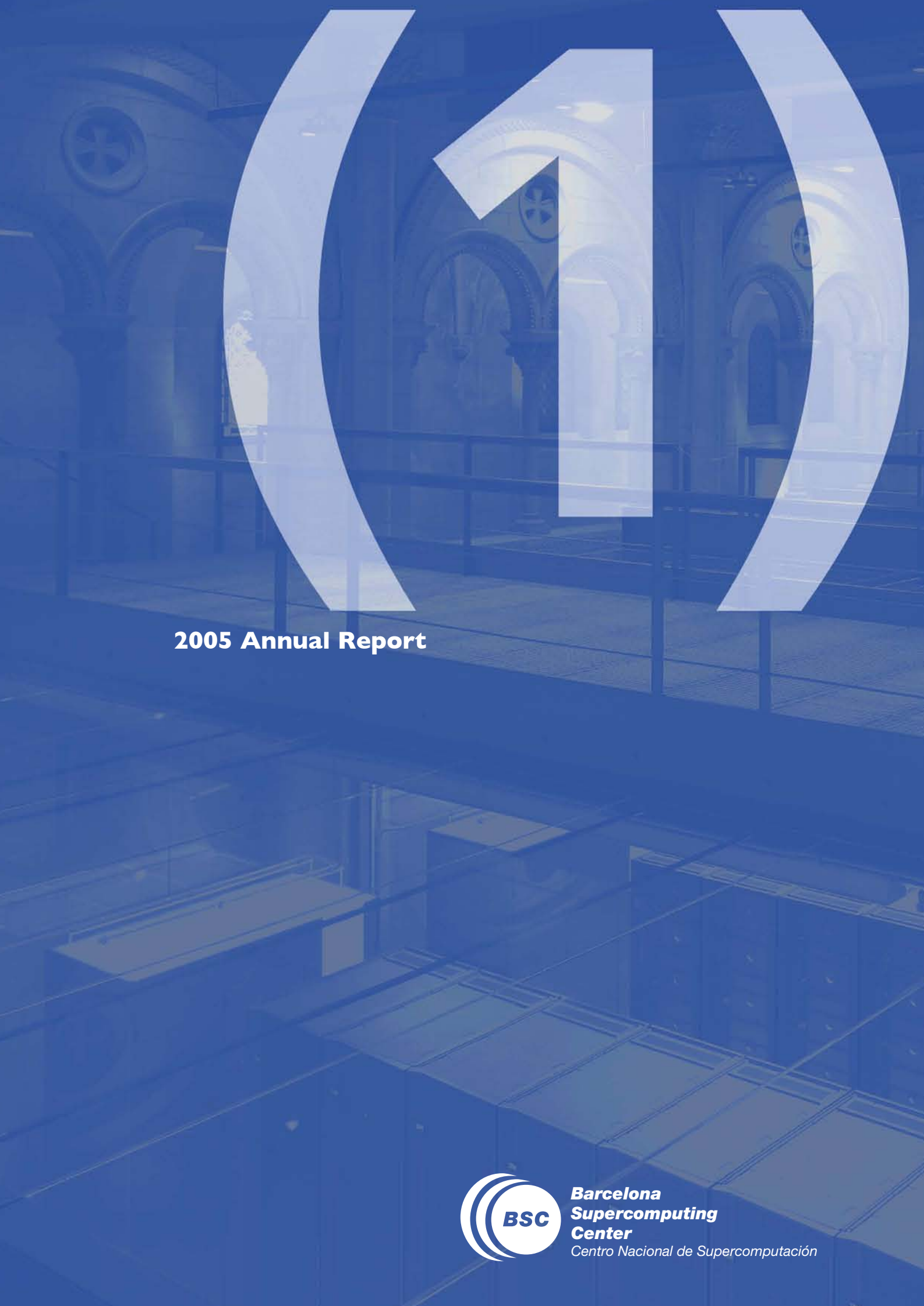

2005 Annual Report

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

You are holding the first edition of the Barcelona Supercomputing Center Annual Report, which contains a summary of our activities as well as a short description of our organization.

2005 Annual Report

Barcelona Supercomputing Center
Centro Nacional de Supercomputación


BSC

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Nexus II Building, BSC headquarters

1 Executive Summary

Research is the goal of our organisation

The Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS) is a public consortium that includes the Spanish government (MEC, 51%), the Catalonian government (DURSI – Generalitat de Catalunya, 37%) and the Technical University of Catalunya (UPC, 12%).

BSC-CNS started operations in April 2005 with the basic objective of being a significant contributor to the advancement of science in Spain, providing it with a capacity for supercomputing.

BSC-CNS has its own research departments in Computer, Life and Earth Sciences:

- the Computer Sciences team focuses its research activity on system software and hardware for future supercomputers;
- the Life Sciences team focuses its research activity on simulations related to genomics and proteomics;
- the Earth Sciences team focuses its research activity on simulations of the Earth's dynamic processes.

The work carried out by the research teams during 2005 resulted in 92 publications, 56 communications and the development of new IT technology.

BSC-CNS runs MareNostrum (MN), the most powerful European supercomputer, with 4,812 processors, 9.6 TB of main memory, a high-speed network, 233 TB of disk and Linux as its operating system, which provides for 42.35 TFlop/s.

BSC-CNS manages MN as a tool for external research, pro-viding scientific computing assistance and user support. MN started public operation in June 2005. Before this date, and since January 2005, system was installed, scaled and tuned. Since June, approximately 70 external research teams have worked on MN from the areas of Biomedicine, Health Sciences, Astronomy, Space, Earth Sciences, Physics, Engineering, Chemistry, Material Science and Information Technology.

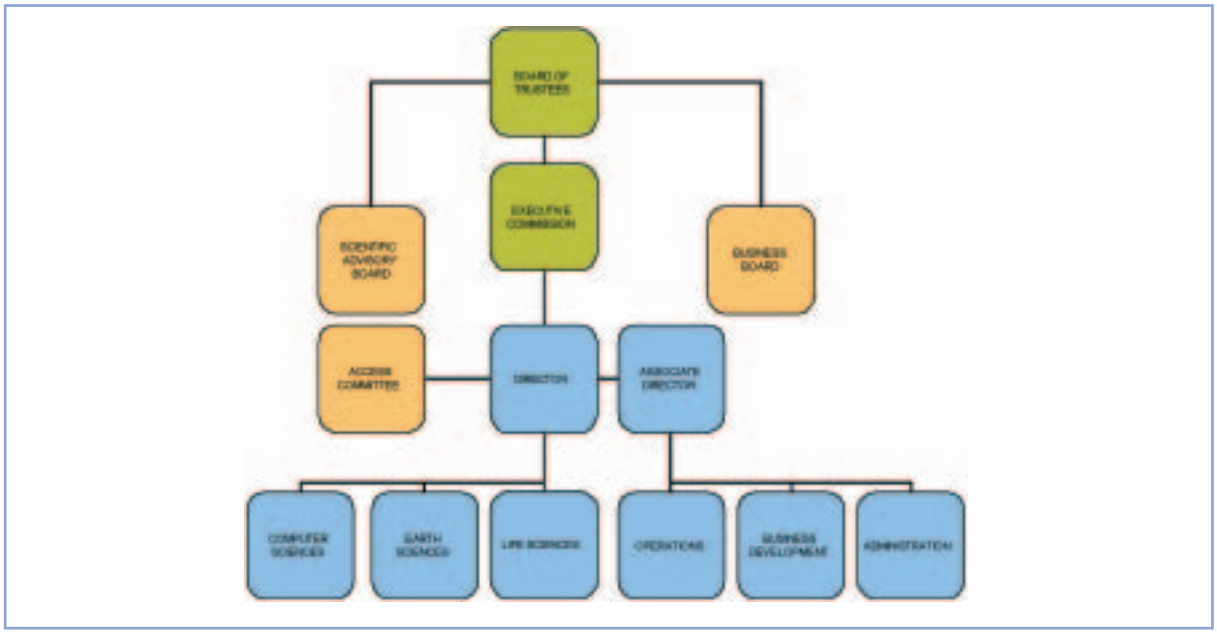
MN had a system utilization stable value of 80% during the later stages of the year, this is a really high percentage. During 2005, BSC-CNS cooperated with institutions and enterprises, signing agreements with public institutions such as CIEMAT, UPM, INB, JSCC (HPC Centre of the Russian Sciences Academy), CESGA and IAC; and private companies such as IBM, Bull, Gas Natural and Airbus.

Lastly, BSC-CNS was a partner on two projects from the VI Framework Programme of the European Commission: DEISA, whose aim is to establish a persistent HPC infrastructure in Europe, joining the 11 main European supercomputing centres, and HPC-Europa, the European mobility program for HPC. In the last quarter of the year, another six projects funded by the European Commission involving BSC-CNS as a partner were approved.

Members of the BSC Management Board

2 Structure

BSC-CNS is a public Consortium working at international scale



The figure above describes the different Governance Bodies and departments that constitute the Barcelona Supercomputing Center – Centro Nacional de Supercomputación:

The main governance body of the BSC-CNS Consortium is the **Board of Trustees**, formed by members of the three shareholder institutions of the Consortium: Ministerio de Educación y Ciencia (MEC), Departament d'Universitats, Recerca i Societat de la Informació de la Generalitat de Catalunya (DURSI) and Universitat Politècnica de Catalunya (UPC).

Members of the Board of Trustees

Chairman	**Salvador Barberá** *General Secretary of Policies on Science and Technology, MEC*
Vice-Chairman	**Ramón Moles** *Secretary of Universities and Research, DURSI*
Members (MEC)	**Carlos Alejaldre** *General Director of Policies on Technology* **José Luís Martínez** *Deputy Director of Research Projects* **Ernest Quingles** *General Deputy Director of Promotion and Technology Infrastructures and Large Installations*
Members (DURSI)	**Ramón Vilaseca** *General Director of Universities* **Xavier Hernández** *General Director of Research* **Josep Mª Vilalta** *General Deputy Director of Research*
Members (UPC)	**Josep Ferrer Llop** *Rector* **Juan Jesús Pérez** *Vice-Rector of Research* **Sebastià Sallent** *Director of Fundació I2Cat*
Director	**Mateo Valero**
Secretary	**Francesc Subirada**

BSC staff and researchers

The **Executive Commission** has the aim of monitoring and executing all the activities of the BSC-CNS.

Members of the Executive Commission

Chairman	**Ernest Quingles** *General Deputy Director of Promotion and Technology Infrastructures and Large Installations*
Vice-Chairman	**Xavier Hernández** *General Director of Research*
Member (MEC)	**Ramon López de Arenosa** *Head of the Department of Production Technologies and Communications General Sub-department of Research Projects*
Member (DURSI)	**Josep Mª Vilalta** *General Deputy Director of Research*
Member (UPC)	**Juan Jesús Pérez** *Vice-Rector of Research*
Member (UPC)	**Cristina Barrado** *Assistant Vice-Rector IT*
Director	**Mateo Valero**
Secretary	**Francesc Subirada**

The **Scientific Advisory Board** and the **Business Board** are being created to offer advice on scientific and business matters. The **Scientific Advisory Board** will be made up of international scientists of prestige. The **Business Board** will be made up of companies that collaborate and fund the center. Decisions concerning the scientific use of MareNostrum are taken by the **Access Committee**, made up of prestigious Spanish scientists outside the BSC-CNS.

BSC-CNS is governed by the Director, Mateo Valero and the Associate Director, Francesc Subirada.

The people that worked at BSC-CNS at the end of the year 2005 are:

Director:	**Mateo Valero**
Associate Director:	**Francesc Subirada**

Computer Sciences Director:	**Jesús Labarta**
Computer Sciences Associate Director:	**Eduard Ayguadé**
Computer Architecture Head:	Álex Ramírez
Senior Researcher:	Francisco Cazorla
Junior Researcher:	Miquel Pericas
Tools of performance analysis Head:	Judit Giménez
Junior Researcher:	Pedro González
Junior Researcher:	Eloy Martínez
Junior Researcher:	Harald Servat
Programming models Head:	Xavier Matorell
Junior Researcher:	Jairo Balart
Junior Researcher:	Roger Ferrer
Junior Researcher:	David Ródenas
Grid computing and clusters Head:	Rosa M. Badia
Junior Researcher:	Francesc Guim
Junior Researcher:	José M. Pérez
Junior Researcher:	Iván Rodero
Junior Researcher:	Raúl Sirvent
Resident Student:	Peter Bellens
Autonomic systems and e-Business platforms Head:	Jordi Torres
Junior Researcher:	Vicenç Beltran
Junior Researcher:	Kevin Hogan
Storage systems Head:	Toni Cortés
Application optimization Head:	José Maria Cela
Senior Researcher:	Rogeli Grima
Senior Researcher:	Guillaume Houzeaux
Junior Researcher:	Raúl De La Cruz
Junior Researcher:	Xavier Sáez

Life Sciences Director:	**Modesto Orozco**
INB – Computational Node 2 Head:	Xavier Messeguer
Computational Genomics:	David Torrents
INB Technical Support Engineer:	Jordi Camps
INB Technical Support Engineer:	David Garcia
INB Technical Support Engineer:	Carles Pons
INB Technical Support Engineer:	Francisco Javier Vera
Resident Student:	Romina Royo
Resident Student:	Alexis Torrano

Earth Sciences Director.	**José María Baldasano**
Air Quality Head:	Pedro Jiménez
Numerical Weather Prediction Head:	Oriol Jorba
Engineer Technical Support:	Eugeni López

Operations Director:	**Sergi Girona**
System Administration:	Javier Bartolomé
System Administration:	Xavier Fustero
System Administration:	Sergi Moré
Networking:	Carles Kishimoto
Security:	Juan Carlos Sánchez
Resource Management:	Ernest Artiaga
Helpdesk:	Carlos Vicente
User support:	David Vicente
Webmaster:	Augusto Izquierdo
Maintenance Assistant:	Albert Riera

Business Development Head:	**Felipe Lozano**
Project Manager:	Toni Moreno
Marketing Leader:	Renata Giménez
Marenostrum's Visitor Manager:	Oriol Riu
Mobility Program Assistant:	Anna Monrós

Human Resources, Administration and Finance Head:	**Mercè Calvet**
Account Officer:	Cristina Calonge
Administration Assistant:	Laura Gutierrez
Administration Assistant:	Neus Jiménez

Members of the Earth Sciences research team

3 Research

The effort of more than 25 teams

3.1 Computer Sciences

The Computer Sciences department focuses its research activities on areas covering lower levels of system software and hardware for future supercomputer systems, as well as kernel and application optimization. Some of the teams (TP, PM, GC, eB, PA) have inherited most of the research topics, projects, knowledge and researchers that previously formed the CEPBA (European Center for Parallelism of Barcelona) and the CIRI (CEPBA-IBM Research Institute). The CA team has inherited some research topics from the Computer Architecture Department (DAC) at the UPC (Technical University of Catalunya) and some recent doctors from its PhD program. Finally, the SS team is of new creation (activities started in the last quarter of 2005) and just include the head of the team.

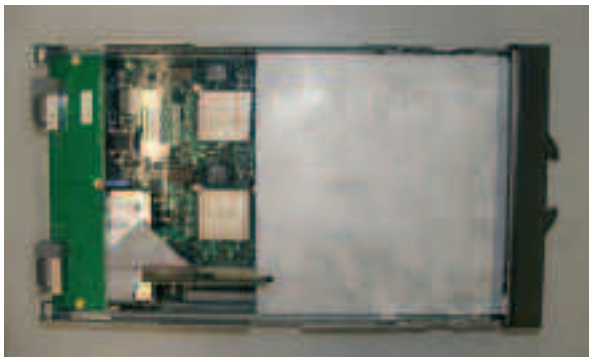
The activities carried out during 2005 are presented for each research team in the Computer Sciences department:

- Computer architecture (CA)
- Tools for performance analysis (TP)
- Programming models (PM)
- Grid computing and clusters (GC)
- Autonomic systems and e-Business platforms (eB)
- Storage systems (SS)
- Application optimization (AO)

Computer Architecture (CA)

The team is exploring three different processor/system architectures for future-generation supercomputer systems:

· MULTITHREADED PROCESSORS: in a simultaneous multithreading (SMT) processor, instructions of several threads (either from the application itself or belonging to a workload of applications) can be issued simultaneously to the back-end pipelines of a processor yielding a dynamic, cycle-by-cycle reconfiguration of the assignment of pipeline resources to threads, based on the decision of scheduler hardware. SMT can be used in real-time embedded environments, posing additional constraints on their design. In an SMT processor, the interaction between threads, and therefore, the execution time of each thread, becomes highly unpredictable, which is an undesirable feature in embedded systems. To tackle this problem, the team has developed two mechanisms that allow the use of SMTs in soft real-time systems. The first, called Predictable Performance, allows the OS to execute up to two time-critical jobs at a predetermined IPC (instructions per cycle rate), regardless of the workload being executed by these threads. The second, called Low-variability Performance, gives results similar to Predictable Performance and, in addition, is suitable for a wider range of applications. The use of one of these two proposals depends on certain properties of the applications themselves, the amount of hardware available to provide soft real-time functionality, and the required success rate. In the near future, the team will include mechanisms and policies at kernel level to dynamically exploit the above processor features when there are more software threads than available hardware contexts.



Cell blade with 2 chips per blade

· KILO-INSTRUCTION PROCESSORS: the continuously increasing gap between processor and memory speeds is a serious limitation to the performance achievable by future microprocessors. Currently, processors tolerate long-latency memory operations largely by maintaining a high number of in-flight instructions. In the future, this may require supporting many hundreds or even thousands of in-flight instructions. Unfortunately, the traditional approach of scaling up critical processor structures to provide such support is impractical at these levels due to area, power, and cycle-time constraints. To solve these problems, the team has proposed a new processor architecture called Kilo-Instruction Processors. The team is working on the following aspects:

- *Decoupled Kilo-Instruction Processor*: this is an improvement of the original idea in which two different processors are included: the first (out-of-order processor), called the cache processor, deals with the instructions that are ready in a short period of time. Therefore, these instructions basically do not depend on any load miss; and the second processor, called the memory processor (an in-order processor), which deals with the instruction that depends on a load miss. The two processors are connected through a FIFO called a Low Locality Instruction Buffer, where the instructions that are not executed in the cache processor are stored and await ready to be executed by the memory processor.

- *Kilo-instructions multiprocessors*: the checkpointing mechanism in kilo-instruction processors introduces the possibility of using the emerging transactional memory programming model. In addition, kilo-instruction multiprocessors can efficiently implement speculation over the critical sections and support sequential consistency models to allow complete unsorted loads and store between checkpoints.

· VECTOR PROCESSORS: these processors increase performance by executing the same operation in parallel over multiple data elements (vectors). Where traditional vector computers are no longer the preferred platform to build high-performance computing systems due to their high cost, they have experienced a new golden era with the introduction of SIMD multimedia extensions (single instruction, multiple data). These new instructions execute the same operation on short vectors, suitable for the most common multimedia applications, such as JPEG image and MPEG-2 video encoding/decoding. However, current SIMD extensions do not prove so useful for other (non-multimedia) applications. The team is evaluating novel application domains such as bioinformatics and high-definition media applications in order to determine the requirements of a next-generation SIMD extension suitable for a wider range of applications. The objective for 2006 is to identify and evaluate possible SIMD extensions that benefit the analyzed applications, such as unaligned memory access and wider vector registers.

Within the framework of the European Union, two projects were prepared during year 2005:

- The SARC project: this project is on scalable computer architecture and was proposed jointly with the PM team at BSC. It was submitted in June, and the proposal passed the negotiation stage in October. SARC starts on 1 January 2006.

- The ACOTES project: the proposal for this STREP project, jointly with the PM team, was also submitted in September 2005, and is currently at negotiation stage; it is expected to be approved and started in June 2006.

The team is also preparing a proposal in the framework of the contract signed with IBM Research, mainly related to SMT processors. This project is expected to start during 2006.

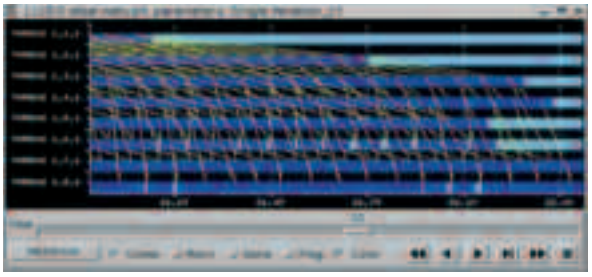
Tools for Performance Analysis (TP)

The main objective for the tools for Performance Analysis team is to increase the scalability of the tools for performance analysis. During 2005 the team focuses in the following areas:

· INSTRUMENTATION PACKAGES: the size of the collected data traces becomes an important issue when considering the execution of applications with thousands of processes. Although each process may generate a small trace, the merging of thousands of such traces could cause a bottleneck. To deal with this issue, one possibility is to have more control on the information that is collected (e.g. by eliminating redundant information) to guarantee that the resulting trace to be analysed is of a reasonable size. The team has designed and implemented a set of mechanisms that control/reduce the size of the generated trace. These mechanisms can be classified depending on the phase in which they are applied: dynamically at runtime (to decide what, when and/or which processes to instrument) or statically during the merging process. The team has ported the MPIDtrace package to the CRAY-XT3 platform, together with a very simplified version of Paraver tracing to the Cell architecture. The team is also in the process of integrating all the tracing packages to share a common source, avoiding the doubling-up of development efforts.

· UTILITIES: the problem of handling large traces (Gigabytes) can be handled post-mortem with a set of utilities that allow the generation of views/traces with different levels of detail, maintaining the original full trace as a reference. The utilities enable the cutting, filtering, transformation and fusion of the original trace records through an XML specification.

· PARAVER: the visualization tool has no restrictions with regard to the number of processes or events frequency it can work with, but it is limited in relation to the trace size it can load. For this reason, the team has worked to optimise the use of memory, reducing the trace records and improving the memory used by the analysis module. As the objective of Paraver is to keep or even raise the motivation to go deeper and deeper in the analysis, it is very important to guarantee that the user has a good response time for most of the



Process/thread activity and communications in a Paraver window

interactions. Along these lines, the team has worked to improve the performance of the load trace algorithm and the semantic function engine. But the analysis of a trace with more than 1024 processes also has certain scalability problems other than the performance and memory that is due to the complexity of the information being analysed. The performance analysis can be considered a search within the three-dimensional space defined by the trace file. The

complexity of the search is increased exponentially when analysing large-scale runs. What can be evident with 10 processes, can be hard to analyse with 1,000 processes. To compensate this increase in the complexity, the tool has to provide mechanisms and functionalities to facilitate the work of the analyst. The team has implemented different functions to select the most representative value for a pixel, which can summarize many different semantic values, to highlight the outlier values, find the path of a communication, generate inclusive and exclusive statistics and combine information from two different traces, etc.

· DIMEMAS: the message-passing performance prediction tool can work with the trace out of core, accessing the records in one sequential read. With this option, the limit on the tracefile size is mainly defined by the filesystem and the operating system. The team has extended the Linux file access to work with 64 bit and is analysing the impact of discarding very small cpu bursts (depending on the final results, the tool can decide to eliminate the generation of these bursts to significantly reduce the trace size).

The team has been involved in several collaboration projects: one in the framework of the European Union and two with research laboratories in the USA:

- HPC-EUROPA. Within the framework of HPC Europa, the team participates in two activities. JRA1 is related to Performance Tools and, as well as the work on scalability reported in the previous section, on the definition of methodologies. NA2 is related to AccessGrid and within this activity the objective is to integrate Paraver with the AccessGrid+VNC environment.

- SDSC collaboration. The project with SDSC provides support in the use of the tools and the implementation of new features or functionalities of common interest. During 2005, the most remarkable tasks have been to automatically define Dimemas block events between MPI calls to allow finer control of the CPU time simulation and to instrument and model LAPI Active messages.

- NASA-AMES collaboration. The project with NASA-AMES has two objectives: to port the OpenMP instrumentation to their Columbia system (SGI Altix with Linux) and to collaborate on the analysis of real applications that have certain performance problems.

The team has worked on the definition of a project with IBM Research in the framework of the contract signed with this company. The project on Performance Tools aims at integrating the tools developed at BSC and the HPC-Toolkit developed at IBM Research. This project should start in spring 2006.

Programming Models (PM)

The team new research targets are future architectures, such as multicore multiprocessors or the new IBM Cell architecture. In particular, the following topics have been covered:

· SHARED-MEMORY RUNTIME SYSTEMS: the Nanos OpenMP runtime system has been extended to the full OpenMP 2.5 specification and ported/maintained for Linux on Power and Pentium (both shared-memory and SDSM versions) and Solaris/SPARC. In the CAS project with Toronto, the team has continued with the development and evaluation of some of the proposed extensions to the OpenMP Architecture Review Board on the IBM XLSMP runtime system. NanosDSM has been stabilized during 2005, in such a way that we can presently run all the NAS benchmarks. It is expected to be ported to the 64-bit environment during 2006.

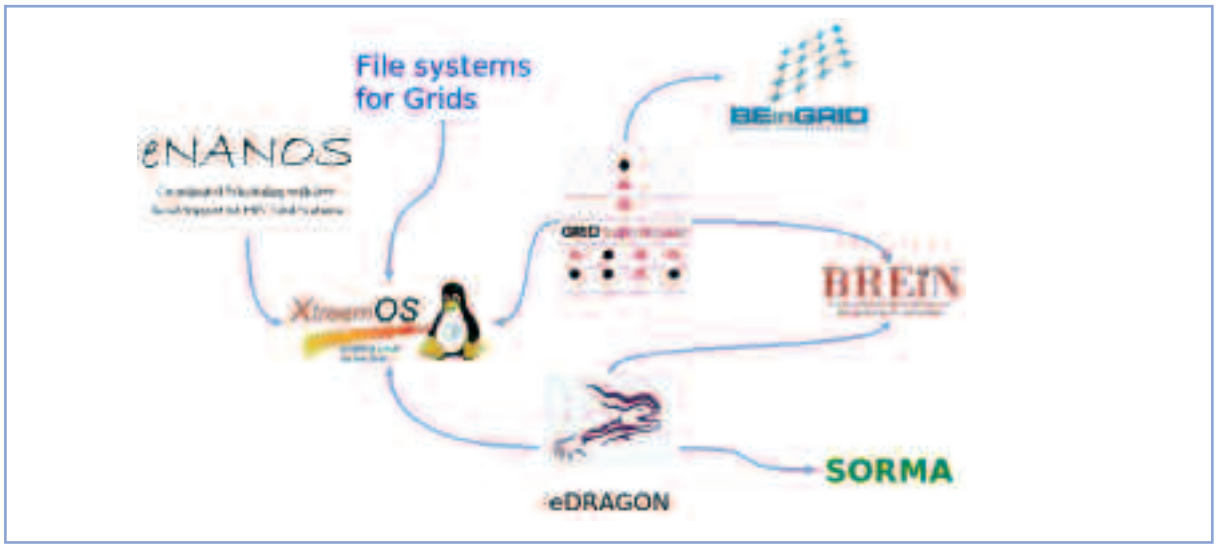
· MESSAGE-PASSING RUNTIME SYSTEMS: there has been ongoing work on the scalability of MPI. The group has been developing techniques to predict the behaviour of the communications system in this programming model and improve the scalability of applications. In addition, the team has also developed a control flow algorithm to allow MPI to scale to systems with thousands of nodes where memory is a scarce resource (such as the IBM Blue Gene/L).

· OPENMP COMPILATION INFRASTRUCTURE: a new compilation infrastructure has been developed to replace the old compilation infrastructure inherited from the CEPBA. The infrastructure includes two new source-to-source translators for C and Fortran 95. C++ is currently being developed. The team has also started the proposal of inspector/executor techniques, with combined efforts at compiler and runtime levels, to provide shared memory in architectures with distributed memory. A first prototype is being developed for MareNostrum and will also target the Cell processor. This will be a topic under development during 2006. Cray Chapel, Sun Fortress and IBM X10 developments are under study, with the goal of tracking new ideas in the field.

· CELL ARCHITECTURE: by the end of October 2005, the BSC received two IBM Cell BE-based blades. BSC was one of the first installations in the world to have this system, which has required an effort to install, configure, understand and evaluate this novel architecture. The Nanos runtime system and compilers will be targeted at Cell during next year.

A number of projects were prepared during 2005, three of them in the framework of the European Union and one with IBM Research:

- SARC project on scalable computer architecture, proposed jointly with the CA team.
- XtreemOS project: this IP project proposal was submitted in September, in collaboration with the GC, SS and eB teams at BSC. This project has been accepted and its starting date will probably be June 2006.
- ACOTES project on stream architectures and programming models, jointly with the CA team.
- IBM proposal on programming models for the Cell architecture: during 2005, the team started the definition, within the framework of the contract signed with IBM Research, of a proposal that we expect to be accepted during 2006. The main objective of this project is to explore different alternatives for the programming of supercomputer systems made from Cell blades, bringing together the activities of the PM and GC teams.



Relation between the recently launched European Projects in the Grid area and the corresponding participating groups at BSC

Grid computing and Clusters (GC)

Research in Grid computing in the BSC is focused mainly on two research projects - GRID superscalar and eNANOS - and on the preparation of the recently accepted projects BEinGRID.

· GRID SUPERSCALAR: this is a grid programming environment that enables the simple programming of applications that will be run efficiently on a computational grid. GRID superscalar is able to parallelize a sequential application at runtime and at task level and execute the application in a computational grid. The approach is able to take advantage of the applications that are composed of coarse grained tasks. These tasks can be of the size of a simulation, a program, a solver... These kinds of applications are very common in bioinformatics, computational chemistry and other scientific fields. Working versions of GRID superscalar were available at the beginning of 2005. The most significant advances during 2005 were:

- Middlewares: working versions with Globus Toolkit version 4 and Ninf-G were developed.
- Implementation of an ssh/scp version: This version has been specially tailored to the MareNostrum supercomputer and several end users are taking advantage of the solution.
- Development of a monitoring graphical interface: We have developed a graphical interface that enables runtime monitoring of application evolution.
- Runtime componentization: This new design enables local tasks and dependencies between any type of task parameter.

· eNANOS: this project is based on the idea of having good low level support for performing good high level scheduling. The eNANOS project is based on these ideas: A fine grain control between scheduling levels, dynamic allocation (MPI+OpenMP jobs) to improve system performance, detailed information about current scheduling and performance for future scheduling decisions, and, based on this accurate information, efficient scheduling (in terms of slowdown) based on performance prediction. During 2005, the team has made the following advances:

- Extension of the resource broker based on GT3 to sup port new functionality such as more information about jobs or cancel/suspend.
- Implementation of the eNANOS scheduler which is an external LoadLeveler scheduler.
- Design and implementation of the mechanism to export fine grain monitoring information to the grid level.
- Implementation of an information system that is able to collect information from monitoring systems such as Ganglia or Mercury
- Design of a prediction service that forecasts job performance

The team is also involved in two projects funded by the European Commission with subjects related to Grid computing: HPC Europa and CoreGRID.

· CoreGRID: this project is a network of excellence on Grid. The research activities are organised into virtual institutes. The team has been involved in the activities of the Institute on Resource Management and Scheduling and on the Institute on Grid Systems, Tools and Environments. In the framework of this network, the group has been working on the integration of its research with the research of other European groups.

· HPC-Europa: The group has been involved in the development of a Grid portal, with the objective of implementing a Single Point of Access to different grid middlewares. To this end, the HPC-Europa Grid Portal, based on the GridSphere portal framework including its GridPortlets mechanism, is being developed. The portal will provide transparent, uniform, flexible and intuitive user access to HPC-Europa resources. This portal will hide the underlying complexity and heterogeneity of these resources and access to them. The team has focused on the implementation of the portal and modifications to the middleware to allow the integration of the eNANOS resource management environment.

The team has actively participated in the last call for European projects, preparing three new European projects that have been recently approved:

- XtreemOS, which aims at developing a Grid aware operating system;
- BEinGRID, which aims to apply current Grid technologies to business applications;
- Brein, which aims to develop a new Grid architecture based on agents and a semantic Grid focused on solving business applications.

Autonomic Systems and e-Business Platforms (eB)

The eB group is currently carrying out research in eBusiness applications and platforms executing on powerful platforms (multiprocessor architectures as well as distributed environments and new architectural proposals).

The year 2005 saw the establishment of the group organization, which was structured into three main interconnected work areas:

· The Self-managed Systems working area focuses on one of the major issues in Autonomic Computing on J2EE platforms: allowing application servers to self-adapt to the execution environment, application characteristics and the workload intensity. In this area, a resource-aware self-management engine for multidomain J2EE application servers was designed and prototyped. A prototype of a global resource manager with self-management facilities that distributes the available resources among the application servers running on the system has also been developed by the team.

· The Systems Architecture working area covers different critical issues for self-managed systems as it is the redefinition of the programming paradigms of the J2EE middleware or the consideration of new features at hardware layer. In this area, the team has redefined middleware architectural paradigms and has designed, prototyped and evaluated the changes. The original multithreading architecture of the server was changed to a hybrid model that combined the benefits of the Java NIO API with the already existing multithreaded architecture.

· The Monitoring and Prediction working area is devoted to extracting knowledge and models from these systems for subsequent incorporation into the core engine when they become autonomous. This area started its activity at the end of 2005 with an extension to the BSC monitoring tools for these environments.

Storage Systems (SS)

The main task for 2005 has been the design of the objectives, the proposal of research projects, and the quantification of the research team needed in the team. The two research projects that will mark this research group's starting point are as follows:

· SCALABILITY OF PARALLEL FILE SYSTEMS. The objective is to study how scalable current parallel file systems are (tested on top of MareNostrum) and once we detect their limitations, propose solutions to the scalability problems encountered.

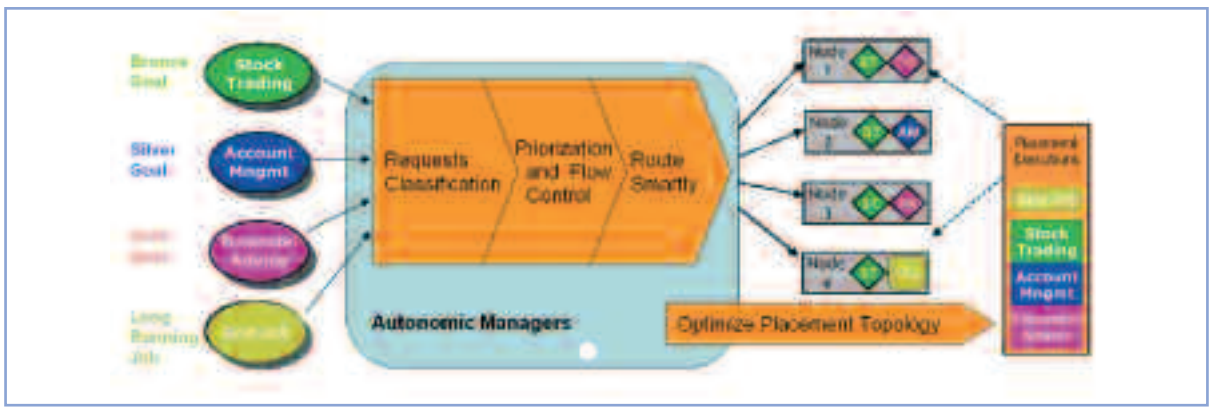
· FILE SYSTEMS FOR THE GRID. This project, done in cooperation with the Grid team, wants to solve the problems currently found in grid systems such as data location, replication, striping, etc. to make grid environments more efficient.

In order to work on the aforementioned projects the team has made contact with industrial and academic partners. On file-system scalability, cooperations with IBM, Bull, and Argone National Lab to test the scalability of their file systems (GPFS, HPSS, Lustre, and PVFSv2) have been started. Regarding the improvement of I/O for grid environments, the team has begun to cooperate with Universidad Politécnica de Madrid to work on an autonomous storage system for the grid. Finally, contacts with the partners of the XtreemOS consortia that will build an operating system for the Grid have been started.

During 2005, the team started the definition of a collaboration with IBM Research in the framework of the signed contract. The "Scalability of HPSS" project has been defined and it is expected to start in 2006. Another project proposal, XtreemOS, was submitted in September, in collaboration with the GC, eB and PM teams at BSC. This project has been accepted and its starting date will probably be June 2006.

Application Optimization (AO)

The team's main objective has been to cover the needs of parallel applications in the starting phase of MareNostrum. In order to achieve this objective the team completed a project of application/libraries porting to the MareNostrum architecture. This project was completely funded by IBM. The main objective of the project was to guarantee that MareNostrum can execute a wide set of the application and libraries required by the users in a highly efficient way. The porting of these applications/libraries requires a variety of actions: MPI/openMP parallelisation, VMX codification, development of patches for



Self-managed systems dynamically adjust resources based on business goals.

proper compilation/installation, etc. The applications ported were reported on the BSC website (www.bsc.es/projects/deepcomputing/pblade/). The applications include:

- Libraries: FFTW (Fast Fourier Transforms and related transforms), ATLAS (Dense Linear algebra), HYPRE (Sparse Iterative Linear solvers), METIS (Graph manipulation library), PETSc (Sparse Linear algebra), SLEPc (Sparse Eigenvalue problems) and SuperLU (Sparse LU solver)
- Bioinformatic Applications: BLAST (Sequence Alignment), BLAT (Sequence Alignment), CLUSTALW (Sequence Alignment), FASTA (Sequence Alignment) and HMMER (Sequence Alignment)
- Image generation applications: POVRAY (Photo-realistic image generator)
- Molecular Dynamics Applications: CPMD (Ab inito molecular dynamics)
- Seismology: CPS (set of tools for seismic data analysis)

3.2 Life Sciences

The effective use of MareNostrum is quite recent, which has limited the amount of data obtained by the computer. The fact that group leaders are still in the process of being hired also limits the output. However, significant progress has been made, shown in several publications in the area, including some in high impact journals). The team focuses mainly on the following areas:

· DYNAMIC PROTEOME

Within the MODEL (Molecular Dynamics Extended Library; http://www.bsc.es/plantillaE.php?cat_id=3) project the team is creating an extensive library of trajectories for all the representative proteins. The current database contains 10 ns trajectories for more than 1300 proteins. The project, the largest of its kind in the world, provides with a complete picture of protein dynamics and helps in drug-design projects. It is expected to have a dramatic impact in the study of protein flexibility.

· PROTEIN-PROTEIN DOCKING

BSC is creating and working on the development of more efficient computational tools for the description of protein interaction patches and for the prediction of the structure of protein-protein complexes. The final objective will be to use MareNostrum to perform massive proteome-scale simulations to predict possible regulatory interactions between proteins.

· LIGAND BINDING AND CATALYSIS

A series of different techniques, from kinetic Monte Carlo to plain molecular dynamics or QM/MM calculations are used to describe the reactivity and ligand diffusion pathways in a variety of biologically important enzymes, including haemoglobins, acentylcholinesterase and cyP450.

· BINDING SITE COMPARISON

The LS Department is deriving an alternative classification of proteins, based on the expected similarity between recognition sites. Calculations based on classical molecular interaction potentials and similarity indexes determined in the reciprocal space will help detect potential secondary interactions in drugs, contributing to the development of new, safer drugs.

· GENOME ANNOTATION AND DATA MINING

Massive techniques are used to scan through genomes to better annotate genes, detect evolutionary routes for genome divergence and to detect pseudogenes. These studies will help gain a better understanding of human genetic-based pathologies.

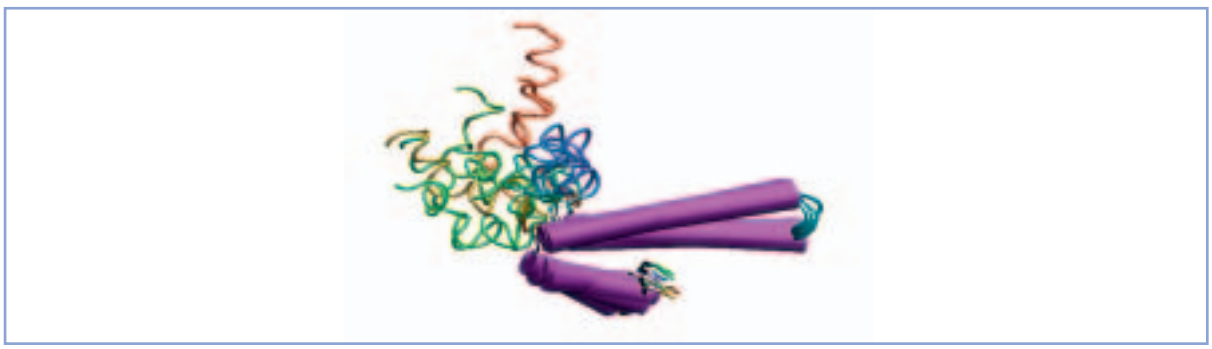
· CHROMATINE SIMULATION

Molecular dynamics and mesoscopic models are used to obtain a fine- to coarse-grain simulation of chromatine in eukaryotic organism, especially humans. Our main goal is to understand how the physical properties of DNA modulate the biological function of this molecule at atom level. Knowing that we will be able to decipher a hidden regulatory mechanism based on the control of chromatine condensation.

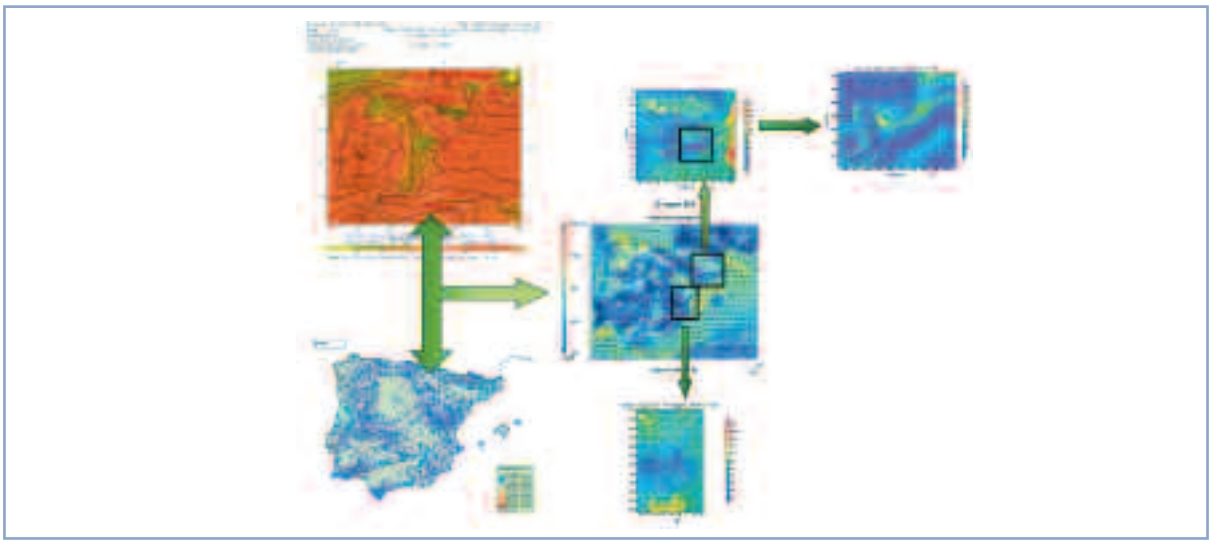
3.3 Earth Sciences

The initial research topics related with Earth sciences at BSC inherits the experience of the Environmental Modelling Laboratory (LMA-UPC). The areas of research are focused mainly on projects that may provide further understanding of the dynamic processes of the Earth, mainly related to the Earth's response to anthropogenic influence and forcing:

- Forecasting of air quality and concentrations of gaseous photochemical pollutants (e.g. tropospheric ozone) and particulate matter.
  Previsions for 2006, operational system in phase of test of an operational system: forecast of the air quality for the Iberian peninsula with high resolution.
- Transport of Saharan dust (outbreaks) from North Africa towards the European continent and its contribution to PM levels.



MODEL Project provides with a complete picture of protein dynamics



Operational air quality forecasting system for the Iberian Peninsula and Balearic Islands

In operation: DREAM transport of Saharan dust to the entire Mediterranean arch (http://www.bsc.es/projects/earthscience/DREAM/)

· Modelling the climate change. This area of research is divided into:
  · Interaction of air quality and climate change issues (forcing of climate change);
  · Impact and consequences of climate change on a European scale.

A wide experience has been acquired in numerical weather prediction (NWP) mesoscale models, both on local and regional scales. They have been applied to regions that present particular characteristics of very complex topography, such as the presence of the land/sea interface, with the existence of near mountain ranges (few kilometres) with altitudes of up to 3000 m. The models MEMO, MM5, ETA, WRF-ARW have been applied using one-way, two-way techniques and nudging, applied to the urban coastal areas, the Mediterranean Iberian coast, the Iberian Peninsula and the Euro-Mediterranean region.

In the field of emission modelling, anthropogenic and biogenic emission models have been developed for the area of Catalonia (LEM/EIM for the city of Barcelona and EMI-CAT2000 for the entire region) and Valencia (EMIVAL2000); they have been applied for the estimation of emissions on the Spanish Levantine Coast. An inventory for the Iberian Peninsula is currently under development, with a resolution of 1 km and 1 hour. This system is currently been developed under a parallel framework for its application and implementation on the MareNostrum supercomputer. The high spatial (1 km^2) and temporal (1 hour) resolutions make these models suitable for use in chemistry transport models. Air quality models and photochemical mechanisms that take into account the photochemical interactions between the different pollutant species have been developed and applied. For their i mplementation, some methodologies for coupling the above emission models and CMAQ have been elaborated.
An extensive experience has been gathered in the analysis of lidar measurements, participating in environmental campaigns of measurements with lidar (summer 1992, in Barcelona, and April 1994 in El Paso (USA), collaborating with Los Alamos National Laboratory (LANL), New Mexico (USA) and summer 1996 and 1997 with ERLAP (European Reference Laboratory of Air Pollution), Environmental Institute, JRC-ISPRA European Commission. From 1993, the UPC lidar group developed two elastic lidar systems: a stationary system working at 532 nm; and a transportable system allowing three-dimensional scans working at the 1064 nm fundamental wavelength and at the 532 nm second harmonic. Based on the experience acquired, the BSC team and the UPC lidar group joined the EARLINET project within the V Framework Programme on Research and Technological Development of the European Union. In this project, 21 lidar stations in Europe collected special data sets to address various topics such as Saharan dust events, forest fires, urban photochemical smog, volcanic aerosol, stratospheric aerosols, diurnal cycle measurements, differences between rural and urban aerosol distributions, and cirrus clouds. From 2002, the Mediterranean Centre on Insular Coastal Dynamics (ICoD) of the University of Malta, established dust operational forecasts within EARLINET with the Dust Regional Atmospheric Modelling (DREAM) system. There was an intensive collaboration with ICoD for the development of the dust model. The works include the simulation and analysis of the transport of natural dust emissions from the Sahara desert to the Euro-Mediterranean region and the Canary Islands, with the milestone of covering the entire planet with high resolution. The DREAM system is fully operative on the Internet on the BSC-CNS website, available for any researcher or interested party.

Signature of specific agreements:

· Agreement with the Spanish National Institute of Meteorology (INM) for the implementation, diffusion and validation of a service of operational prediction of episodes of transport of Saharan dust in the Iberian Peninsula and the Canary Islands and modelling studies, detection, pursuit and characterization of atmospheric particular matter.

· Agreement with Natural Gas (GN): a study of the environmental impact on the quality of the air due to the traffic of the cities of Barcelona and Madrid, with special consideration to the tropospheric ozone and particulate matter.

Interconnection network Myrinet

4 Support

Tools for the research community

4.1 Operations

Operations group has two major missions: system administration and user support.

The system administration area includes pure system administration, security, resource management, networking, helpdesk. This group of people makes the BSC systems available 7 days a week, 24 hours a day. The service is guaranteed via an automatic mechanism which informs at any time of events, and reacts automatically to recover most technical problems. The user support group includes direct user support with knowledge in programming models, libraries, tools, applications, etc. BSC webmaster is integrated in this group. During 2005, the Operations group has focused on the three major areas:

- creation of the adequate infrastructure for the new Supercomputing Centre
- preparation of MareNostrum for operation and its subsequent operation
- maintenance of the infrastructure inherited from CEPBA-UPC

Among these activities, the whole group has participated in DEISA and HPC-Europa. In DEISA with the responsibility for integrating BSC-CNS resources in the DEISA infrastructure, including networking, file system, resource management, user support, system administration and security. In HPC-Europa, providing support for the different visitors, including experience and help in parallelizing their codes.

MareNostrum

BSC-CNS hosts MareNostrum, one of the most powerful supercomputers in Europe, managed by the Operations team that takes care of its availability, security and performance. An important task of this team is to support scientists in the usage of MareNostrum, as well as to help them in the improvement of their applications getting better research results.

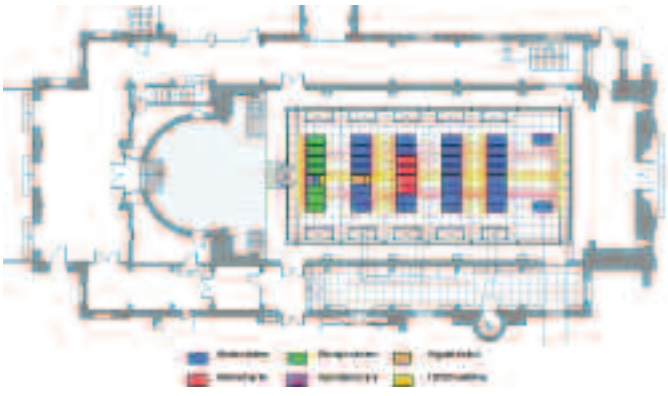
System Architecture

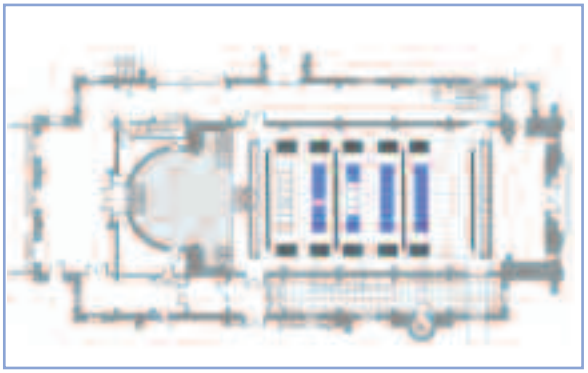
MareNostrum is a supercomputer based on processors PowerPC, the architecture BladeCenter, a Linux system and a Myrinet interconnection. These four technologies configure the base of an architecture and design that will have a big impact in the future of supercomputing.

A brief summary of the system is the next:

- Peak Performance of 42, 35 Teraflops
- 4.812 IBM Power PC 970FX processors at 2.2 GHz (2406 dual 64-bit processor blade nodes)
- 9,6 TB of main memory
- 236 TB of disk storage
- Interconnection networks:
  - Myrinet
  - Gigabit Ethernet
  - Ethernet 10/100

MareNostrum has 42 racks and takes up a space of 120m^2. In the following figure you will see the floor where the supercomputer is located.

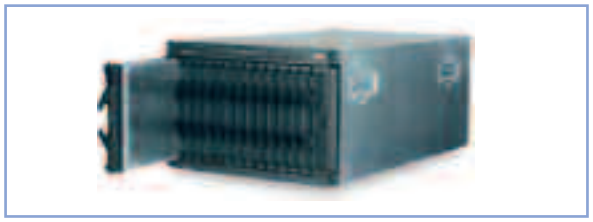




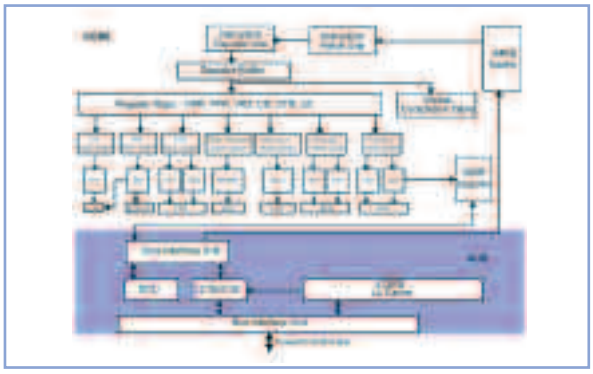
Blade Centers
MareNostrum has 29 racks dedicated to calculate. These racks have a total of 4812 processors PowerPC 970FX with a frequency of 2, 2 GHz and 9.6TB of total memory.
Each rack is formed by 6 Blade Centers. In total, each rack has a total of 168 rocessors and 336 Gb of memory. Each one has a rough peak performance of 1, 4 Tflops

Blade Center:
The nodes JS20 are grouped in a Blade center which is formed by 14 dual nodes with 28 processors in total.
Each Blade Center has two redundant energy supplies. In this

way, if one of the supplies fails there is the other one still working. It also has a switch for the Gigabit, which connects all Gigabit connections to the other nodes JS20.



Server Blade JS20:
Each Blade Center has 14 server blades type JS20. Each of these nodes has 2 processors PowerPC 970 FX at 2.2 GHz, 4 Gb of shared memory between both processors and a local disk IDE of 40 Gb.



PowerPC 970FX Processor:
The processor PowerPC 970FX is a processor with an architecture of 64 bits oriented to a general purpose (Mac G5 contains this type of processor). It is a superscalar processor with vectorial extensions type SIMD (VMX) whose design is based in the processor of high provision Power4.

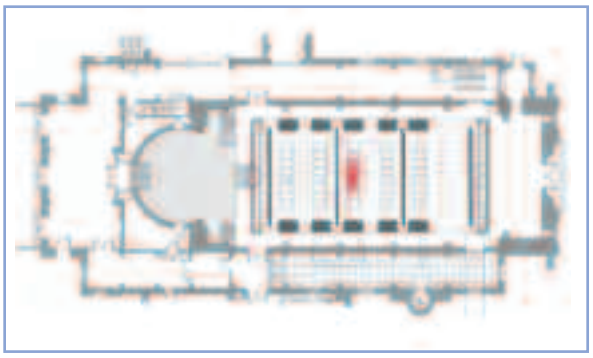
The new PowerPC 970 based in a 90nm technology works with a frequency of 2.2 GHz. It is ready to launch a maximum of 4 instructions per cycle and it's able to have a maximum of 200 in flight instructions.

Myrinet racks:
The 2400 blade nodes JS20 and the 40 nodes that are working as servers (nodes p615 in the storage blades) are interconnected through a high speed interconnection network called Myrinet. The different nodes are interconnected via fibre optic cables.

Four of the 42 racks in MareNostrum are dedicated to network elements which allow to interconnect the different nodes connected to the Myrinet network.
These four racks are located in the center of the room and each node has a fibre optic cable. The network elements connect the different cables allowing the interconnection from one point to another from the different nodes.
The total Myrinet network is connected through:

- 10 elements Clos256+256
- 2 elements Spine 1280

Storage servers:
Further to the local disk of each node with a 40GB capacity, MareNostrum has 20 storage servers arranged in 7 racks. These have a total of 560 disks of 250GB and each one provide a total capacity of 140 TB external storage. These

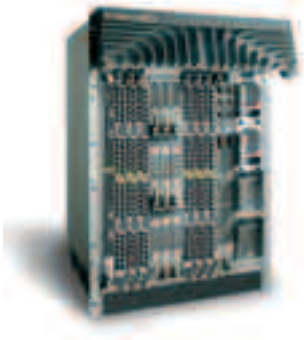


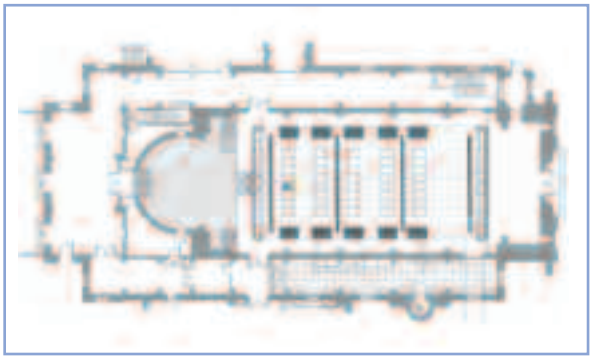
disks are working with GPFS (Global Parallel File System) which offers a global vision of the file system and also allows a parallel access.

The 2406 nodes access the disks through a Gigabit network. Each one of the 20 storage nodes has two nodes p615 in charge of the disk requests, a controller type FAStT100 and one unit EXP100. Each node p615 has a Myrinet connection, Gbit connections and Ethernet 10/100 connection.

Operation rack:
One of the racks is the operation rack where the system can be managed. This rack is located in the machine console. The content of each rack is the following one:

- 1 Monitor 7316-TF3
- 2 nodes p615
- 2 HMC (consoles) 7315-CR2
- 3 remote nodes asynchronous
- 1 Chasis BCIO BladeCenter IO
- 4 Switches Cisco 3550





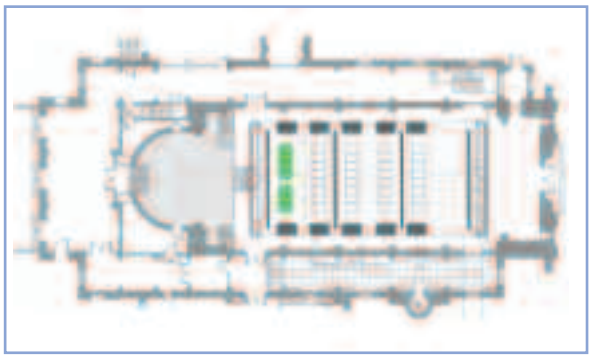
Gigabit switches:
One of the racks of MareNostrum is dedicated to the interconnection of the Gigabit network and one part of the interconnection elements of the Ethernet 10/100 network. The elements are the following ones:

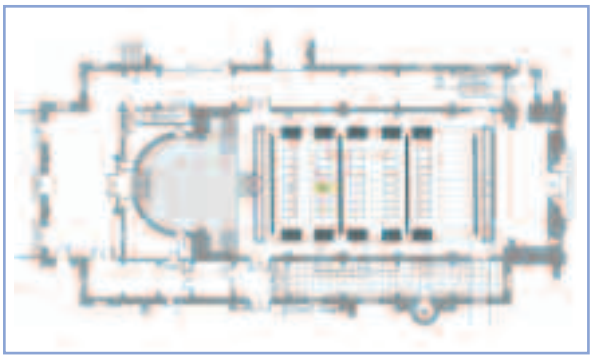
- 1 switch Force10 E600 Gigabit Ethernet.
  It contains 7 slots in total, 6 of them have cards 10/100/1000 Base-T of 48 ports offering a total of 288 ports GigabitEthernet/IEEE 802.3
- 4 Switches Cisco 3550 48-port Fast Ethernet

System administration
From the creation of the centre to June 2005 when MareNostrum started production, BSC system administration staff worked together with IBM technicians on the final setup of MareNostrum and its preparation for general use. The next tasks are worthy of mention:

- Tuning and final adjustment of the Diskless Image Management (DIM) software. This is the software that makes it possible for all blades to be booted remotely.
- Installation and configuration of the IBM General Parallel File system (GPFS) in the whole cluster as a global file system.
- Installation of the Linux Myrinet driver (GM) to enable the use of this network for parallel applications.

Since MareNostrum has been in production mode, the normal operation of the super-cluster began and the policies for the use of filesystems and resources were defined. The hardware machine components were declared Customer Replacement Units (CRUs), so BSC system staff has been responsible for the replacement of these components. Apart from the normal system administrator tasks required by a computer, continuous work has been carried out by the systems team to obtain the best performance of





J20 blade

MareNostrum, modifying and adapting the initial configuration to their optimal values for use.

For instance, at the end of the year, part of the machine was reserved to test the new Myrinet driver (MX), with the idea of a future upgrade.

The BSC system team have been in charge of the administration and maintenance of all the servers that belonged to CEPBA.

Cell processors at BSC

The system staff team has also been involved with projects with IBM. For instance, two Cell blade machines have been installed and configured. This new architecture was initially tested with Fedora Core 3 and has recently been updated to Fedora Core 4.

Networks

The network for BSC internal users has grown from a low-bandwidth, slow and less efficient Ethernet 10 Mbps network to a fully switched gigabit Ethernet network. Physically, the network comprises different locations. The first is the MareNostrum Supercomputer and the second is the offices for most BSC staff, including students, direction and administration and located in the Nexus II building near the supercomputer. Next year, the network is expected to grow in order to accommodate more users and to interconnect computers located in different computer rooms.

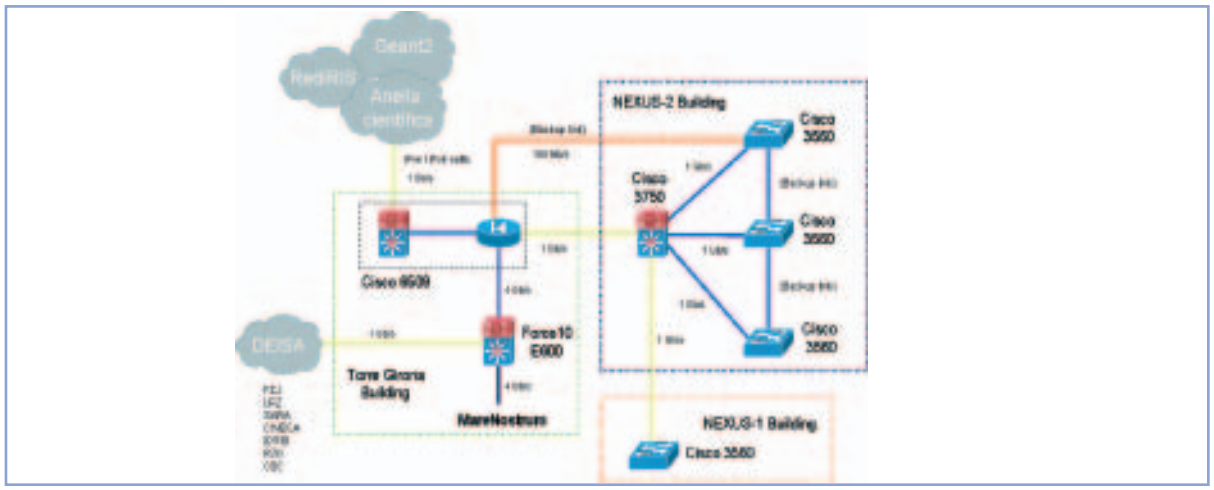
The network can be divided into three layers: at the access layer, gigabit Ethernet Catalyst Switches from Cisco Systems can support traffic from approximately two hundred users using gigabit speeds; at the distribution layer, new Cisco equipment will route all traffic to a powerful Cisco switch/router in the core layer which will provide us with the external connection and firewall functions needed nowadays. This network equipment was shipped with redundancy everywhere, including the routing board and power supplies.

BSC Network is available through the Anella Científica and RedIRIS, the Catalan and the Spanish networks for research and science.

BSC technologies - Characteristics or features of the network:

· (Ipv6) During the "IPv6 Global Summit" (http://www.ipv6-es.com) in June 2005, jointly organized with the Internet Global Congress (http://www.igcweb.net) in Barcelona, the MareNostrum external connection started to work with IPv6 protocol. As most of the academic networks are IPv6 enabled, MareNostrum can be accessed using a native Ipv6 connection as well as with traditional IPv4 protocol. We expect to expand the use of this protocol next year, for which BSC has already reserved a /48 address range, which is approximately equivalent to 1.20 10^24 addresses.

· (Multicast) AccessGrid (http://www.accessgrid.org) is described as a set of tools and resources that allow a collaborative environment through the use of large-format multimedia displays. The access grid is used for large-scale distributed meetings, collaborative work sessions, seminars,



Network logical topology

tutorials and training. The increasing use being made at BSC has led us to move from the unicast version of software that can be run everywhere to the multicast version. Accordingly, a multicast has been deployed on some parts of the network. This will allow the reception of multimedia streams more efficiently than unicast.

· (QoS) The participation in the DEISA (Distributed European Infrastructure for Supercomputing Applications) (http://www.deisa.org) project forced us to acquire a video-conference supporting H.323 and SIP protocols. These protocols are known to be sensitive to parameters such as delay, latency and jitter, and will force us to implement Quality of Service policies in the near future.

Batch Systems, Monitoring and Performance

In order to achieve an efficient use of computing resources, resource managers and schedulers (also known as "batch systems") are needed. During the first year of BSC-CNS, the LoadLeveler batch system was installed in the MareNostrum supercomputer. This software has required several modifications in order to adapt it to the special configuration and the size of MareNostrum, a task that is being carried out in tight collaboration with IBM developers.

On the BSC-CNS site, a number of tools have been developed in order to automate the process of updating the resource manager configuration and distributing it to all the nodes in the cluster, collect execution information, diagnose problems, etc. Some of these tools can automatically change the configuration of LoadLeveler in order to keep the system running even in the event of occasional hardware or software problems.

The current LoadLeveler configuration allows users to submit jobs to several "classes", depending on their requirements. Thus, there are classes for "interactive" jobs and for "debug". Also, depending on the number of processors and time required, jobs are distributed into "small", "medium" and "large" classes. Finally, additional classes exist for jobs with special requirements (e.g. specific configurations, kernel modules, etc.).

The priority of jobs is dynamically adjusted, taking several factors into account (such as the number of resources required, the number of jobs being sent, the expected termination time, the system load, etc.).

Apart from day-to-day production, we must follow the current developments in high performance computing, testing new software and techniques to improve system performance. In this context, the SLURM resource manager has been tested as an alternative to LoadLeveler, especially to support "grand challenge" applications that require the whole supercomputer to run. The Maui scheduler is also under evaluation, as it may provide enough flexibility to adapt to the changing requirements of the applications at BSC-CNS.

Another important tool to improve the performance of our computing resources is the monitoring system, which allows us to detect anomalies, such as hardware problems and system or application malfunctions. Accordingly, Ganglia has been deployed at MareNostrum and adapted and configured to provide real-time information about the 2400+ computing nodes. Several extensions have been added to integrate it with the batch systems (reporting information about the jobs being executed and the resources being used) and several diagnostic tools.

Due to the large number of nodes of MareNostrum, a new visualization tool has been developed to report the monitoring information by showing a synthetic view of the whole supercomputer, highlighting the "hot spots" (as opposed to common visualization tools that show the detailed status of individual nodes).

All these tools are being used to start a characterization of the applications being executed at BSC-CNS, including the amount of resources required (processors, memory, disk, time, etc.). By knowing the needs and behaviour of the applications, we aim to tune our systems to achieve better performance and a more efficient use of our computing resources. BSC is also committed to improving the usability of our systems by final users. In this context, a number of tools and scripts are being developed to provide information to users about the execution of their jobs and to check them before submission. In addition, new interfaces to the system are being tested, such us UniCore, which provides a graphical interface to the batch systems.

Last but not least, BSC aims to collaborate with other supercomputing centres, and actively participated in testing and deploying tools that will allow the integration of our systems in continental-wide clusters, allowing our batch and monitoring systems to interact with those installed at remote sites. PKI/Certificates, LDAP and Web Services are some of the technologies that will enable this integration.

Security

From the security viewpoint, the policy of "Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS)" is to protect information assets from all threats, whether internal or external, deliberate or accidental.

The implementation of this policy is important to maintain our integrity as a supplier of services to internal and external customers. This task is being and will be developed by "The Computer Emergency Response Team – Barcelona Supercomputing Center" (CERT-BSC).

The main objective of CERT-BSC focuses on how the BSC-CNS systems are implemented from the security point of view, and how security affects their properties. It examines systems to establish what information is stored and processed, how valuable it is, what threats exist, and how they can be addressed (Risk Assessment).

This year, the security of the new BSC-CNS network topology was audited and evaluated by CERT-BSC.

User Support

The User Support Staff provides assistance with all aspects of scientific computing and visualization. This assistance includes, but is not limited to, general user support, writing and porting serial and parallel codes to the supercomputers, development of scripts or user-friendly procedures, assistance with software packages, tutorials on specialized topics or programmes, user training, code optimization, parallel model building support, and assistance with developing code for the supercomputers.

The areas of expertise include Earth Science, Computational Chemistry, Computational Fluid Dynamics, Design Optimization, Structural and Molecular Biology, Bioinformatics and Computational Biology.

The number of user support requests received in the period from 1 March to 31 December totals approximately 1600. These can be classified into 9 different groups.

During 2005 approximately 70 external researchers accessed MareNostrum.

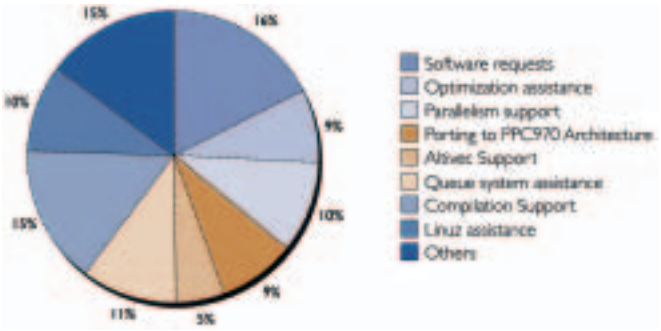
Accounting

MareNostrum began public operation on 23 June 2005. The system has been used for system installation and scalability testing for software such as LoadLeveler and GPFS since January 2005. The first is the resource manager in MareNostrum, and GPFS is the Global Parallel File System. In both, MareNostrum is the largest system in the world due to the number of nodes, and a special setting was required, together with the support of the development team.

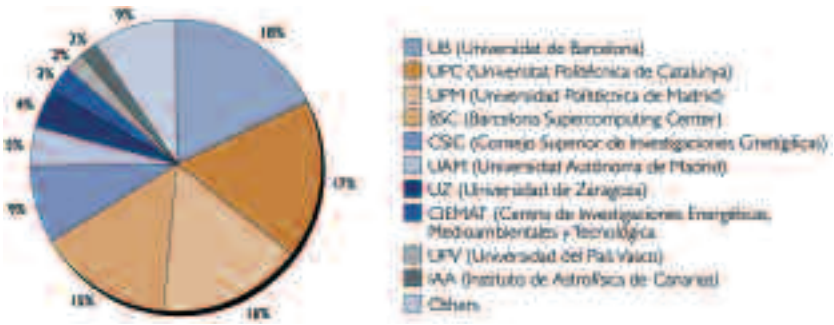
The system use can be defined as follows:

$$\left(\frac{total\_cpu\_hour\_used}{total\_hours}\right) \times 100$$

The system use has certain variations during the year and in the later period of the year it reaches a more stable value of 80%.



User support requests classified per topic

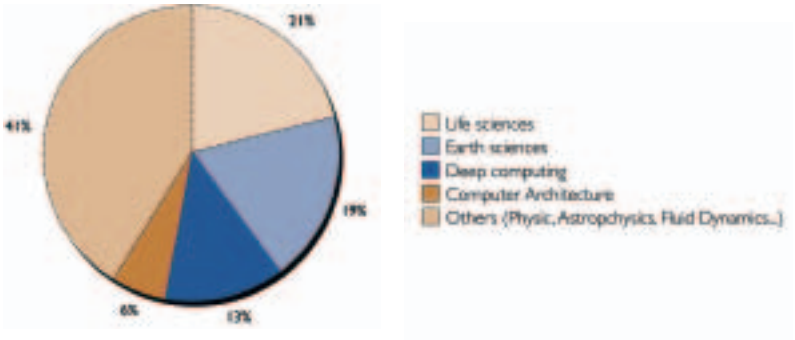


User support requests classified per institution

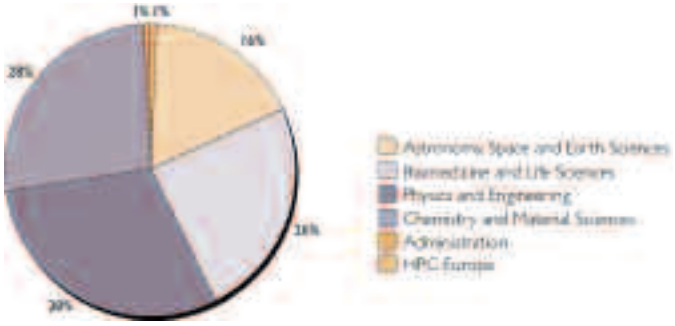
Top 500 list:
In November 2004 Top500 list, MareNostrum reached fourth worldwide place and the first place in Europe (www.top500.org).

In June 2005 Top500 list, MareNostrum continues being the first European supercomputer and descended to fifth worldwide.

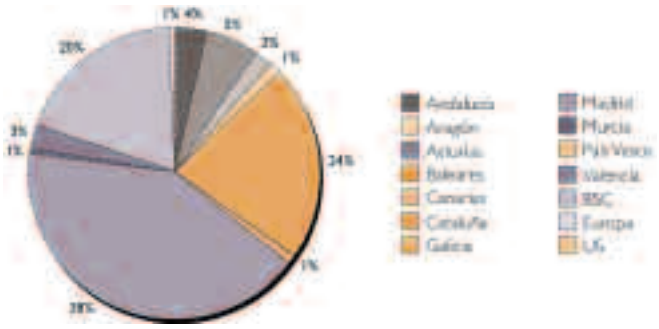
In November 2005, MareNostrum continues being the first European supercomputer and descended to eighth worldwide.



User support requests classified per area



Use of MareNostrum classified per science area



Use of MareNostrum classified per geography

4.2 Business Development

Business Development Group has two main responsibilities: Project Management and Marketing.

- The Project Management area is in charge of promoting, looking for opportunities, starting and, finally, manage any scientific or industrial external funded project in the Center.
- The Marketing area is in charge of the corporate image at Barcelona Supercomputing Center, what includes the communication and dissemination of our activities to the Academia, the industry and the Society.

In addition the group coordinates the areas of Technology Transfer and Training.

Project Management

International Activities

BSC-CNS has kept an intense record of participation in international activities during 2005. The involvement in activities belonging to the VI Framework Programme of the European Commission has been particularly relevant. During 2005, BSC-CNS has participated in two projects - DEISA and HPC-Europa - and has been involved in several European project proposals.

- DEISA Project

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

BSC-CNS joined the DEISA project (http://www.deisa.org) in May 2005. The project has secured funds until the end 2007 and a proposal for extended activities in 2007 and 2008 (eDEISA) is currently being negotiated.

During 2005, the main activities in which BSC-CNS has been involved are management, participating in the Executive Committee, dissemination, service activities and life science joint research activities, led by BSC.

In addition, seven proposals have been submitted to the DEISA Extreme Computing Initiative (DECI) from Spain (the total number of proposals submitted by the 12 partners was 52). Four of these proposals were selected for execution.

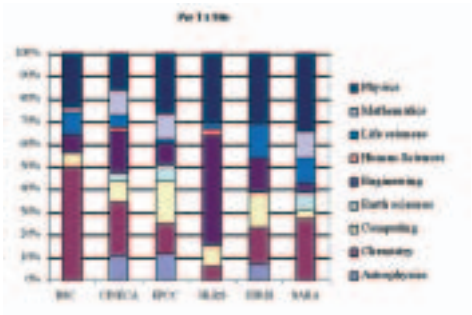
- HPC-Europa project

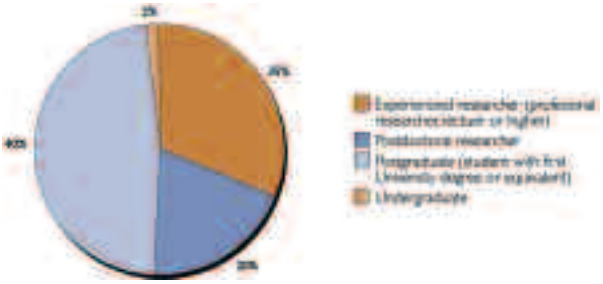
HPC-Europa is a consortium of six leading High Performance Computing (HPC) infrastructures, including BSC, and five centres of excellence. This consortium aims to provide advanced computational services in an integrated manner to the European research community. The culture of cooperation fostered by the consortium's joint research and networking activities generates critical mass for computational science.

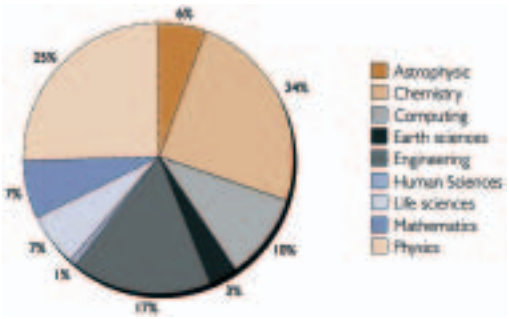
It enables researchers working in any eligible country in Europe to visit a participating research institute to carry out a collaborative visit of up to 3 months' duration and to gain access to some of the most powerful High Performance Computing (HPC) facilities in Europe.

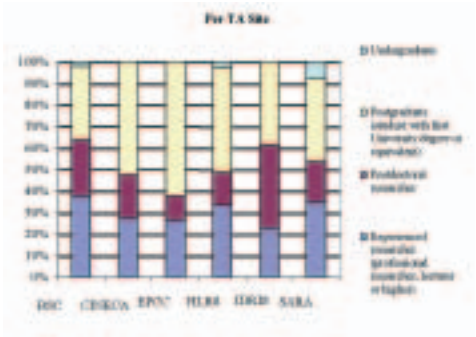
During 2005 the BSC-CNS welcomed 50 researchers through the European Commission's HPC-Europe Transnational Access programme. These researchers have visited and used BSC facilities.

The following graphs offer information about the distribution of visitors for 2005, for the whole Consortium and for each HPC Center:









Technology Transfer

During 2005, BSC started up technology transfer projects with IBM, Bull, Gas Natural and Airbus:

Several projects in Deep Computing and Computer Architecture are continuing the research lines that UPC and IBM carried out over the last 5 years through their joint initiative, CEPBA-IBM Research Institute (CIRI).
The aim of the project is to cooperate with Bull in its Lustre technology, where BSC will supply its expertise on storage systems.

Air quality studies in cities like Barcelona or Madrid are taking place within the scope of this project.
BSC is helping Airbus to improve its eLSA code (fluid dynamics), developed by ONERA in France and used worldwide by Airbus.

Memorandums of Understanding

During 2005, BSC signed five Memorandums of Understanding:

CIEMAT – UPM: CIEMAT (Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas), one of the main players on the Spanish eScience scenario, and UPM (the Technical University of Madrid) with an excellent background in Supercomputing and Computer Architecture areas. The objective of the agreement related mainly to sharing experiences and resources in these areas.

· INB (Instituto Nacional de Bioinformática), one of the key players in Life Sciences in Spain. BSC is one of the Technical nodes, that related to Supercomputing, of the INB.

· JSCC (Supercomputing Centre of the Russian Sciences Academia). The objective of the agreement related mainly to acting as a hub in both countries, in order to bring the respective scientific communities together.

· CESGA (Supercomputing Centre in Galicia), one of the supercomputing centres that existed in Spain before the establishment of BSC. The objective of the agreement related mainly to sharing experiences and resources in Supercomputing.

· IAC (Instituto de Astrofísica de Canarias) one of the three main astrophysics centres in the world. The objective of the agreement is to help this scientific community advance through the use of BSC Supercomputing resources (Human and Computing resources).

Image

Visits to MareNostrum

During 2005, BSC-CNS received a total of 500 people from national and international centres, including universities, research centres, industry and non-profit organizations. MareNostrum in addition to be a tool for a Scientific research is a new way to obtain the interest of Society in Science.

Conferences
BSC members participated in different conferences and courses to disseminate BSC-CNS activities:

International:
HPC Europa. 2nd Transnational Access Meeting (TAM), HLRS, University of Stuttgart (Germany)
JSSC seminar Power.org. Moscow, Russia.
IBM. Boblingen, Germany.
LA Grid. Miami, USA.
Grid@Large Workshop. Lisbon, Portugal.
Forum ORAP. Paris, France.
Machine Evaluation Workshop. Daresbury, UK.

National:
Cercle de la FIB, Facultad de Informática de Barcelona. UPC, Barcelona.

Workshop on Scientific Cases for European HPC Initiative. Barcelona.

XV Ciclo de Divulgación Científica. Caja de Burgos. Burgos.
JOCS: Jornada Catalana de Supercomputación. Universitat Rovira i Virgili. Tarragona.

Grandes usuarios de Supercomputación. BSC, Barcelona.
Centre de Regulació Genòmica. PRBB, Barcelona.

Fundación Valenciana de Estudios Avanzados. Valencia.
Jornadas españolas de e-Ciencia. Santiago de Compostela.
SPOC, Barcelona.

IGC 2005. Internet Global Conference. Barcelona.
Universidad de Las Palmas de Gran Canaria.

Fundación "Zaragoza Ciudad del Conocimiento". Zaragoza.
II Jornada para el profesorado de Secundaria. Universidad Politécnica de Catalunya.

Jornada de Aeronáutica. CIMNE - Universitat Politécnica de Catalunya.

Ministerio de Medio Ambiente. Madrid.

Instituto de Astrofísica de Canarias. La Laguna.

Cosmocaixa. Barcelona.

Universitat Pompeu Fabra. Barcelona.

Universidad de la Rioja. Logroño.

Events organized by BSC
The centre also organized different seminars and workshops during the year:

- 3 November 2005 – Conference on Forecast Air Quality in Spain (1 day)
- 22 November 2005 - Opening BSC (1 day)
- 28 and 29 November 2005 - 1st Workshop on Scientific Cases for European HPC Initiative (2 days).

4.3 Human Resources, Administration and Finance

The Human Resources, Administration and Finance Unit covers 3 areas:

- Human resources: manages selection processes, hiring and training; prepares job descriptions, looks after labour relations and collective bargaining, plannes careers and internal promotion, and prevents work-related accidents.

- Administration support: deals with reception and logistics, space allocation and new offices, purchasing and secretarial support for directors.

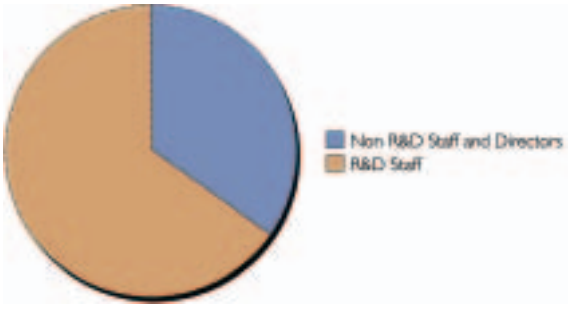
- Finance and accounting: manages the financial resources of the center, calculates and pays expenses, meets budgetary obligations according to existing financial legislation and accountancy norms, manages and safeguards acquired patrimony. It prepares budgets, the annual accounts report, the balance sheet, the liquidation of budget deficits, and the processes of accounting audits. Detects and analyzes budget deviations. Acts as treasurer, managing relations with banks, deals with suppliers, receiving payments.

2005 saw the setting up and launch of the staff structure in BSC-CNS, involving the creation of six departments (as outlined in the attached organizational chart), and the hiring of 63 staff.

It should be emphasized that the staff includes staff from other public institutions with close ties to the centre, complying with established norms and according to established agreements of collaboration with each one.

The following is a breakdown of staff in the BSC-CNS Consortium at the end of the year 2005:

Departament	Number of staff
Director and Associate Director	2
Administration and Finance	4
Operations	11
Business Development	5
Earth Sciences	4
Life Sciences	9
Computer Sciences	28
TOTAL	63



Incorporating all the new staff and welcoming visiting researchers meant finding and adapting the necessary space for their activities. Two types of areas have been established: those that entail no additional financial expense, and those that entail a financial cost for the right to use.
The areas given by the UPC, according to the established collaborative agreement, consisting of the rooms which house the supercomputer and the energy and refrigeration equipment, and the work rooms of the staff directly responsible for the physical operation of the machine. The facilities are located in the Edificio Capilla de Torre Girona ("the Chapel"), in Calle Jordi Girona 31, 08034 Barcelona.

The building initially housed a chapel, which explains its architectural structure. It has undergone two extensions, one in a nearby basement which houses the energy equipment, water tanks, generators, etc.; and the other in the South facing part of the building, which houses the computer itself. At the end of 2005 the renovation work, including the provision of office space for the operational staff, was completed. The total space available for use is 1,864.79 square metres.

Rented Areas are in the Nexus II building, managed by the Zona Franca Consortium. 710 square metres have been rented on the first and third floors. Additionally, negotiations with other institutions lodged in the same building have taken place in order to accommodate the many researchers who, according to the plan for 2006, will soon be hired.

MareNostrum Supercomputer

5 MareNostrum Users

Research leaders with access to the supercomputer

This section details some of the external researchers that have accessed MareNostrum, as well as the title of the projects performed during 2005. Papers derived from the work done in 2005 and published before the printing of this Annual Report has been included. They have been classified in accordance with the different areas of knowledge in which the Access Committee is organized.

· **Biomedicine and Life Sciences**
- Ángel Ramírez Ortiz, Universidad Autónoma de Madrid. "Protein structure prediction".
- Carme Rovira i Virgili, Universidad de Barcelona. "Unravelling the mechanism of drug activation in Mycobacterium tuberculosis catalase-peroxidase by means of first principles Car-Parrinello simulations."
- Ernest Giralt, Universidad de Barcelona. "Evolutionary Algorithms and de Novo Peptide Design".
- Francisco Javier Luque, Universidad de Barcelona. "Ligand exit pathways in Mycobacterium tuberculosis truncated haemoglobin"
- Jordi Garcia Ojalvo, Universitat Politècnica de Catalunya. "Nonlinear and stochastic aspects of gene regulation"
- Jordi Villa Freixa, Institut Municipal d'Investigació Mèdica. "ByoDyn: parameter estimation of multicellular models of gene regulatory networks"
- Juan Jesús Pérez González, Universitat Politècnica de Catalunya. "Molecular dynamics simulations of G-protein coupled receptors"
- Julio Rozas, Universidad de Barcelona. "Detecting the impact of natural selection on a genome-wide scale"
- Natalia Díaz, Universidad de Oviedo. "Matrix Metalloproteins: Modelling of Substrate Binding and Enzyme Catalysis"

· **Astronomy, Space and Earth Sciences**
- Allen Bateman, Universitat Politècnica de Catalunya. "Study of debris flows, associated with extreme rain events."
- Álvaro Viúdez Lomba, CSIC. "Generation of inertia gravity waves by balanced geophysical flows"
- Fernando Moreno Danvila, CSIC. "Calculation of scattering matrices for large and irregular particles with the Discrete Dipole Approximation method"
- Fernando Moreno Insertis, Instituto Astrofísico de Canarias. "Eruptive phenomena in the atmosphere of the sun and cool stars"
- Gustavo Yepes, Universidad Autónoma de Madrid. "Cosmological Simulations of Large-Scale Structure formation in the Universe"
- Romain Teyssier, Comissariat à l'Énergie Atomique (CEA), HORIZON Consortium, DEISA. "HORIZON@MareNostrum: Galaxy formation in a cosmological context"
- Jordi Torra i Roca, Universitat de Barcelona. "Gaia: Simulation of Telemetry Stream"
- Jose Maria Ibáñez, Universidad de Valencia. "Stability of extragalactic jets"
- Josep Maria Solanes – Universitat de Barcelona. "Investigation of the Diffuse Light Component in compact groups of galaxies (IDILICO)"
- Juan García Bellido, Universidad Autónoma de Madrid. "Cosmological Parameter Estimation from CMB and LSS data"
- Pablo Fosalba, Universitat Autònoma de Barcelona. "Large numerical simulations for dark-energy surveys"
- Rolando R. Garcia, University Corporation for Atmospheric Research. "Simulation of changes in atmospheric climate and chemical composition 1950-2050"

· **Physics and Engineering**
- Antonio Huerta, Universitat Politècnica de Catalunya. "Large-Scale Simulations of Dynamic Fracture"
- Asensi Oliva, Universitat Politècnica de Catalunya. "Direct Numerical Simulation of Turbulent Flows"
- Domingo Giménez Cánovas, Universidad de Murcia. "Parallel routines optimization and applications"
- Iñigo Toledo, Desafio Español Copa América. "Desafio Espanol Challenge 2007 – America-s Cup Yacht CFD Research"
- Javier Jimenez Sendín, Universidad Politécnica de Madrid. "DNS in turbulent channels"
- Josep Maria Porta, Universitat Politècnica de Catalunya. "Isolating configuration spaces of polycyclic robots and molecules by extended bound smoothing"
- Markus Uhlmann, CIEMAT. "Direct Numerical Simulation of Turbulent Flow with Suspended Solid Particles"

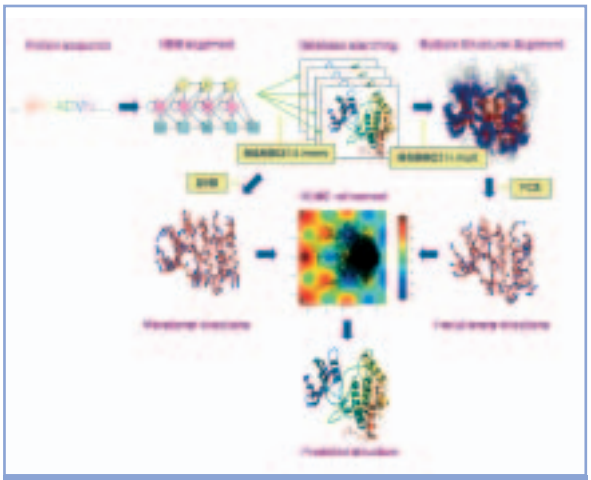
- Monty Newborn – McGill University, Montreal. "Parallel Automated Theorem Proving"
- Pilar Hernández, Universidad de Valencia. "Non-perturbative aspects of QCD in flavour physics"
- Richard J. Duro, Universidade da Coruña. "Automatic designo f wind turbina blades"
- Vincent Gimenez Gómez, Universidad de Valencia. "Monte Carlo numerical computations of the properties of hadrons"

· **Chemistry and Material Science**
- Andrés Arnau, Universidad Politécnica de Valencia. "Adsorption of alkanethiols on Au(111) at different coverages up to one monolayer"
- Ángel Rubio, Euskal Herriko Unibertsotatea. "Spectroscopic properties of biomolecules, nanostructures and extended systems"
- Antonio Luque López, Universidad Politécnica de Madrid. "Study of the nonradiative recombination"
- Carlos Alemán, Universitat Politècnica de Catalunya. "Nanotechnology: De Novo Design using the Self-Assembly of Biomolecules"
- Carlos Alemán, Universitat Politècnica de Catalunya. "Dynamics of an Artificial Muscle based on Conducting Polymers and Calix[4]arene Scaffolds"
- Eduardo Hernández, Institut de Ciència de Materials de Barcelona. "Phase diagrams of complex materials from first principles simulations"
- Eliseo Ruiz, Universitat de Barcelona. "Magnetic Properties of large Single Molecule Magnets: Mn25 and Mn32"
- Feliu Maseras Cuni, Institut Català d'Investigació Química. "A DFT computational approach to supramolecular catalysis"
- Francesc Illas, Universitat de Barcelona. "Scalability of the VASP code and applications to heterogeneous catalysis"
- Isabel Campos, Universidad de Zaragoza. "Computational studies on Kinetics transport in stellerator TJ-II"
- Jordi Faraudo, Universitat Autònoma de Barcelona. "Molecular Dynamics Simulations of Electrostatic Interactions between Macromolecules and/or Macroions in Aqueous Solution"
- Josep Maria Poblet, Universitat Rovira I Virgili. "First-principles molecular dynamics simulations of the formation mechanisms of polyoxometalates with low nuclearities"
- Maria José Caturla Perol, Universidad de Alicante. "Atomistic simulations of materials with nano-features and the behaviour of materials under irradiation and extreme conditions of pressure and temperature"
- Pedro de Andrés, CSIC. "Molecular adsorption on metallic and oxide surfaces".

5.1 Biomedicine and Health Sciences

Ángel Ramírez Ortiz - Universidad Autónoma de Madrid
"Protein structure prediction"

Proteins are the "horsepowers" of the organism, nanomachines in charge of most biological functions. Many diseases are related to alterations in a particular protein, and as a result most drugs fulfil their pharmacological action by interacting with specific proteins. As with any machine, to really understand how it works and how it can be pharmacologically modulated it is important to know its three-dimensional structure. We know the sequence of many proteins, i.e. their building blocks, but we lack information about their structure, i.e., how these building blocks are organized in space. This is because experimental methods for protein structure determination are too expensive and time consuming in comparison with the speed at which protein sequences are determined. The long-term research goal is to devise computational methods to obtain high quality structural models from sequence information to bridge this gap.

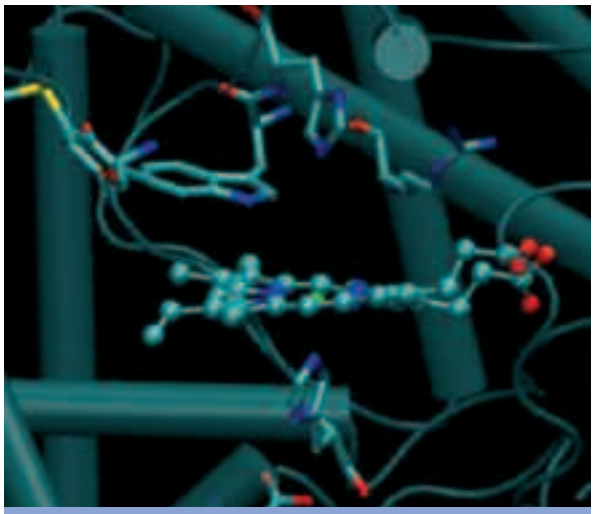


Protein Structure prediction process.

Carme Rovira i Virgili - Universidad de Barcelona

"Unravelling the mechanism of drug activation in Mycobacterium tuberculosis catalase-peroxidase by means of first principles Car-Parrinello simulations."

Catalase-peroxidases (CatPs) are bifunctional heme-dependent enzymes belonging to the class I peroxidase family. Despite the sequence homology, CatPs are the only members of the family displaying catalatic activity, which dominates the peroxidatic reaction. The Mycobacterium tuberculosis CatP is a target of pharmacological interest, as it activates isoniazid (INH), a drug used to treat tuberculosis. In particular, when the enzyme decreases the activity, the resistance to the drug increases. Therefore, the precise knowledge of the enzymatic mechanism is of fundamental importance to understanding both the activation process of the drug and the significance of variations in the enzyme (mutations) which may be directly responsible for INH-resistance. The project is intended to model the enzyme mechanism and find the most likely binding site for the INH drug in order to understand the drug activation mechanism. To this aim, the project performs several simulations with varying conditions (e.g. protonation state of the residues in the binding pocket) in order to see how they could affect the enzymatic activity through changes on the electronic structure of the reactive species. The analysis is performed in both monofunctional catalases (e.g. Helicobacter pylori catalase) and bifunctional catalases (CatPs). The intermediate reaction for monofunctional catalases basically shows the typical oxoferryl pophyrin radical, i.e. mostly delocalized on the porphyrin ring. However, slight changes in the radical location are found for other catalases, including CatPs, which could be related to differences in enzyme activity. The calculations are performed using the so-called Car-Parrinello molecular dynamics method, as implemented in the CPMD program. The project usually runs on 64-256 MN processors. Thanks to increasing supercomputing capabilities such as MareNostrum, it is feasible to do projects that involve a large number of atoms to be treated quantum mechanically. Only by using a large number of processors can the project obtain the results on appropriately, which is what makes the project feasible.



Molecular view of the active centre of the catalase-peroxidase enzyme. The heme group is shown in ball and stick and the catalytic residues are shown as sticks

Papers:

C. Rovira. "The Study of ligand-protein interactions by means of Density Functional Theory and first-principles molecular dynamics" in Methods in Molecular Biology, Vol 305, Protein-Ligand Interactions: Methods and Applications, ed.: G. U. Nienhaus, Humana Press, Totowa NJ, pp. 527-566 (2005)

C. Rovira. "Structure, protonation state and dynamics of the compound II intermediate of catalase. Chemical Physics Chemistry. 6, 1-8 (2005).

C. Rovira, M. Alfonso, X. Biarnés, I. Fita, P. Loewen, "A first principles study of the binding of formic acid in catalase complementing high resolution X-ray structures". Chemical Physics. 323, 129-137 (2006).

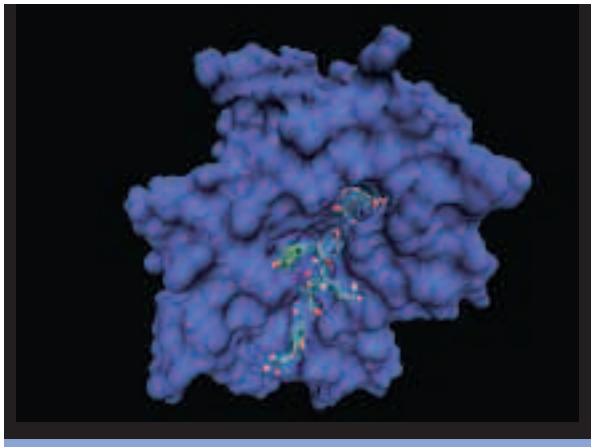
Ernest Giralt - Universidad de Barcelona

"Evolutionary Algorithms and de Novo Peptide Design"

The project is developing the program "Evolutionary structure de Novo Peptide Design Algorithm" (ENPDA). Given a user-defined target protein surface, ENPDA is able to design peptides able to recognize this surface, i.e., bind to it with good binding energies. In particular, the project focus falls in the implementation of novel features into ENPDA such as its capacity to design variable length peptides, reliable and fast docking strategies, and new parallelization architectures to achieve higher speed-ups. In addition, and as part of our testing problems, ENPDA was used to design peptide inhibitors for prolyl oligopeptidase, an important enzyme related to several neuropathologies such as schizophrenia, bipolar disorder, bulimia nervosa, etc.

Papers:

Ignasi Belda, Sergio Madurga, Teresa Tarragó, Xavier Llorà, and Ernest Giralt. Evolutionary computation and multimodal search: a good combination for tackling molecular diversity in the field of peptide design. Journal of Molecular Diversity, 2006 (in press).



Structure of the best peptide (EKYKEK) proposed by ENPDA that recognizes MHC H-2Kb surface. ENPDA evaluated 9500 different peptides to propose this final sequence.

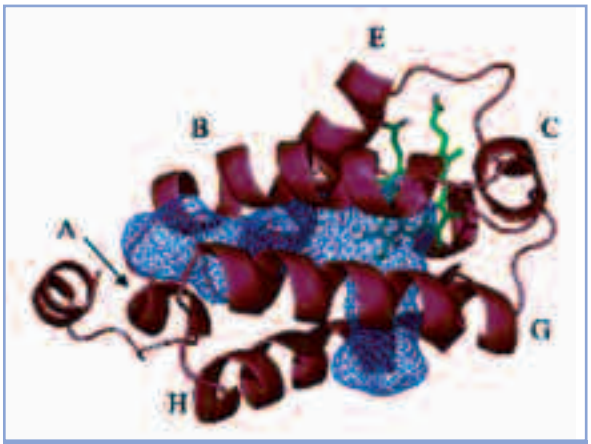
Francisco Javier Luque - Universidad de Barcelona

"Ligand exit pathways in Mycobacterium tuberculosis truncated haemoglobin"

Mycobacterium tuberculosis, the causative agent of human tuberculosis, is forced into latency by nitric oxide produced by macrophages during infection. In response to nitrosative stress M. tuberculosis has evolved a defence mechanism that relies on the oxygenated form of "truncated haemoglobin" N (trHbN), formally acting as NO-dioxygenase, yielding the harmless nitrate ion. X-ray crystal structures have shown that trHbN hosts a two-branched protein matrix tunnel system, proposed to control diatomic ligand migration to the heme, as the rate-limiting step in NO conversion to nitrate. Extended molecular dynamics simulations (0.1 μs), employed here to characterize the factors controlling diatomic ligand diffusion through the apolar tunnel system, suggest that O_2 migration in deoxy-trHbN is restricted to a short branch of the tunnel, and that O_2 binding to the heme drives conformational and dynamical fluctuations promoting NO migration through the long tunnel branch. In turn, this is achieved by modulating the conformation of the residues TyrB10 and GlnE11, which regulate the dynamical behaviour of helices B and E. The simulation results suggest that trHbN has evolved a dual-path mechanism for migration of O_2 and NO to the heme to achieve the most efficient NO detoxification.

Papers:

A. Bindon-Chanal et al. "Ligand-Induced Dynamical Regulation of NO Conversion in Mycobacterium Tuberculosis Truncated haemoglobin-N", volume 64, issue 2, Wiley InterScience, pages 457-464, 2006



Structure of trHbN showing the two branches of the tunnel system.

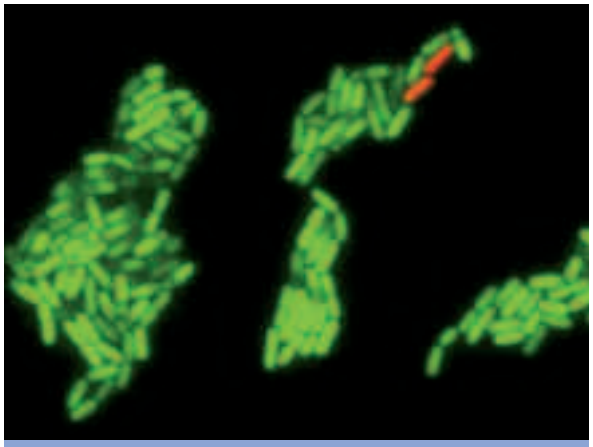
Jordi Garcia Ojalvo - Universitat Politècnica de Catalunya

"Nonlinear and stochastic aspects of gene regulation"

One of the most fundamentals aspects of cellular behaviour is phenotypic variability, through which a collection of genetically identical cells behave in strongly different ways. Cells use nonlinear and stochastic mechanisms for that purpose: nonlinearity leads to multistability, through which different cellular states coexist, and stochasticity allows for sampling of the different stable states. An important example of this phenomenology is the stress response of bacteria, through which these prokaryotic cells deal with a lack of nutrients. The project has studied the mechanism underlying the development of competence in the bacterium Bacillus subtilis. A combination of fluorescence microscopy experiments and numerical simulations has made it possible to identify the gene circuit module underlying this behaviour. The statistical analysis of the properties of such a genetic module is very time consuming from a computational point of view, due to the highly different time scales involved.

Papers:

G.M. Süel, J. García-Ojalvo, L.M. Liberman, M.B. Elowitz "An excitable gene regulatory circuit induces transient cellular differentiation" Nature 440, 545-550 (2006)

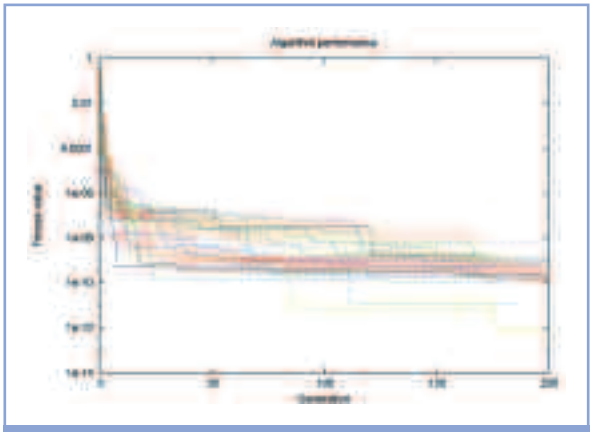


Behavior of a B. subtilis colony under stress. Green represents normal vegetative cells, red are competent cells.

Jordi Villa Freixa - Institut Municipal d'Investigació Mèdica

"ByoDyn: parameter estimation of multicellular models of gene regulatory networks"

Integrating multilayer biological/biomedical information is setting the ground for what is known as biomedical informatics. This field is partially based on systems biology approaches, where the research focuses on systemic rather than reductionist views. Within this framework, ByoDyn is an open source computational package aimed at studying the dynamical behaviour of small to massive biochemical networks (input as SBML files). The model can be simulated, the sensitivity of the system with respect to the parameters can be analysed and, more relevantly for the project, kinetic parameters can be estimated using experimental time course data. The project carried out on the MareNostrum aims at developing a parallel framework for the optimization techniques implemented in the programme. Thus, MPI tools are being developed to parallelize the critical aspects of the hybrid optimization algorithms used to find the optimal sets of parameters that fit a given set of experimental data.

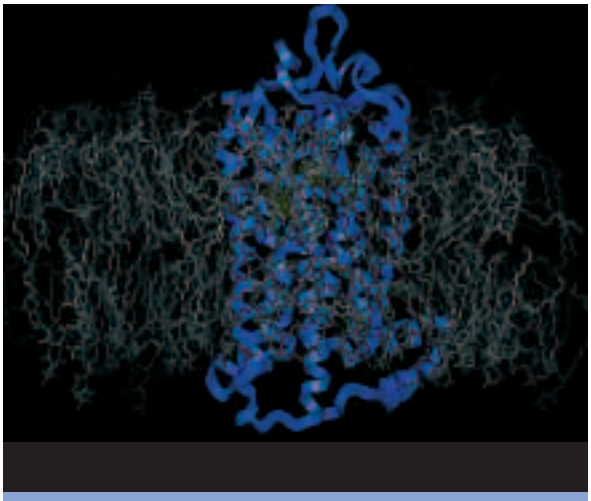


Multiprocessor hybrid optimization of the kinetic parameters for a model of two cells displaying lateral inhibition through a Notch/Delta interaction. The genetic algorithm (GA) is coupled with local gradient searches in each member of each GA generation.

Juan Jesús Pérez González - Universitat Politècnica de Catalunya

"Molecular dynamics simulations of G-protein coupled receptors"

The study carried out involves a comparative analysis of a set of five 16 ns MD simulations of rhodopsin embedded in a DPPC lipid bilayer using different simulation protocols. The simulations were carried out using periodic boundary conditions on a system consisting in a molecule of rhodopsin, 197 lipid molecules and 15,817 water molecules. Calculations were carried out considering two different approximations for the treatment of long-range electrostatics: on the one hand, the use of a cutoff and on the other, the PME method in combination with two different sampling ensembles: the canonical (NVT) and the constant pressure (NPT). The results seuggest that special care must be taken when selecting the statistical ensemble and the type of treatment for long-range electrostatics. The use of NPT is necessary for the bilayer equilibration and for the process involving the bilayer rearrangement around the protein. The use of the PME method provides a better description of lipids and ions but with a higher computational cost.



View of the system subject of the calculations. Water molecules are removed for clarity.

Julio Rozas - Universidad de Barcelona

"Detecting the impact of natural selection on a genome-wide scale"

The analysis of DNA sequence variation within and among species is a powerful approach to understanding the evolutionary forces underlying nucleotide variation. Currently, the comparative analysis of the non-synonymous and synonymous rate ratio (_) is the major tool for detecting genes or genomic regions under different selective constraints, or promoted by natural selection, using DNA sequence data from different species. Using this approach, the project is trying to identify genes, lineages and functional GO-categories with high and low constraints. Present analysis is being conducted using the complete genome information from 12 Drosophila species.

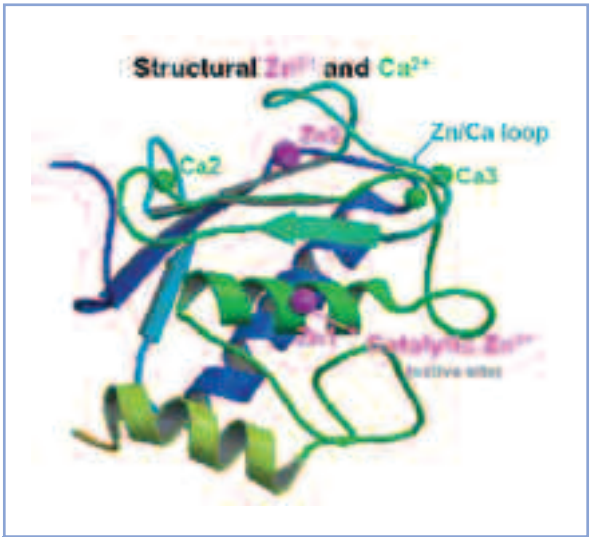
Natalia Díaz - Universidad de Oviedo

"Matrix Metalloproteins: Modelling of Substrate Binding and Enzyme Catalysis"

The computational work carried out in the Mare Nostrum supercomputer during 2005 is framed into a long term research project devoted to the study of the matrix metalloprotease enzymes (MMPs), a family of zinc-dependent endopetidases capable of hydrolyzing virtually all kinds of extracellular matrix proteins. Initially, it was characterized the coordination environment around the catalytic zinc ion using QM and QM/MM methodologies. Subsequently, it was analyzed by means of Molecular Dynamics simulations the role performed by the additional zinc and calcium ions observed in the crystallographic structures (the so called "structural metal ions"). The results point out that the structural zinc ion contributes to stabilize the catalytic domain, whereas the presence of the calcium ions seems to modulate the accessibility to important anchorage points of the active site groove.

Papers:

Natalia Díaz, Dimas Suárez, and Tomás L. Sordo. "A Quantum Chemical Study on the Coordination Environment of the Catalytic Zinc Ion in MMPs". Submitted to J. Phys. Chem. B.



Ribbon representation of the catalytic domain of MMP-2 (gelatinase A). The catalytic zinc ion (Zn1) and the structural metal ions (Zn2 and Ca1-Ca3) are also presented.

5.2 Astronomy, Space and Earth Sciences

Allen Bateman - Universitat Politècnica de Catalunya

"Study of debris flows, associated with extreme rain events"

GITS (Grupo de Investigación en Transporte de Sedimentos, DEHMA-UPC) has developed FLATModel, a numerical model for 2D shallow water equations; this model was designed to compute floods. Making some modifications to the equations and mainly in the geologies, it is possible to compute debris flows. These flows are associated with extreme rain events. To obtain precise results in this kind of simulation, a fine mesh (~1m2) is required and the total area of the computations is on a scale of Km2. Accordingly, it is typical to work with grids with more than four or five millions of nodes. With these floods and debris flow computations, it is possible to define risk areas. If the areas are urban, the results enable the design of control structures to avoid or reduce the damage.

The implementation of the model is designed to include the flow computations and the hydrological computations. The fact that the model works over a structured uniform grid enables the integration of a distributed hydrological model working with information such as meteorological radar or rain gauges, some of these coupled models compute the hydrological results and terrain stability values. This makes it possible to delimit landslides risk zones.

There are two different computing modes: the first computes flows or debris flows only; the second computes hydraulic flows and hydrological results. Together with hydrological results, we can obtain a simple landslide risk map. The main difference between two modes is the cell scale: hydrological scales are larger than hydraulic scales. Therefore, to couple both computations, it is again necessary to work with big domains and compute on small scales. Consequently, it is necessary to use parallel computing techniques. As an improvement of the model, GITS is developing a FLATModel with AMR (Automatic Mesh Refinement). This mesh refinement allows the use of different resolution scales in the domain and dynamically changes the cell size to adapt it to a resolution criterion defined by modeller.

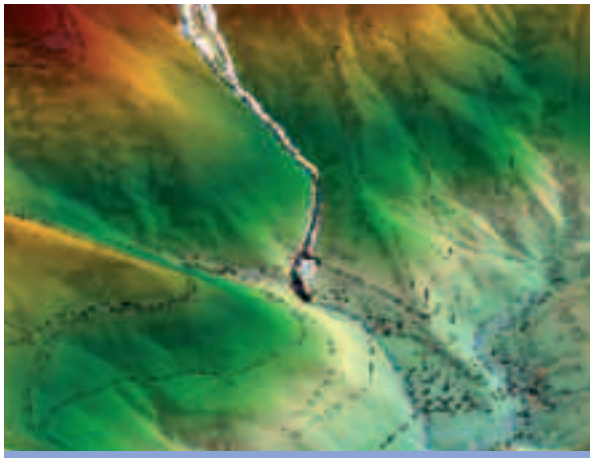
The hydrological models that can be connected to FLATModel include TRIGRS (Baum and Savage, 2002) and TOPMODEL (Beven and Kirkby, 1979). Other specific slope stability models that can be connected are SINMAP (Pack and Tarboton, 1998) and SHALSTAB (Dietrich, 1995).
The FLATModel uses the finite volume method (FVM) to solve the shallow water equations with modifications to include steep slope situations and debris flow geologies. The Godunov method is used, which explicitly solves Riemann problems on every cell face. The equation system is unsteady so the model computes a transitory system in an explicit way. As a consequence, the time step is small, which requires a lot of iterations to simulate a complete event.

The fact that it has a large computation mesh and simulation periods makes computer parallelization necessary. To parallelize an

explicitly structured grid is easy; all that is required is to divide the computation domain and assign every subdomain to a computation node. Then, during the computation, it is necessary to exchange information between subdomains as boundary conditions. To parallelize the code MPI (Message Passing Interface) and OpenMP was used.

Papers:

Bateman, A., Medina, V., Hürlimann, M., (2006). Modelo bidimensional para simulación de flujos detríticos: FLATModel. Ingenieria Hidráulica de Mexico. Under revision.



3D Picture of the debris flow simulation

Álvaro Viúdez Lomba - CSIC

"Generation of inertia gravity waves by balanced geophysical flows"

High-resolution three-dimensional numerical experiments carried out at the Supercomputer MareNostrum showed that initially balanced, static and inertially stable geophysical flows (void of waves) generate spiral patterns of inertia-gravity waves (IGWs).

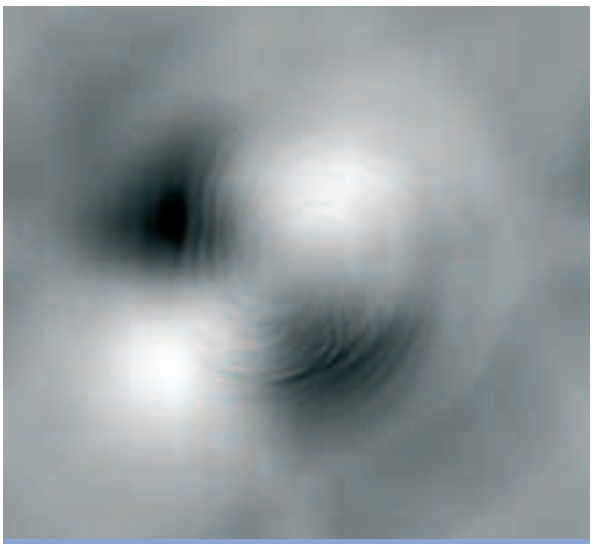
The spiral wave patterns are due to the spontaneous generation of IGW packets emitted from fluid volumes experiencing large local changes in potential vorticity.

The IGW packets spread away from the vortical flow and cause spiral wave patterns in the same direction as the spiral, i.e. cyclonic or anticyclonic, similar to the moving IGW sources.

The generation of the spiral wave patterns was observed in many numerical simulations, including the single ellipsoidal vortex (cyclone and anticyclone), the merging of two spherical vortices, the dipole, the tripole and the shear and baroclinic instability.

Papers:

Viúdez, A., 2006: Spiral patterns of inertia-gravity waves in geophysical flows. J. Fluid Mech. 562, 73-82.



The image shows the spiral patterns in the vertical velocity field produced by the anticyclone in a vortex dipole in a numerical simulation with 512 x 512 x 512 grid points.

Fernando Moreno Danvila - CSIC

"Calculation of scattering matrices for large and irregular particles with the Discrete Dipole Approximation method"

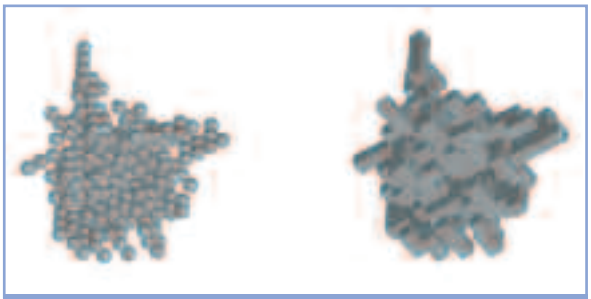
MareNostrum supercomputer was used to make calculations of scattering matrices of several irregular particles for blue and red incident wavelengths, for several values of the refractive indices, and for different structures, ranging from compact to fluffy (aggregate) particles, with the Discrete-Dipole Approximation code. The results are still preliminary, but some conclusions can already be stated:

1) The scattering of large-size aggregates of individual strongly absorbing spherical monomers (up to 512 spherules of 0.1 micrometer in radius) do not reproduce the observed properties of the linear polarization in comets, as has been previously suggested.
2) The shape of the phase function depend on whether the monomers are spherical or non-spherical. In particular, in the latter case, the backward lobe becomes less prominent. Therefore, in general, the scattering properties of aggregates as being represented by a collection of glued spherules may not be representative of real aggregate structures.
3) The calculations of the scattering matrices with MareNostrum show, for the first time, that the amount of circular polarization observed in comets may be largely due to the fact that the particles have not any symmetry. However, additional calculations must be done to exclude other possibilities, such as the particle alignment by electromagnetic or solar radiation forces.

Papers:

Guirado, D., Hovenier, J.W., and Moreno, F. "Circular polarization of light scattered by asymmetrical particles" 9th International Conference on Electromagnetic and Light Scattering by Non-Spherical Particles, 59-62, June 5-9 2006, St. Petersburg.

Moreno, F., Muñoz, O., Molina, A., Vilaplana, R., and Guirado, D. "Can a distribution of compact particles reproduce the observed properties of cometary particles at visible wavelenghts ? 9th International Conference on Electromagnetic and Light Scattering by Non-Spherical Particles, 199-202, June 5-9 2006, St. Petersburg.

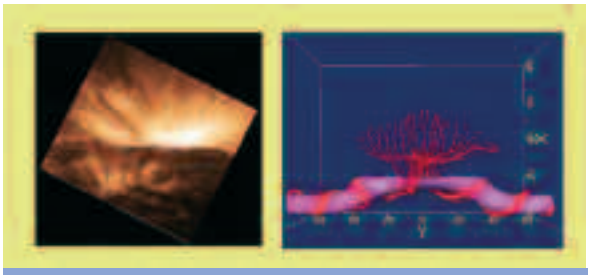


A sample of aggregates of spheres (left) and cubes (right) used in the simulations. These aggregates were grown by a diffusion-limited aggregation scheme. Each configuration is composed by some 250.000 dipoles. The calculations with the MareNostrum supercomputer reveal that the orientationally-averaged scattering matrices are significantly different in these cases, so that the monomer shape is influencing the global scattering properties of the whole aggregate.

Fernando Moreno Insertis - Instituto Astrofísico de Canarias

"Eruptive phenomena in the atmosphere of the sun and cool stars"

In 2005 the team carried out a preliminary phase of our use of the MareNostrum computer. In the project the team is using three different, large parallel magnetohydrodynamic codes adequate to run in massively parallel architectures. In 2005, the team implemented in the MareNostrum (MN) one of those codes. The implementation involved a number of optimizations; it also included extensive scaling tests. The conclusion, for large computational grids, like the ones needed for these experiments, is that code shows excellent scaling in the MN up to (at least) 512 CPUs. A few complete runs were carried out for comparatively small setups but for research-relevant experiments, which have helped in the planning of the larger experiments being run in 2006.



(left) image taken by the solar space mission TRACE showing very hot gas that delineates magnetic field lines in the solar corona (outer part of the solar atmosphere).
(right) snapshot from a numerical simulation of magnetic flux emergence into the solar atmosphere showing the magnetic field line distribution; the uppermost field lines, located in the corona, strongly resemble the satellite image.

Gustavo Yepes - Universidad Autónoma de Madrid

"Cosmological Simulations of Large-Scale Structure formation in the Universe"

The scientific objective of the project is to understand how galaxies and larger structures are formed in the Universe from cosmological initial conditions and to determine the relevant physical processes responsible for the formation and evolution of the objects we see in the universe today and in past times. Accordingly, the project employs state-of-the art numerical codes (called GADGET) that simultaneously take into account the gravitational evolution of density disturbances in an expanding universe and the hydrodynamic and shorter scale processes acting on the visible component of the matter: the baryonic gas.

The codes are fully parallel (with MPI) and can treat a large number of particles representing the collisionless dark matter and the collisional baryonic gas fluid. They also have a module to include all the extra physical processes (non-adiabatic) acting on the baryon component related to electromagnetic and nuclear interactions. The multiphase nature of the ISM is also taken into account, as well as chemical enrichment modelling. This makes the code very useful for studies of cosmic structure formation on different scales, ranging from large-scale distributions in which the non-adiabatic effects have less importance, to the formation of galaxies themselves, in which a very detailed modelling of the baryonic processes is required.

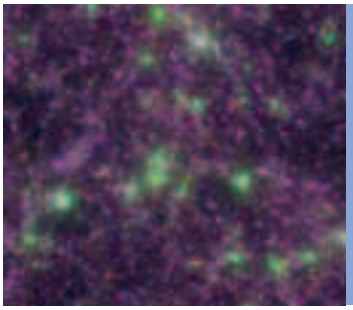
The first application of GADGET in MN has been able to simulate the largest-known SPH simulation of large-scale structure formation. The so called MareNostrum Universe simulation consists of more than 2 billion particles (half dark matter and half SPH) distributed in a 500 /h Mpc comoving box. The project used 256 nodes (512 processors) of MareNostrum.

Papers:

Stefan Gottlöber, Gustavo Yepes, Christian Wagner & Raúl Sevilla The MareNostrum Universe. Proceedings of XXVI Astrophysics MoriondMeeting. La Thuile, 2006.(in press).

Stefan Gottlöber, Gustavo Yepes, Christian Wagner & Raúl Sevilla. Baryon distribution in the Mare Nostrum Universe. Proceedings of DSU 2006 The Dark Side of the Universe. Madrid 2006.

Gustavo Yepes, International Conference: Bernard's Cosmics Histories: From Primordial Fluctuations to Cosmological Structures. The MareNostrum Universe. The biggest SPH simulation up to now. Valencia 2006.



This picture shows 13 billion years of evolution of the gas density in a small portion of the MareNostrum Universe Simulation. The formation of clusters of galaxies can be clearly seen in this animation.

Roman Teyssier. Comissariat à l'Énergie Atomique (CEA). HORIZON Consortium - DEISA

"HORIZON@MareNostrum: Galaxy formation in a cosmological context"

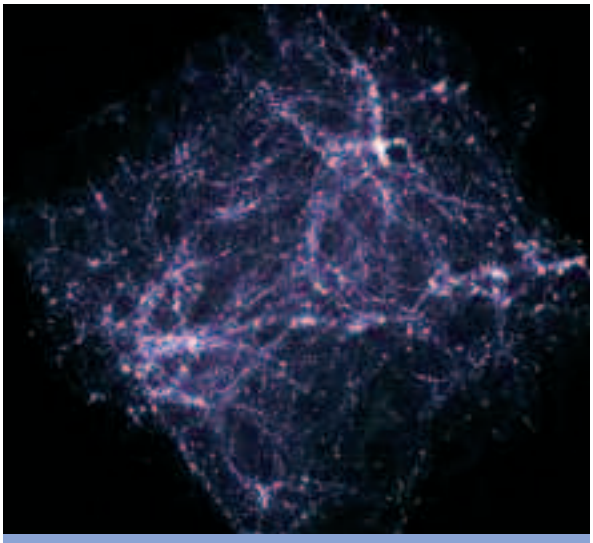
The Horizon Project is led by a French consortium whose objective is to tackle the key astrophysical issue of galaxy formation in the explicit cosmological context of an expanding universe dominated by dark matter and dark energy. To achieve this goal, the project runs the largest and most resolved N-body and hydrodynamic simulation to date with state-of-the-art subgrid physics modelling to describe star formation and feedback processes. For this purpose, the project uses an Adaptive Mesh Refinement (AMR) code called RAMSES (R. Teyssier, A&A, 2002, 385, 337), which is a tree-based, high-order Godunov solver with self-gravity. Its parallelization strategy relies on MPI-based adaptive domain decomposition, using a "space-filling Peano-Hilbert curve". To be more specific, this project provides the first opportunity to perform a 20 billion grid cell simulation, allowing for the first time to resolve the formation of "dwarf galaxies" within a large enough volume fraction of the universe to beat the cosmic variance. The requirements for this extreme run are around 8 Terabyte of RAM memory and 4096 processors.

Papers:

Teyssier, Fromang & Dormy, 2006, "Kinematic dynamos using constrained transport with high order Godunov schemes and adaptive mesh refinement", Journal of Computational Physics, 218, 44

Fromang, Hennebelle & Teyssier, 2006, "A high order Godunov scheme with constrained transport and adaptive mesh refinement for astrophysical magnetohydrodynamics", Astronomy and Astrophysics, 457, 371

"The Universe in a Box", Liberation, June 17th, 2006 "Computational Cosmology", Les Houches School of Physics 2006, "The Fabrics of Space Time".

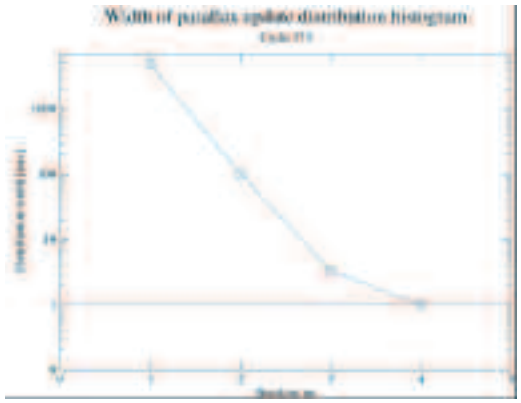


Redshift evolution and travelling

Jordi Torra i Roca - Universitat de Barcelona

"Gaia: Simulation of Telemetry Stream"

Gaia is an ESA astrometric mission whose main goal is the measurement of the position and velocity of approximately one billion stars. The simulation of the telemetry stream generated by Gaia is of extreme importance in the current phase of the project. The simulation on MareNostrum was for 1.2 millions of stars up to a magnitude of 12 over a period of 18 months. These data were used by several research teams in order to prepare and test the Gaia Main Data Base and the data reduction algorithms. This was the first step to an almost-complete simulation of the mission data, scheduled for 2009-2010.



Convergence of the Astrometric Global Iterative Solution (AGIS) of Gaia using the data generated at MareNostrum and processed by the Gaia team at ESAC.

Jose Maria Ibáñez - Universitat de Valencia

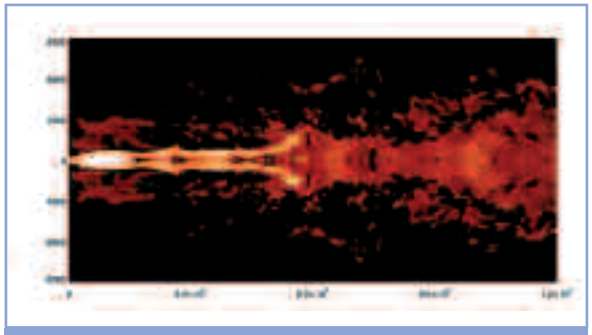
"Stability of extragalactic jets"

The study of the stability of extragalactic jets is a powerful tool to understand the physics and derive the physical parameters involved in extragalactic jets from Active Galactic Nuclei. Work on this topic has been mainly done in two dimensional simulations, where high numerical resolutions have been shown to be needed in order to reproduce successfully the growth of small instabilities. These requirements make very difficult fully three dimensional simulations without the use of high performance computers. Full parallelization of a three dimensional hydrodynamic code with MPI libraries has been performed in the Barcelona Supercomputing Center (BSC). This will allow not only to study the stability of relativistic jets in three dimensions but also to perform simulations on the long term evolution of jets in their motion through interstellar and intergalactic media. In the picture shows a map of one of these simulations for a two-dimensional axisymetric jet. The code is now under testing phase.

Papers:

Perucho, M., Lobanov, A., Martí, J.Mª, Simulations of the parsec-scale relativistic jet in 3C 273, Proceedings of the workshop Multiband Approach to AGN, Mem. S. A. It., 76, p.110-113.// (2005).

Perucho, M., Martí, J.Mª, Hanasz, M., Nonlinear stability of relativistic sheared planar jets_, Astronomy and Astrophysics, 443 863-881 (2005).



Snapshot of Lorentz factor from a long term simulation at t = 7:2 106 yrs. The color scale stands for the values of the Lorentz factor, ranging from 1 (black) to 5 (white). Coordinates are in parsecs.

Josep Maria Solanes - Universitat de Barcelona

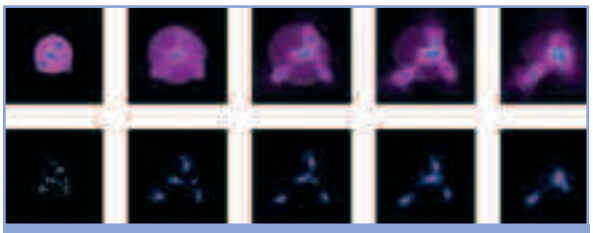
"Investigation of the DIffuse LIght COmponent in compact groups of galaxies (IDILICO)"

The IDILICO Project (Investigation of the DIffuse LIght COmponent in compact groups of galaxies) is an international collaboration involving researchers from Universitat de Barcelona, Universitat Rovira i Virgili, and Instituto de Astrofísica de Andalucía in Spain and Observatoire Astronomique de Marseille-Provence in France.
IDILICO is a basic research project specifically oriented towards studying the role of gravitational interactions on the evolution of galaxies in the highest density regions of the universe, known as compact groups of galaxies.
Preliminary simulations performed with the MareNostrum supercomputer have shown that compact groups of galaxies (CGGs) of the local universe might come from small galaxy systems that are just now collapsing, and whose dynamic evolution is mainly driven by mergers that selectively destroy intermediate mass galaxies. This scenario could provide a sensible explanation for both the observed bimodal nature of the luminosity function of CGGs and the origin of the large amount of diffuse visible light found recently in the intergalactic medium of some of these systems.

Papers:

Toribio, M.C., Athanassoula, E., Bosma, A., García-Gómez, C., Lambert, J.C., del Olmo, A., Perea, J., and Solanes, J.M. IDILICO: Studying the properties of compact groups of galaxies with a supercomputer. Proceedings of the XLIst Rencontres de Moriond, XXVI Astrophysics Moriond Meeting: 'From dark halos to light', eds. L. Tresse, S. Maurogordato, & J. Tran Thanh Van (Gif sur Yvette: Éditions Frontières), in press (2006)

Solanes, J.M., Athanassoula, E., Bosma, A., García-Gómez, C., Lambert, J.C., del Olmo, A., Perea, J., and Toribio, M.C. Supercomputer Simulations of Compact Groups of Galaxies: the IDILICO project 'Nuevos Retos de la Astrofísica Española', Proceedings of the VII Reunión Científica de la SEA, eds. xxx et al., in preparation (2006)



These two series of 5 images each show the evolution of the dark (top) and luminous (bottom) matter density in a simulation of a compact group of galaxies performed at the MareNostrum machine with 1 million particles initially distributed among 30 galaxies of various sizes and a uniform background.

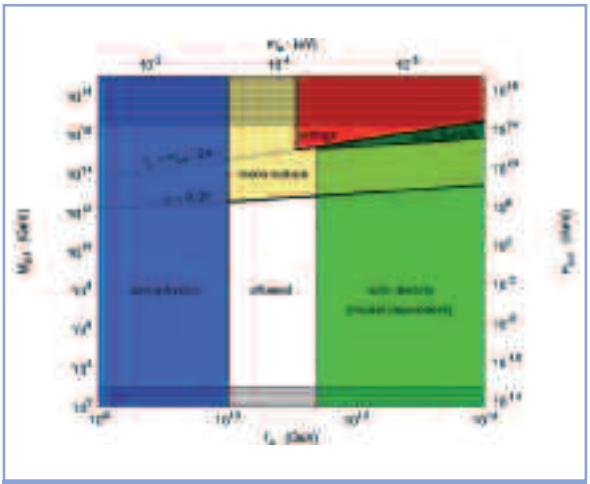
Juan García Bellido - Universidad Autónoma de Madrid

"Cosmological Parameter Estimation from CMB and LSS data"

Recent technical improvements and intensive engineering work have provided cosmologists with access to an important amount of experimental data. The anisotropies in the Cosmic Background Microwave (CMB) and catalogues of galaxies, clusters and superclusters that make up structure on large scales in the universe contain extremely valuable information about the origin and evolution of the universe.
With the development of a code that generates Monte Carlo Markov chains (MCMC) from the likelihood of the given data and the computational power provided by MareNostrum, an estimation of the value of many of the parameters that govern the dynamics of the universe was given. In particular, the project focused on the search for a hypothetical particle, the axion, by constraining the possible signature it may have imprinted on the visible universe under certain very general assumptions, such as the occurrence of inflation. Most of the area in the relevant parameter space is ruled out by the observations.

Papers:

Maria Beltran, Juan Garcia-Bellido (Madrid, Autonoma U.), Julien Lesgourgues (Annecy, LAPTH). "Can isocurvature bounds rule out the axion?" LAPTH-1149-06, Jun 2006. 22pp.



The figure describes the bounds that different observations put on the relic abundance of cosmic axons as cold dark matter.

Pablo Fosalba - Universitat Autònoma de Barcelona

"Large numerical simulations for dark-energy surveys"

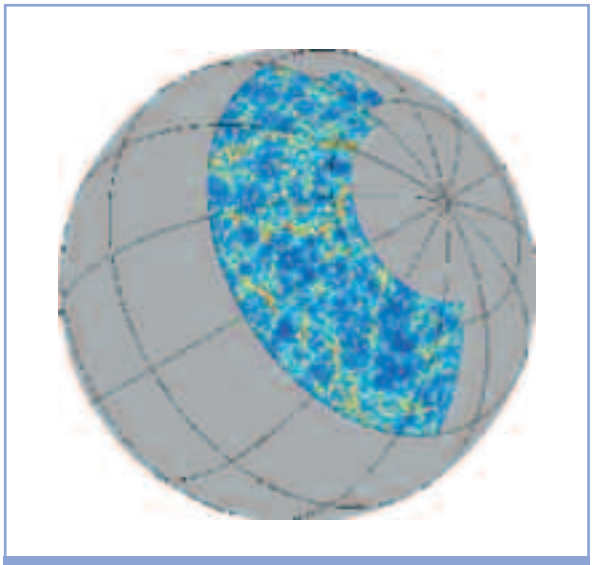
The evolution and ultimate fate of the universe is determined by the so-called dark-energy, which represents about 75% of the total energy-density of the universe today.

IEEC (ICE-CSIC) has undertaken a long-term project to understand the properties of this form of energy through its imprints on the large-scale distribution of matter and radiation in the universe.

In the project, the team is developing the largest N-body simulations to date to build mock galaxy catalogues for the new generation of surveys, such as the Dark-Energy Survey in which our group participates along with other Spanish and international institutions.

The project involves simulating 10,000 million dark-matter particles filling the entire observable universe and following its gravitational evolution immediately after the big bang to present day.

This poses a serious computational challenge.
For this project, the MareNostrum supercomputer used up to 1000 computers in parallel to achieve 1 TeraByte of memory and several Terabytes of disk storage, which is a requirement for developing these cutting-edge numerical simulations.



Projection of the simulated dark-matter distribution onto the Dark-Energy Survey (DES) area. DES will cover 12% of the sky in the south galactic hemisphere and it will observe light emitted by galaxies up to 10,000 million years ago.

Rolando R. Garcia - University Corporation for Atmospheric Research

"Simulation of changes in atmospheric climate and chemical composition 1950-2050"

This project consists of two parts:

(1) Simulation of the period 1950-2003. The comparison of model results and observations, in particular for the period since 1980, which is very well covered by both conventional and satellite observations, is both a test of model performance and a means of interpreting the physical/chemical mechanisms that have led to the changes observed from 1950 to date.

(2) Prognostic simulation up to 2050. This simulation covers the years 1980-2050, with the period 1980-2000 being used as a control against observations, and will be used to assess the future state of the atmosphere as ozone-depleting compounds are reduced (leading to ozone recovery), while greenhouse gases continue to increase (leading to further warming in the troposphere and cooling in the middle atmosphere).

Initial results have been submitted to J. Geophys. Res. and are currently under review (see reference below). The full set of simulations at BSC is expected to be completed some time in late 2006 or early 2007 and will be reported in future journal articles.

Papers:

Garcia, R.R. and co-authors, 2006: Simulation of secular trends in the middle atmosphere, 1950-2003. J. Geophys. Res., submitted.

5.3 Physics and Engineering

Antonio Huerta - Universitat Politècnica de Catalunya

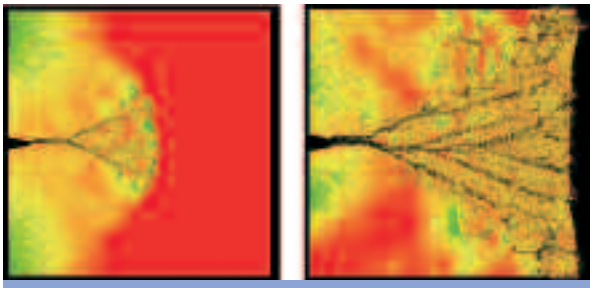
"Large-Scale Simulations of Dynamic Fracture"

Dynamic fracture is ubiquitous in nature, yet its fundamental physics are poorly understood, particularly when it comes to crack branching and fragmentation processes. The goal of the project is to further understand the physics of high-energy dynamic fracture and massive fragmentation through large scale finite element simulations. Supercomputing is required to resolve in a single computation the enormous scale disparity between the processes at the crack tip and the macroscopically relevant sample sizes. In the first set of runs on MareNostrum, a scale disparity of 4 orders of magnitude has been reached. This allows us to extract preliminary, physically meaningful scaling laws that characterize this complex phenomenon.

Papers:

Arias, J. Knap, V. Chalivendra, S. Hong, M. Ortiz and A.J. Rosakis, "Validation of large scale simulations of dynamic fracture", Proceedings of the III European Conference on Computational Mechanics, Lisbon, 2006.

Arias, J. Knap and M. Ortiz, "On the physics of massive crack branching", Proceedings of the Third International Conference on Multiscale Materials Modeling, Freiburg, 2006.



Dynamic fracture process of a 2D brittle plate subjected to an initial strain rate in the vertical direction: dynamic crack propagation, branching and fragmentation.

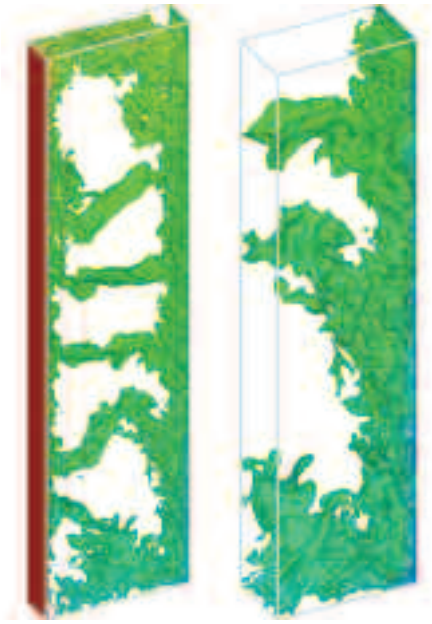
Asensi Oliva - Universitat Politècnica de Catalunya

"Direct Numerical Simulation of Turbulent Flows"

Direct numerical simulation (DNS) is an important area of contemporary fluid dynamics, because it is of interest for improving the understanding of the physics of turbulence and because it is an essential tool for the development of better turbulence models. Recently, relevant improvements to turbulence modelling based on symmetry-preserving regularization models for the convective (non-linear) term have been developed. They basically alter the convective terms to reduce the production of small scales of motion by means of vortex-stretching, precisely preserving all inviscid invariants. They have been successfully tested for relatively high Rayleigh (Ra) numbers [1, 2]. At this stage, high resolution DNS results at higher Ra-numbers are of extreme importance for further progress.
To do so, the team is currently using the new version of the DNS code developed by CTTC on the MareNostrum supercomputer to carry out a simulation of a differentially heated cavity with Ra=10e11, Pr=0.71 (air) and height aspect ratio 4 using a mesh of 111M points. To the best of the authors' knowledge, this will be by far the largest DNS simulation with two wall-normal directions ever performed. Moreover, due to the complex behaviour exhibit, an accurate turbulence modelling of this configuration remains a great challenge. These new DNS results shall give new insights into the physics of turbulence and will provide indispensable data for future progresses on turbulence modelling.

Papers:

F. X. Trias, M. Soria, A. Oliva and R. Verstappen, "Regularization models for the simulation of turbulence in a differentially heated cavity", ECCOMAS CFD'06, Egmond aan Zee (The Netherlands), September 2006.(under revision).



Instantaneous isotherms at Ra=1011. Left: general view of the cavity. Right: zoom around the bottom right corner.

Domingo Giménez Cánovas - Universidad de Murcia
"Parallel routines optimization and applications"

MareNostrum has been used to study two problems with high computational capacities:

The parallelization of algorithms for the solution of Inverse Eigenvalue Problems has been studied. The performance of the system has been characterized by studying the value of parameters that appear in the modelling of algorithms. The model of the execution time has been used to determine optimal conditions.

Algorithms for the solution of Simultaneous Equation Models have been developed. SEM are used in the simulation of economical models, but the algorithms have so far been used only to solve simulated systems.
The use of MareNostrum has enabled the study of larger problems than those previously studied, together with a deeper study of the scalability of the developed algorithms.

Papers:

Georgina Flores Becerra, Algoritmos Secuenciales y Paralelos para la Resolución del Problema Inverso de Valores Singulares, Ph. D. Thesis, Universidad Politécnica de Valencia, May 2006.

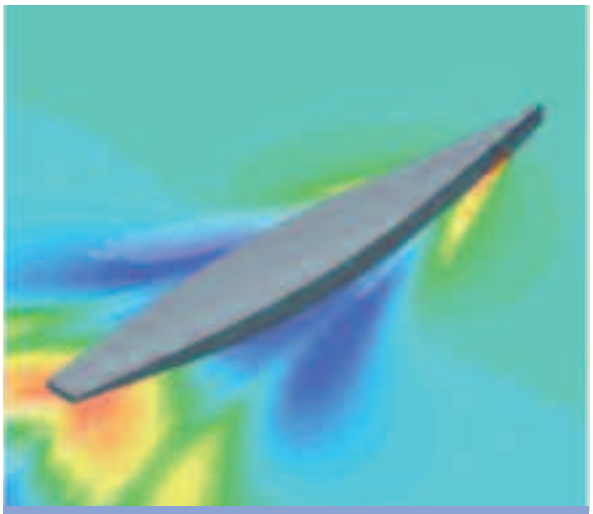
José-Juan López-Espín, Domingo Giménez, Solution of Simultaneous Equations Models in high performance systems, In XXIX Congreso Nacional de Estadística e Investigación Operativa, 15-19 May 2006, Tenerife, Spain.

José-Juan López-Espín, Domingo Giménez, Solution of Simultaneous Equations Models in high performance systems, in PARA06, WORKSHOP ON STATE-OF-THE-ART IN SCIENTIFIC AND PARALLEL COMPUTING, Umeå, Sweden, June 18-21, 2006.

Iñigo Toledo - Desafio Español Copa América
"Desafio Espanol Challenge 2007 - America's Cup Yacht CFD Research"

The objective of Desafio Español 2007 America's Cup Yacht CFD Research project is the development of the fastest America's Cup Class yacht for the 2007 America's Cup challenge. Modern America's Cup class yachts are highly refined sailing yachts that represent the product of millions of dollars of aero and hydrodynamic research by experts in their respective fields. The performance of these yachts is defined by an extremely complex balance of aero and hydrodynamic forces, where the difference in performance between the top performing yachts is less than 10 meters per km, or less than approx 1%. Since these performance differences are so small, extremely accurate and consistent performance predictions are required to identify design features which further improve performance. Traditionally, America's Cup yacht hull-form development has principally relied on a combination of potential flow analysis methods and towing tank experiments. However, the accuracy of these traditional techniques is no longer sufficient to reliably advance hull-form design. Over the past 5-10 years Reynolds Averaged Navier Stokes (RANS) codes have evolved to where they can accurately simulate complex free-surface flows, however these codes require significant computational resources.

The top teams competing for the America's Cup have had the benefit of well-funded, continuous research and development programmes since the end of 2003. The resources available at BSC were of immense benefit to the Desafio Español 2007 effort by providing the team access to state-of-the-art CFD capability. The computational resources at BSC gave the team the opportunity to substantially close the R&D technology gap with the top teams and should allow the Desafio Español 2007 sailing team to compete on an equal or better basis with the fastest America's Cup yachts developed by other competing countries.



Hull form design applying Computational Fluid Dynamics (CFD).

Javier Jimenez Sendín - Universidad Politécnica de Madrid

"DNS in turbulent channels"

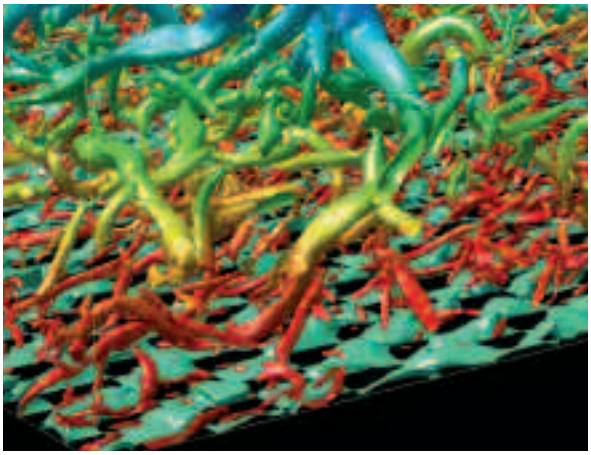
The main aim of this grand challenge application is to contribute to understand the physics of turbulent boundary layers at high Reynolds numbers. Special attention is paid to the multiscale character of the intermediate layer that is present in these flows. This is where the longest flow structures are found, and where the range of scales is widest. The purpose of this experiment is to extend the available simulation to a Reynolds number two times higher than at present. Wall-bounded turbulence has been studied for a long time, but it is only recently, in fact only with this experiment, that we are beginning to be able to represent the logarithmic layer linking the near-wall and outer flow regions. This is the location of the self-similar energy and momentum cascades that are the essence of turbulent flows.

The problem is not just of scientific interest. Wall-bounded turbulence is the interface between the ambient fluid, water or air, and moving vehicles, and between flows and pipes and channels. It is also a key ingredient of the atmospheric boundary layer. Large scales, for example, play an important role in the dispersion of chemical agents in the atmosphere. Due to their associated low frequencies, their pressure fluctuations are responsible for undesirable aerodynamic loads which may result in structural fatigue, and for long-range noise in vehicles. More than half the friction drag in vehicles resides in the near-wall and intermediate layers. The hopes of controlling and alleviating all these phenomena pass through the understanding of their dynamics.

Papers:

Sergio Hoyas and Javier Jiménez, School of Aeronautics, Universidad Politécnica de Madrid, 28040 Madrid, Spain. Scaling of the velocity fluctuations in turbulent channels up to Re_ = 2003, Received 25 October 2005, accepted 1 December 2005, published online 11 January 2006. 2006 American Institute of Physics. DOI: 10.1063/1.2162185.

Hoyas et al (2006) "Reynolds number effects in the Reynolds stress statistics and balances", J. of Fluid Mech, in preparation.



Josep Maria Porta - Universitat Politècnica de Catalunya

"Isolating configuration spaces of polycyclic robots and molecules by extended bound smoothing"

The project developed algorithms able to provide complete characterizations of the conformational spaces of molecules. The conformational space of a molecule determines the possible movements of the said molecule. Therefore, this information is basic for finding out the possible interactions between different biological structures (protein-ligand docking, drug-design, virus-cell assembly).

The algorithm will be used for geometric virtual screening. This application is computer intensive and requires significant software development: new algorithms that perform better high-dimensional conformational spaces.
Thanks to the supercomputing capabilities of MareNostrum, it is possible to obtain completed characterization of conformational spaces of complex molecules in reasonable times.

The conformational space of cycloctane. Red areas correspond to conformations with higher energy.

Markus Uhlmann - CIEMAT

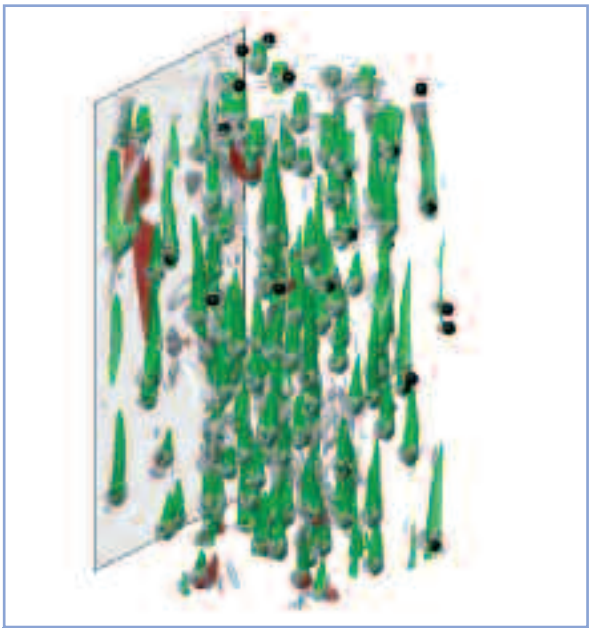
"Direct Numerical Simulation of Turbulent Flow with Suspended Solid Particles"

The team has simulated low-Reynolds-number turbulent flow in a vertical plane channel containing a dilute suspension of heavy spherical particles (0.5% solid volume fraction) that are fully resolved. The conditions are adjusted so that the particles are on average at rest, having a diameter equivalent to 10 times the smallest flow scales near the wall. The runs on MareNostrum so far have revealed the formation of very large-scale flow structures in the form of streamers, which are absent in the single-phase flow. Further simulations and theoretical analysis will be necessary in order to discover their origin and characteristics.

Papers:

M. Uhlmann. An immersed boundary method with direct forcing for the simulation of particulate flows. J. Comput. Phys., Vol. 209, Number 2, pp. 448-476, 2005

M. Uhlmann. DNS of finite-size heavy particles in vertical turbulent channel flow. Bulletin Am. Phys. Soc., Vol. 50, Number 9, p. 133, 2005.



Visualization of the flow field near a wall-plane in vertical turbulent channel flow with heavy particles (0.5% solid volume fraction; particle Reynolds number 135). The green isosurfaces correspond to particle wakes, the red ones to high-speed coherent structures; the grey surfaces indicate regions of high vorticity.

Monty Newborn - McGill University, Montreal

"Parallel Automated Theorem Proving"

Programming and experiments were carried out on the parallel automated theorem-proving program called Octopus. Octopus carries out resolution-refutation proofs on theorems presented to it in first-order predicate calculus. It can run on as many processors as available. On MareNostrum, several tests were carried out using as many as 256 processors.

Octopus has been in existence for almost a decade and has participated in several of the annual conferences on Automated Deduction's ATP System Competition; it will do so again this August. Each of the processors carries out an independent effort to find the proof of a theorem by trying to prove a simpler, or weaker, version of the given theorem. The more processors, the more weakened versions. Some theorems have thousands of weakened versions. The efforts on MareNostrum were aimed to improve Octopus's criteria for selecting weakened versions. The results of this effort will be put to the test soon as discussed above. During the competition, Octopus will run on a network of over 100 processors located in the School of Computer Science at McGill University.

Pilar Hernández - Universidad de Valencia

"Non-perturbative aspects of QCD in flavour physics"

The aim of the project is to compute the amplitudes for non-leptonic kaon decays from first principles in the well-established theory of Quantum Chromodynamics. The prediction of these quantities is a very important contribution to the field of flavour physics, which tries to reveal the origin of the fundamental parameters of the Standard Model. An unresolved problem in this field is the striking hierarchy between the two isospin amplitudes, the so-called Delta I=1/2 rule, whose origin after many years of research remains unknown. In the time allocated to the project during 2005, the team computed these amplitudes in a particularly interesting limit of a light charm quark. The fact that the charm quark is so heavy with respect to the up, down and strange quarks has been proposed as a possible source of the hierarchy. Results show that a significant hierarchy remains in the case where the charm is light, challenging the old law.

Papers:

L. Giusti, P. Hernandez, M. Laine, C. Pena, J. Wennekers and H. "On the K->pipi amplitudes with a light charm quark" Wittig arXiv: hep-ph/0607220. Recently published in a preprint that has been sent for publication to Physical Review Letters.

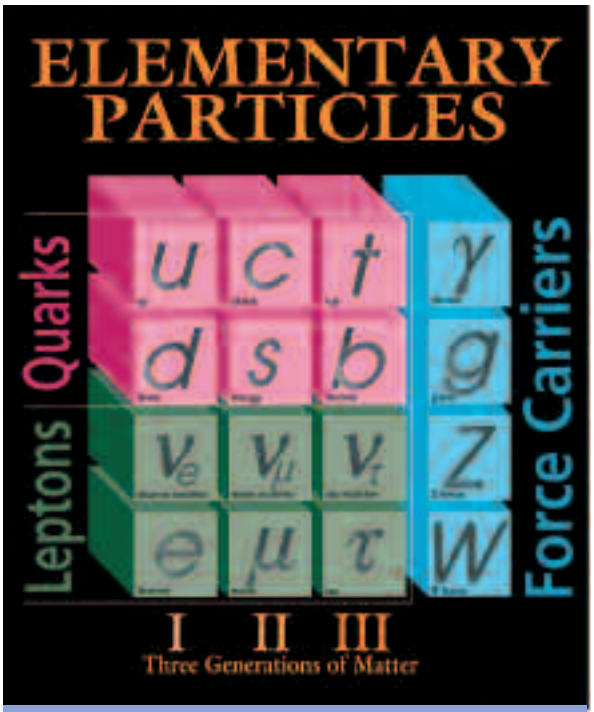


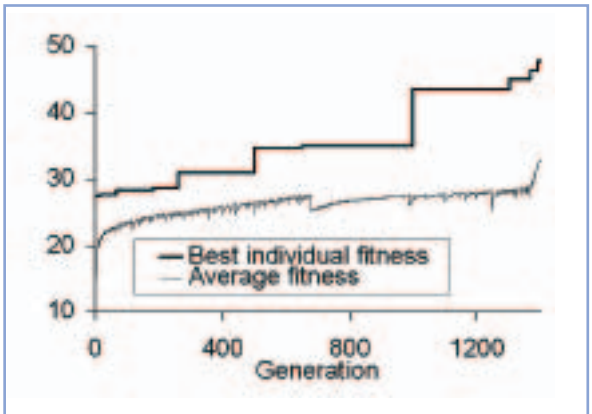
Table of elementary particles of the Standard Model. The particles are classified in three families or generations identical except for the flavour sector.

Richard J. Duro - Universidade da Coruña

"Automatic design of wind turbine blades"

In this work we have developed an automatic design environment in order to obtain the optimal wind turbine blade profiles for a given geographic location. This automatic design environment has two main parts: a search module that is based on Macroevolutionary Algorithms (MAs), and an evaluator module that is based on an aerodynamic simulator. The aerodynamic simulator obtains the forces and moments generated by the wind turbine blade and then calculates the resulting power generated by the turbine. The simulator is also divided into two parts; the first one, a potential solver corrected by neural networks, computes the performance of two-dimensional airfoils and the second one applies blade element theory in order to obtain the resulting forces and moments exerted on the blade.

The MAs used in the largest experiment considered a population of 40960 individuals distributed into 32 races. Each individual chromosome consisted of 115 genes representing different parameters of the blade configuration. The time necessary to evaluate each individual oscillated between 5 and 20 seconds. MAs were selected due to their good balance between exploitation and exploration, but they showed a slow selection phase when using populations with many individuals and this forced us to make changes in the algorithm in order to adapt it to such large populations.



Population average fitness and best individual fitness value during an evolution process.

Vincent Gimenez Gómez - Universidad de Valencia

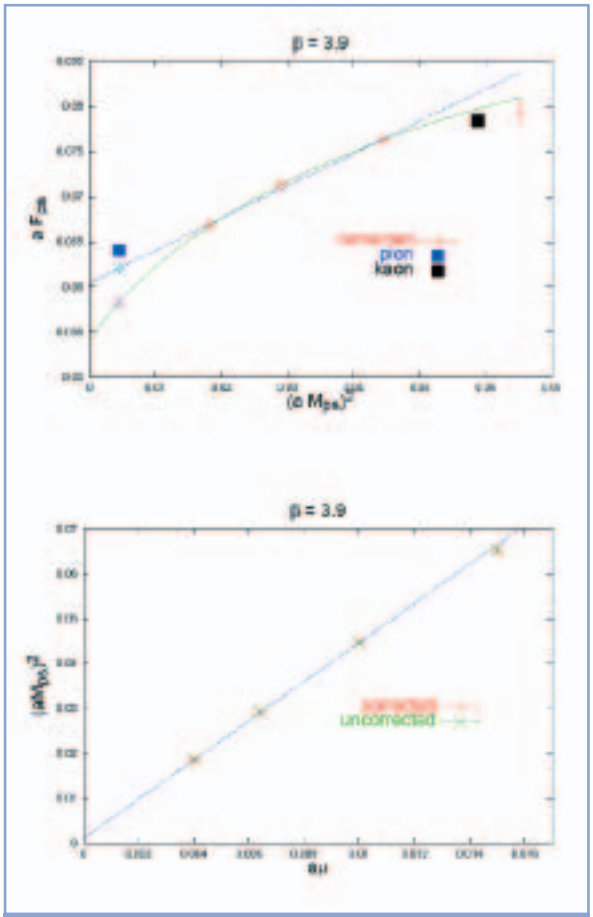
"Monte Carlo numerical computations of the properties of hadrons"

Quantum Chromodynamics (QCD) is presently the best model of the strong interaction of particle physics. However, it is not clear that it describes all its aspects. In particular, non-perturbative phenomena such as the confinement of quarks, the symmetry-breaking of chiral massless quarks and the old puzzle of K- meson decays are still unresolved problems.

To address such questions, it is necessary to resort to non-perturbative methods. Large scale numerical simulations in a discretized version of QCD, i.e. lattice QCD (LQCD), is the most powerful tool available today to perform such a study. The aim of our project is to perform the first realistic simulations of LQCD. This means using dynamical fermions taking the strange quark mass into account and running at light quark masses, as close as possible to the physical pion mass, in a sufficiently large lattice box, at least 2 fm. This demanding setup can be realized by using a new formulation of LQCD, the so-called maximally twisted mass fermions. With the MareNostrum supercomputer, as many as 1500 gluon configurations have been generated on large lattices, with which the team have calculated the hadron spectrum and meson decay constants, and shown that the method used allows for simulations that rival those with staggered fermions, which were unthinkable only a few years ago. The project's main result is that once the system is tuned to full twist, simulations become possible at pion masses as small as 270 MeV. The team have also tested the approach adding the strange and charm quarks to the lightest up and down doublet and such simulations have been found to be perfectly feasible. This MareNostrum project is a member of a larger international collaboration, the European Twisted Mass Collaboration (ETMC).

Papers:

B. Blossier, Ph. Boucaud, P. Dimopoulos, F. Farchioni, R. Frezzotti, V. Giménez, G. Herdoiza, K. Jansen, V. Lubicz, G. Martinelli, C. McNeile, C. Michael, I. Montvay, M. Papinutto, O. P`ene, J. Pickavance, G.C. Rossi, L. Scorzato, A. Shindler, S. Simula, C. Urbach, A. Vladikas, U. Wenger, Summary of Twisted Mass Results from the ETMC collaboration, XXIV International Symposium Lattice 2006 held at Tucson, Arizona, USA from 23 to 28 July 2006.



The chiral extrapolation of the pseudoscalar decay constant as a function of the pseudoscalar mass with finite size (FS) corrections.

The pseudoscalar mass as a function of the twisted mass without and with finite size (FS) corrections.

5.4 Chemistry and Material Science

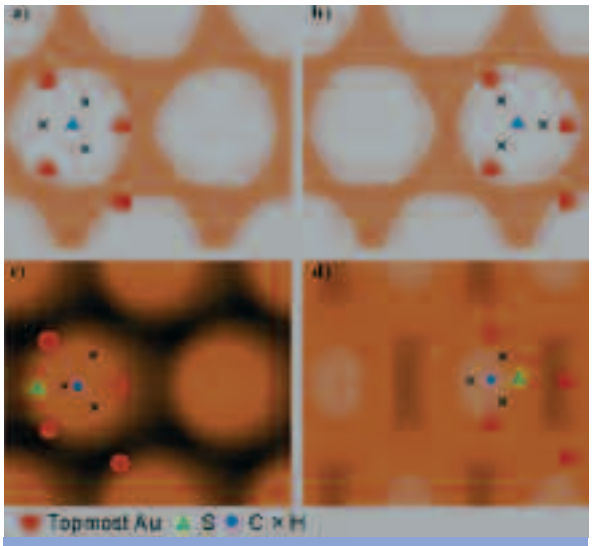
Andrés Arnau - Universidad Politécnica de Valencia

"Adsorption of alkanethiols on Au(111) at different coverages up to one monolayer"

In this project, several aspects of the interaction between short chain alkanethiols on Au(111) were studied. A detailed characterization of the S-Au bond was made using ab initio methods, as well as the vibrational modes and simulation of STM topographical images. The tool used is a plane wave based DFT code (VASP) that allows us to characterize the structure of the adsorbate-metal system and the electron charge density at the surface. The first paper addresses the high coverage (1 ML) structure and in the second we also consider the low coverage (0.25 ML) structure that requires four times larger unit cells. Results show that no dimerization of thiols is taking place on Au(111) in agreement with recent results published in Physical Review Letters 97 (2006) 045505.

Papers:

Nora Gonzalez a, Nicolas Lorente b,1, Andres Arnau a,b,c,*, Methylthiolate adsorption on Au(111): Energetics, vibrational modes and STM imaging. Surface Science (2006)



Simulated STM images for fcc-vertical staggered orientation (a), fcc-vertical eclipsed (b), bridge-fcc (c) and fcc-hollow tilted (d). The local density of states (LDOS) has been integrated up to 1eV, and the contours have been plotted for the integrated LDOS value of 1 x 10-5 e-/Å3. The corrugation is ~0.6 Å for fcc vertical phases, ~0.8 Å for the tilted fcc and ~1.3 Å for the bridge-fcc phase.

Ángel Rubio - Euskal Herriko Unibertsotatea

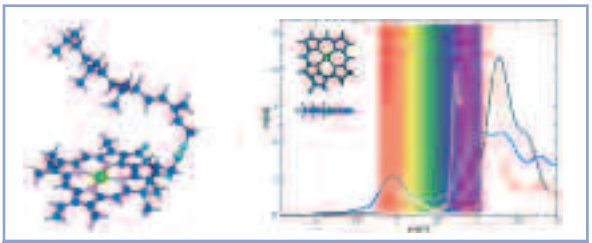
"Spectroscopic properties of biomolecules, nanostructures and extended systems"

The project combines quantum mechanical simulations in order to understand the properties of nanoscale advance materials and to control them to design new devices: molecular transistors, opto-electronic devices, electromechanical actuators, chemical sensors, organic photovoltaics, biological sensors and markers. The main systems under study are inorganic nanotubes and nanowires together with biochromophores and nano-magenetic particles. All the studies address the interaction of nanoscale objects with light (i.e. description of photosynthesis or fluorescent chromophores and their integration with macroscopid devices).

Papers:

K. Ishioka, M. Hase, M. Kitajima, L. Wirtz, A. Rubio and H. Petek Femtosecond Coherent Quasiparticle Correlations of a Nonequilibrium Plasma in Graphite. Submitted (2006)

K. S. Thygesen and A. Rubio, Non-equilibrium GW Approximation for Electron Transport in Nanoscale Contacts, submitted for publication.



Performance of the numerical modelling tools

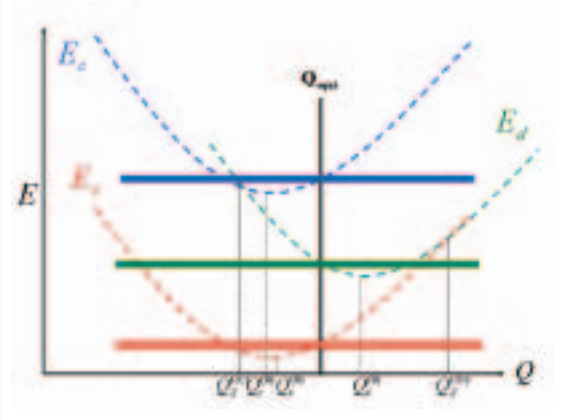
Antonio Luque López - Universidad Politécnica de Madrid

"Study of the nonradiative recombination"

One mechanisms of nonradiative recombination is related to a sufficiently large lattice vibration. In a complete nonradiative cycle the levels move across the entire energy gap. First-principles calculations allow us to explicitly calculate the dependence of the bands on the positions of the atoms without making any additional approximations. This has been the main objective of the work carried out in MareNostrum. Nevertheless, initially it has been necessary to choose and to characterize a material with a deep level that gives place to an intermediate band when increasing the impurity concentration. The results of this work are actually in publication phase.

Papers:

C. Tablero, Phys. Rev. B 74 (accepted for publication).



Configuration coordinate diagram for non-radiative recombination

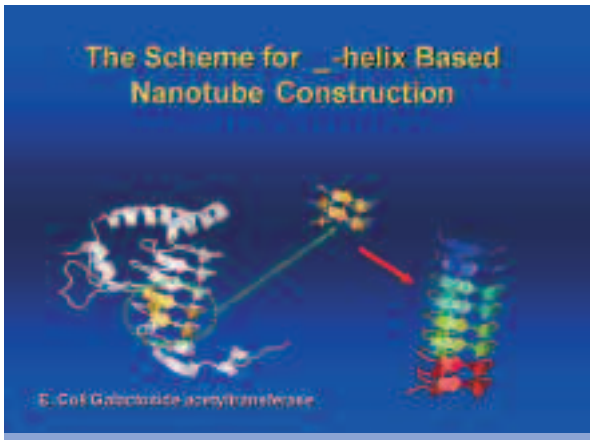
Carlos Alemán - Universitat Politècnica de Catalunya

"Nanotechnology: De Novo Design using the Self-Assembly of Biomolecules"

Molecular dynamics simulations have been used to construct nanofibers based on motifs taken from left-handed beta-helical protein motifs . Thus, the goal was to design nanosystems that show structural stability and can be used as templates for the experimental construction of novel systems. Results showed that a system constructed of four self-assembled replicas of residues 131-165 of galactoside acetyltransferase exhibit remarkable stability under the simulated conditions.

Papers:

N. Haspel, D. Zanuy, C. Alemán, H. Wolfsom, R. Nussinov "De Novo Tubular Nanostructure Design based on the Self-Assembly of beta-Helical Protein Motifs", Structure 2006, 114, 1137-1148.



Nanotube constructed by self-assebling four copies of the left-handed _-helix building block motif of E. coli galactoside acetyltransferase.

Carlos Alemán - Universitat Politècnica de Catalunya

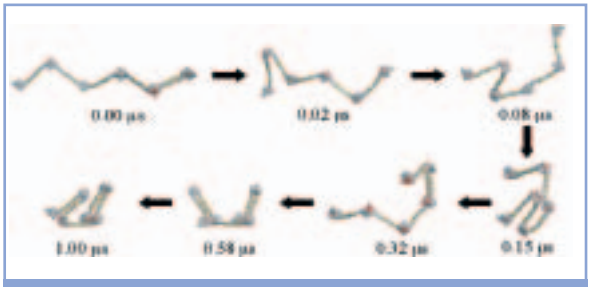
"Dynamics of an Artificial Muscle based on Conducting Polymers and Calix[4]arene Scaffolds"

The electromechanical actuation of an artificial muscle based on redox-active polymers and flexible calix[4]arene scaffolds has been investigated using molecular dynamics (MD) simulations. Initially, short MD simulations were performed to describe each electronic state involved in the actuation mechanism in terms of flexibility/rigidity, as well as to characterize the initial (accordion-like) and final (fully-contracted) conformational states. After this, the accordion-like-to-fully-contracted transition was fully characterized through a 1 ms MD simulation. The results made it possible to describe the dynamics of the molecular actuator from a microscopic point of view and also to identify secondary conformational transitions that may reduce the efficacy of the artificial muscle.

Papers:

D. Zanuy, J. Casanovas, C. Alemán. "Conformational Features of an Actuator Containing Calix[4]arene and Thiophene: A Molecular Dynamics Study". J. Phys. Chem. B 2006, 110, 9876.

D. Zanuy, C. Alemán. "Phenomenological Description of the Contraction Process of an Electroactive Actuator Based on a One Microsecond Atomistic Molecular Dynamics Simulation". Submitted 2006.



Atomistic representation of selected snapshots to illustrate the contraction of the actuator through the 1_s MD simulation.

Eduardo Hernández - Institut de Ciència de Materials de Barcelona

"Phase diagrams of complex materials from first principles simulations"

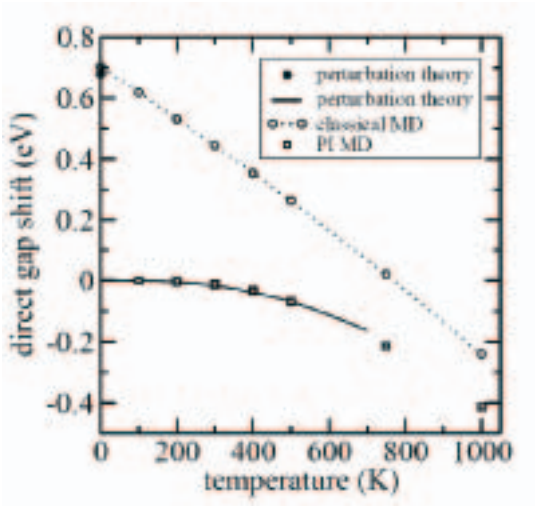
The project performed intensive simulations along two different research lines, namely: path-integral molecular dynamics studies of pure and hydrogen-doped diamond; and ab initio studies of the thermal behaviour of sodium and lithium. The path-integral simulation technique allows for a correct quantum treatment of the atomic degrees of freedom, which are normally treated approximately by means of classical mechanics. This is particularly important in the case of light atoms such as carbon and hydrogen, where quantum effects are most appreciable. The thermal behaviour of simple metals Li and Na is currently a topic of great interest in the condensed matter physics community, and the project's results will be timely and attract much attention.

Papers:

Rafael Ramirez, Carlos P. Herrero and Eduardo R. Hernandez, Path-integral molecular dynamics simulations of diamond. Physical Review B, vol. 73, 2452202 (2006).

Carlos P. Herrero, Rafael Ramirez and Eduardo R. Hernandez, Hydrogen and muonium in diamond: a path-integral molecular dynamics simulation. Physical Review B, vol. 73, 245211 (2006).

Eduardo R. Hernandez and Jorge Iniguez On the nature of the melting line of Sodium. Submitted.

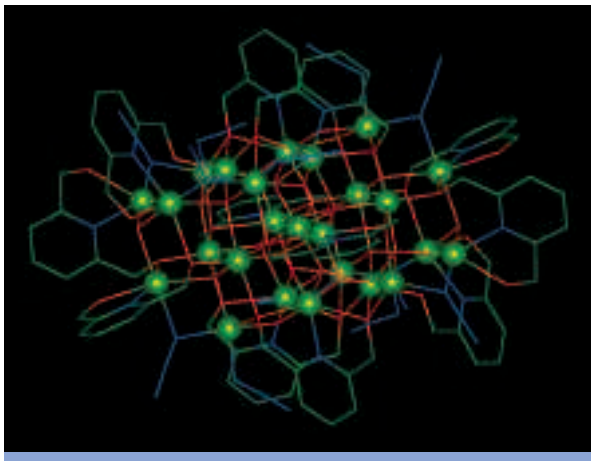


Behaviour of the direct forbidden electronic gap in diamond as a function of temperature.

Eliseo Ruiz - Universitat de Barcelona

"Magnetic Properties of large Single Molecule Magnets: Mn25 and Mn32"

Some isolated molecules behave like a magnet (single-molecule magnets) and are excellent candidates to storage the information at nanoscopic level. In order to have such properties, we need a high-energy barrier that fixes the magnetic moment (spin) of the molecule to avoid the change of the spin direction that would cause a loss of the stored information. Due to the complexity of the magnetic interactions present in such systems up to now, improving their properties was basically a serendipitous process. However, the use of theoretical methods based on density functional theory allows a detailed knowledge of the microscopic magnetic interactions. Such information allows a rational design and synthesis of new molecules, such as Mn25 and Mn32 complexes, with very high energy barriers.



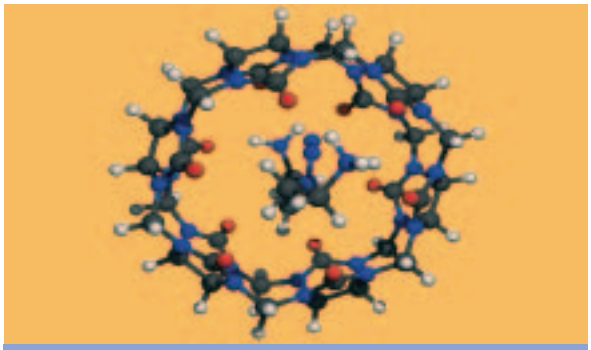
One molecule of the Mn25 complex behaves like a nanomagnet.

Feliu Maseras Cuni - Institut Català d'Investigació Química

"A DFT computational approach to supramolecular catalysis"

The pumpkin-shaped macrocycle cucurbit[6]uril or CB6 ($C_{36}H_{36}N_{24}O_{12}$) was first synthesized in 1905 but its chemical nature and structure was not revealed until 1981. Although less famous than its structurally similar cousins cyclodextrin and calixarene, it has still found a wide range of applications, such as molecular recognition and catalysis. The synthesis of several new CBn homologues has sparked renewed interest and research into cucurbiturils since the beginning of the new millennium. The project has focused on the catalytic ability of CB6. It has been found to be able to catalyze a cycloaddition reaction, turning a slow and unselective reaction into one that is fast and regiospecific. The reason of interest in this reaction is twofold. The existence of experimental and, most importantly, kinetic data for the reaction is a way of evaluating the computational methods available. This will enable us to learn what to use in future projects which might not include as much experimental detail, i.e. using computations as more of a predictive tool. Secondly, our computations will gain insight to the catalytic function of CB6 on a molecular level, to answer questions that are beyond today's experimental tools.

In choosing the project's computational method, the team found the use of DFT (density functional theory) to be the best choice for studying the cycloaddition reaction catalyzed by CB6. Cheaper methods, such as hybrid methods (e.g. ONIOM) were not accurate enough. The stationary points were fully optimized and further characterized by frequency calculations, a tremendous task, considering the size of the system (up to 1400 basis functions) that required nearly 60.000 cpu hours. The enzyme-like reaction mechanism of the cucurbituril was elucidated together with energy data for the actual cycloaddition step not accessible through experiments. The calculations showed that the rate-limiting step is the release of product from CB6 (in accordance with experiments), the cylcoaddition step was found to have an activation energy of 20 kcal/mol, a rate-enhancement of 5.5¥104. Since the results obtained are agree with experiments, the team believe the project's computational approach to be good. In the future, it could therefore be used in a more predictive manner. For example in the rational design of new supramolecular catalysts.

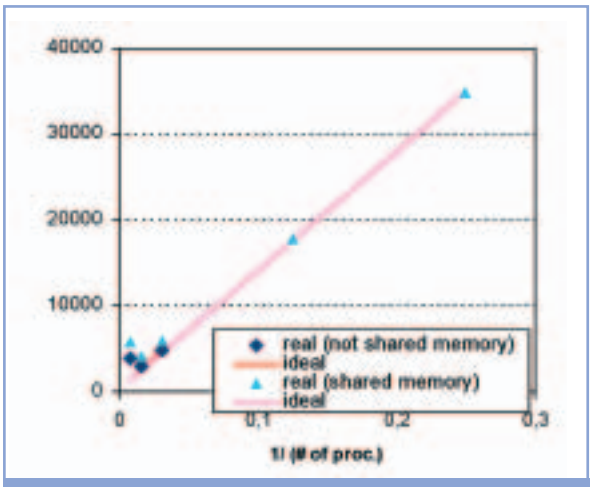


DFT calculations allow the characterization of the process where two small organic molecules undergo a Diels-Alder reaction inside a cucurbituril supramolecule.

Francesc Illas - Universitat de Barcelona

"Scalability of the VASP code and applications to heterogeneous catalysis"

Periodic density functional calculations have been carried out in order to study the performance of VASP code on the MareNostrum computer. Several systems have been chosen to carry out the scalability tests ranging from small to large systems containing up to 580 atoms and considering different types of usual calculations in heterogeneous catalysis applications: geometrical optimization, molecular dynamics simulations, nudged elastic band method and vibrational frequency determination. Results show that the scalability of VASP code depends largely on the size of the system. For production jobs, a scalability up to 64 processors is substantially acceptable. Good performance may still be attained for systems with a very large unit cell.



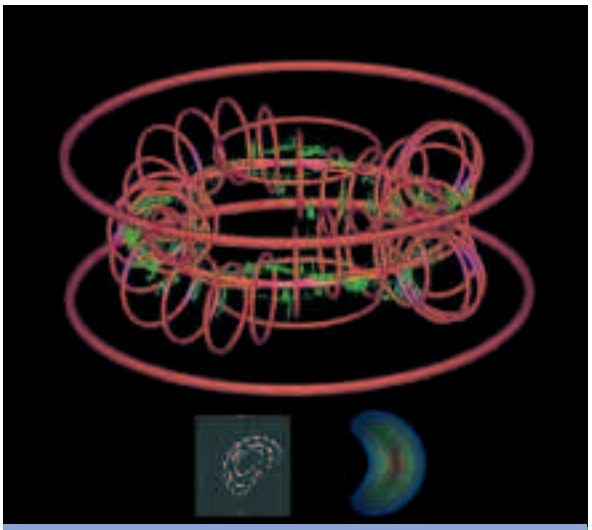
VASP CPU time versus the reciprocal number of processors for a system containing 256 atoms (geometry optimization, E_{cutoff}=415 eV, G-point mesh).

Isabel Campos - Universidad de Zaragoza

"Computational studies on Kinetics transport in stellerator TJ-II"

This research project studies the physics of magnetically confined plasmas from a theoretical point of view using computational methods, complemented by access to the experimental data of TJ-II from the national fusion laboratory of the CIEMAT (LNF). MN is needed to approach the problem numerically.

In collaboration with the LNF, the project analyzes the physics of transport in magnetically confined plasmas. This area of work has been a constant in all the research groups in the world dedicated to research on fusion magnetic plasmas. Transport is a key phenomenon in plasmas because it permits particle and energy leakage from the device, adds problems to the fusion reaction and forces the construction of bigger devices. Plasma-like systems can be analyzed from the point of view of a complex system, that is, its properties depend crucially on the details of the interaction. It is also expected to find chaotic phenomena and self-organization. Due to the geometry of the magnetic fields, in a first approach, the transport problem can be considered one-dimensional. However there are problems that are exclusively three-dimensional, which have been observed in the stellerator TJ-II and other devices. This invalidates a purely one-dimensional study. This is the case of particle injection and derive. An important part of the project consists of the study of transport in 3D by Monte Carlo simulations. Interactions between particles and interactions with the turbulent electromagnetic fields generated by the plasma or by the microwaves introduced to heat the plasma are included. Accordingly, it is possible to elaborate microscopic descriptions of the interaction between the electromagnetic turbulent fields and the wave-particle stochastic interaction. Some of these descriptions exist already; others have yet to be modelled.



Distribution of collisions of the plasma particles inside the TJ-II Stellerator Fusion Reactor (green dots).

From the application point of view and in the light of the ITER project, the project results and methodology have a deep impact on the design and construction of future fusion devices, specifically the stellerator Wendelstein VII-X, currently under construction in Germany, and which will start operation in 2010. Also, such a computing tool is a natural testbed for all three-dimensional computing codes in the fusion community, either computation of turbulent flux or any other magnitude requiring a 3D treatment.

The project was performed using two applications: plasma evolution and Eirene, which scale up to 200 nodes.

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F. Castejon et al., Ion orbits and ion confinement studies on ECRH plasmas in TJ-II Stellerator. Nuclear Fusion (to appear 2006).

I. Campos, L.A. Fernandez, V. Martin, D. Sciretti, A. Tarancon and J.L. Velasco, Numerical study of the enlarged O(5) symmetry of the 3-D antiferromagneti c RP2 spin model. Physics Letters B628 2005 (281-290).

I. Campos, M. Cotallo, V. Martin, S. Perez and A. Tarancon, Kosterlitz-Thouless scaling of the 3-D Heisenberg spin glass. cond-mat/0605327.

Jordi Faraudo - Universitat Autònoma de Barcelona

"Molecular Dynamics Simulations of Electrostatic Interactions between Macromolecules and/or Macroions in Aqueous Solution"

Electrostatic interactions are essential in determining the behaviour and functionality of large molecules or nanoparticles in solution. Applications of interest include nanofunctionalized materials, bio-inspired materials and the design of certain pharmaceutical drugs to mention only a few examples.

In the project, the team study how explicit effects due to the molecular details of the solvent dramatically modify electrostatic interactions at short distances between the interacting molecules or nanoparticles, originating the so-called hydration forces. Simulations of films and monolayers of SDS surfactant adsorbed in water and gold nanoparticles covered by surfactant at water/air interface were performed. In both cases, the molecular detail is accessible only with the fastest supercomputers such as MareNostrum.

Now, the results obtained for large and very large systems in this project on MareNostrum allow the team to demonstrate that the specific behaviour of electrostatic interactions due to the modification of the solvent structure near amphiphilic interfaces is even more important than expected and extends far from the interface.

These new effects observed in the simulations are expected to appear at the nanoscale in many chemical systems in aqueous environments. This is particularly important in the design of chemicals and materials tailored on a nanoscale acting in aqueous environments (such as biomedical and chemical applications).

Papers:

J. Faraudo and F. Bresme "Origin of the Short-Range, Strong Repulsive Force between Ionic Surfactant Layers", Phys. Rev. Lett. 94, 077802 (2005), ibid 92, 236102 (2004).

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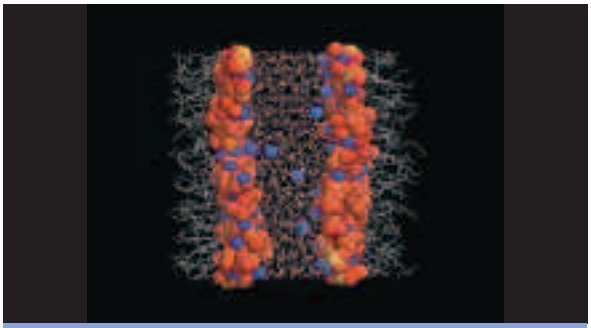


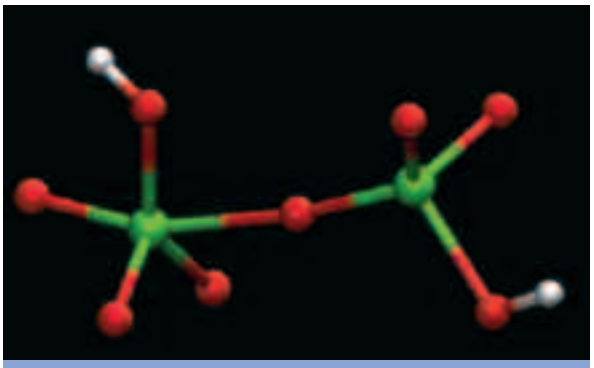
Snapshot of interaction between two surfactant layers: Two layers of SDS surfactants separated by a thin film of water. Red and yellow spheres correspond to the SDS headgroups, brown lines are the SDS tails and blue spheres are sodium ions. The water molecules are shown as red and white dots.

Josep Maria Poblet - Universitat Rovira I Virgili

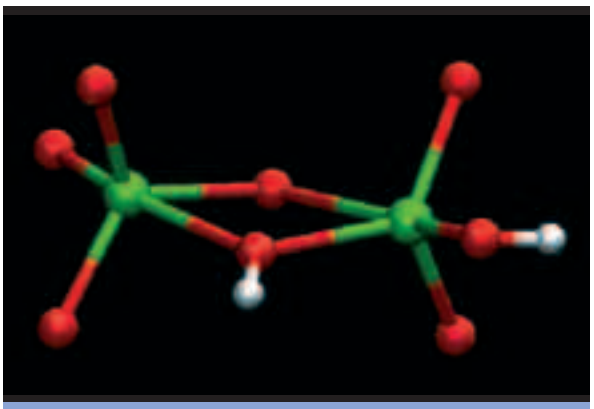
"First-principles molecular dynamics simulations of the formation mechanisms of polyoxometalates with low nuclearities"

The aim of the project is to elucidate the mechanism of formation of the polyoxometalates (POMs) with low nuclearities from the tetrahedral WO3(OH)- building blocks. The project employs first-principles molecular dynamics techniques (Car-Parrinello molecular dynamics, CPMD) including explicitly the solvent molecules, water in this case. Therefore it is possible to model processes involving formation and breaking of bonds (i.e. chemical reactions). In particular, the project uses the metadynamics method, which allows for an acceleration of the dynamics thus making possible the observation of activated processes in reasonable simulation times.

In the simulations was observed that the dinuclear structures that show the lowest barriers of formation are not the ones postulated for the first step of the aggregation process. The dinuclear species in which the tungsten atoms are four- and five-coordinated were found, formed by one tetrahedron and one square pyramid that share a vertex (4-5 structure) and species in which both W atoms are five-coordinated, formed by two square pyramids that share an edge (5-5 structure).



4-5 structure



5-5 structure

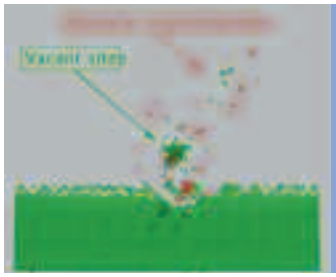
Maria José Caturla Terol - Universidad de Alicante

"Atomistic simulations of materials with nano-features and the behaviour of materials under irradiation and extreme conditions of pressure and temperature"

Understanding the relationship between microscopic features and macroscopic behaviour is crucial to developing new materials with specific properties. In particular, the atomic scale defects produced under irradiation can significantly modify the mechanical, electrical and optical properties of materials. Using molecular dynamics simulations with millions of atoms, the team have studied the formation of defects in Ni, Cu and Fe during irradiation at energies from 20 to 100 keV. In Cu and Ni, vacancies are produced by the irradiation agglomerate in clusters that collapse in stacking fault tetrahedra, as observed experimentally, while in Fe, vacancies remain mostly isolated. The higher energies show the interaction between sub-cascades. The effects of irradiation close to microstructural defects such as nanocracks have also been studied. In particular a nanocrack is partly healed by the defects produced in the irradiation. These results have been presented at the EMRS'06 meeting and will be published shortly.

Papers:

Z. Yao, M. J. Caturla, R. Schäublin, Study of cascade damage in Ni with MD by different interatomic potentials, accepted for publication in J. of Nuclear Materials.



Defects produced by a 20keV cascade in Cu close to a nanocrack. Green represents vacant sites in the lattice and red represents atoms located at interstitial sites.

Evolution of a 20keV Cu cascade in Cu close to a nanocrack at (a) 1.4 ps (b) 2.3ps (the shock wave produced by the collisions can be observed) and (c) at 20ps. The morphology of the crack-tip has changed close to the cascade, probably being healed by the arrival of self-interstitials.

Pedro de Andrés - CSIC

"Molecular adsorption on metallic and oxide surfaces"

Density Functional Theory was used to study surfaces with or without adsorbed chemical species. These systems are relevant as catalytic models, but they can be important in other fields too, like electronic devices, corrosion, etc. As a way of example, the surface TiO2(110)-(1x2) from a structural and electronic point of view [1] was characterized (fig. 1,2). The results include finding a potentially active site for catalysis, and the existence of quasi-1D metallic chains. On the methodological side, the project has taken advantage of MareNostrum parallel power to devise a structural multidimensional minimization algorithm where different parameters are simultaneously optimized [2]. This new algorithm shows a Poisson-like distribution (fig. 3), i.e. it performs a most efficient search unlike previous ones showing Gaussian-like distributions. The project has also studied the conductivity of a single H2 molecule pinched between two Pt tips [3] (fig. 4), and the adsorption of large PTCDA molecules on Ag(110) [4].

Papers:

M. Blanco-Rey, J. Abad, C. Rogero et al; Structure of Rutile TiO2 (110)-(1x2): Formation of Ti2O3 Quasi-1D Metallic Chains; Phys. Rev. Lett. 96, 055502 (2006).

M. Blanco-Rey, P. de Andres; Surface Diffraction Structure Determination from Combinatorial Simultaneous Optimization; Surf. Sci. Lett. 600, L91 (2006).

J.A. Verges, P. de Andres; Electron Transport Through Simple Molecules From Band Structure Formalism; 3rd Nano Spain Workshop (Pamplona, March 2006).

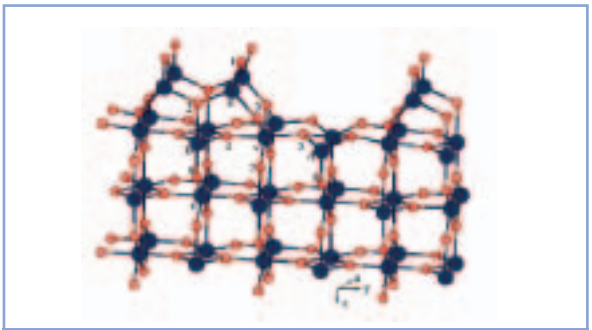


FIG. 1 (color online). Model for 1 x 2 TiO2 (110) (best fit to LEED, RP = 0.28). Large anda small spheres represent Ti(a-e) and O(1-8) atoms, respectively. The lowest layer has been frozen to optimized bulklike positions.

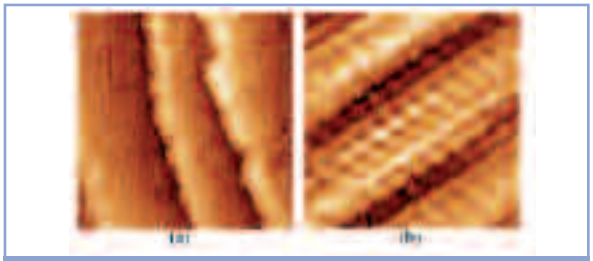
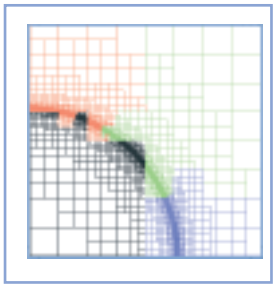


FIG. 2 (color online). Constant current STM images of 1 x 2 TiO2 (110), V = +1.5 V. (a) Monatomic steps and large terraces on a 500 x 500 A2 area (I = o.146 nA). (b) A high-resolution image on a 30 x 30 A2 area (I = 0.178 nA).

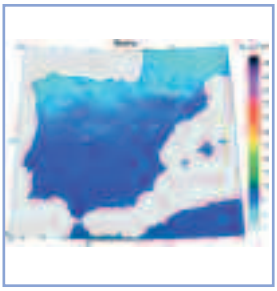
5.5 Success Stories

The following success stories are from 2005:
"The MareNostrum parallel supercomputer has proved to be an invaluable piece of equipment to carry out the largest simulation performed so far. The large number of processors available and the high-speed interconnection among them enables the simulation of cosmological volumes filled with billions of particles representing both the baryons (gas) and the collisionless dark matter." The MareNostrum Universe, Gustavo Yepes, Univ. Autónoma de Madrid.

"Using up to 2100 processors on MareNostrum, we have run the code for more than 5M hours, obtaining approximately 25TB of data." Channel 2000, Javier Jiménez Sendín, Univ. Politécnica de Madrid.

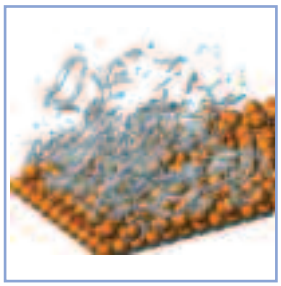


"MareNostrum provides the first opportunity to perform a 20-billion cell simulation of galaxy formation, allowing for the first time to resolve the formation of dwarf galaxies within a large enough field of view, necessary in order to decrease the cosmic variance." The Horizon Project, CEA.



"Thanks to the increasing supercomputer capabilities of MareNostrum, it is feasible to make a high-resolution global dust modelling, which is essential to describe important features of the dust processes, such as cloud-aerosol interaction and dust emissions." Dream, Earth Sciences team BSC-CNS.

"Thanks to increasing supercomputing capabilities such as MareNostrum, it is feasible to make an extensive use of molecular dynamics simulations to derive properties of protein structures that are not accessible through the analysis of a single structure as contained in the PDB.", MoDEL, Life Sciences team BSC-CNS.



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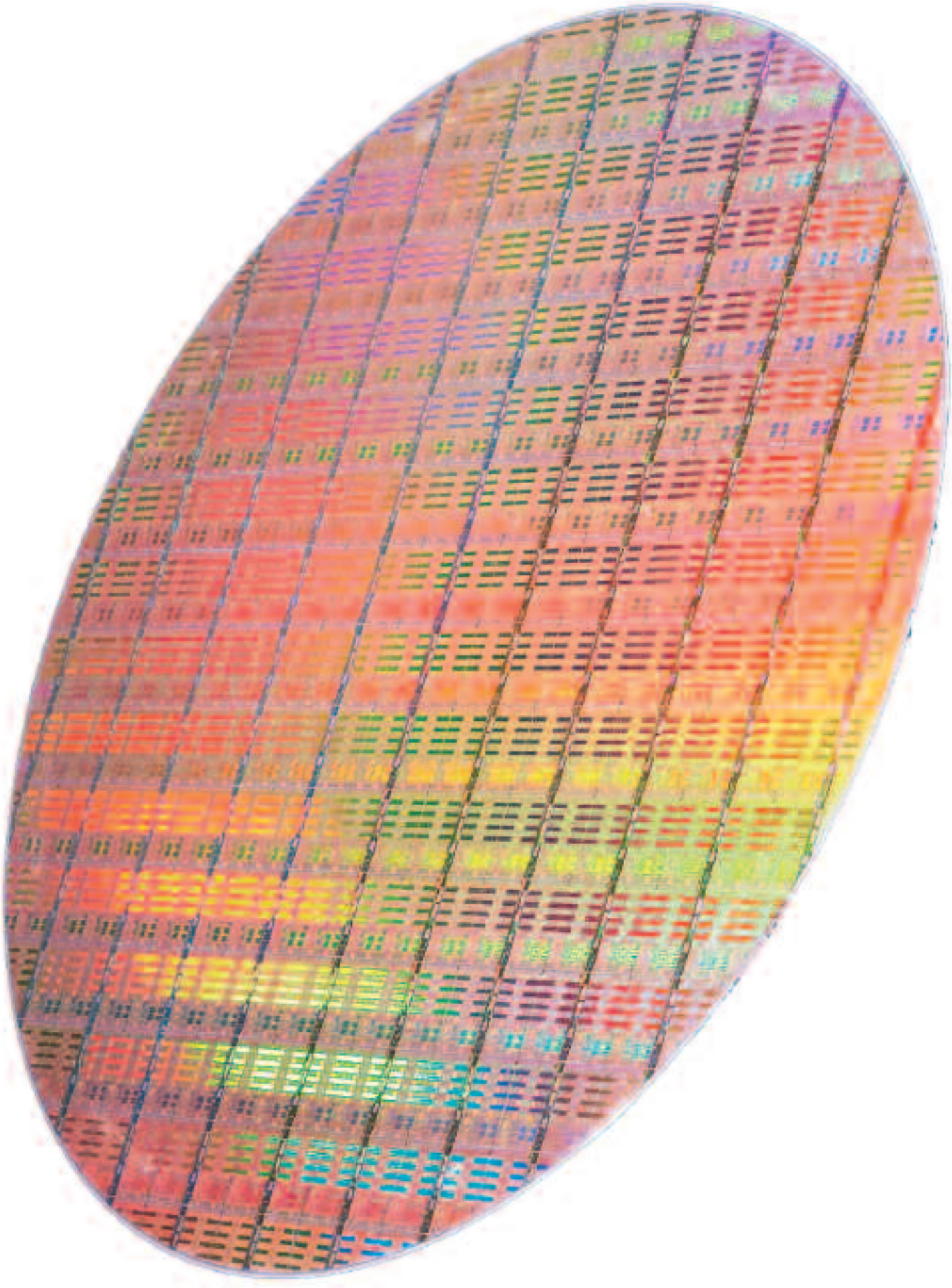

IBM Cell BE processors

6 Research Results

Publications, papers and communications

6.1 Computer Sciences

Publications

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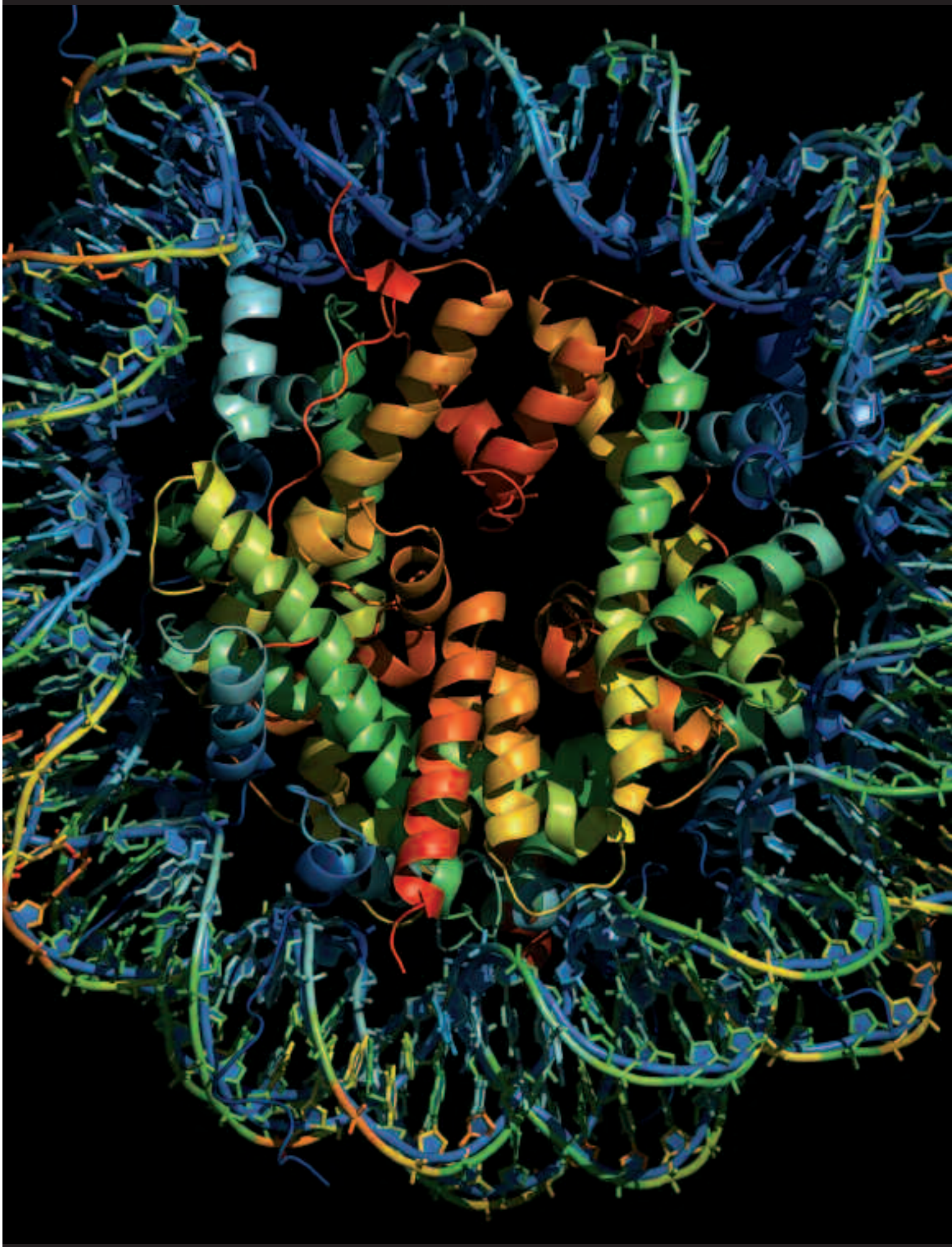

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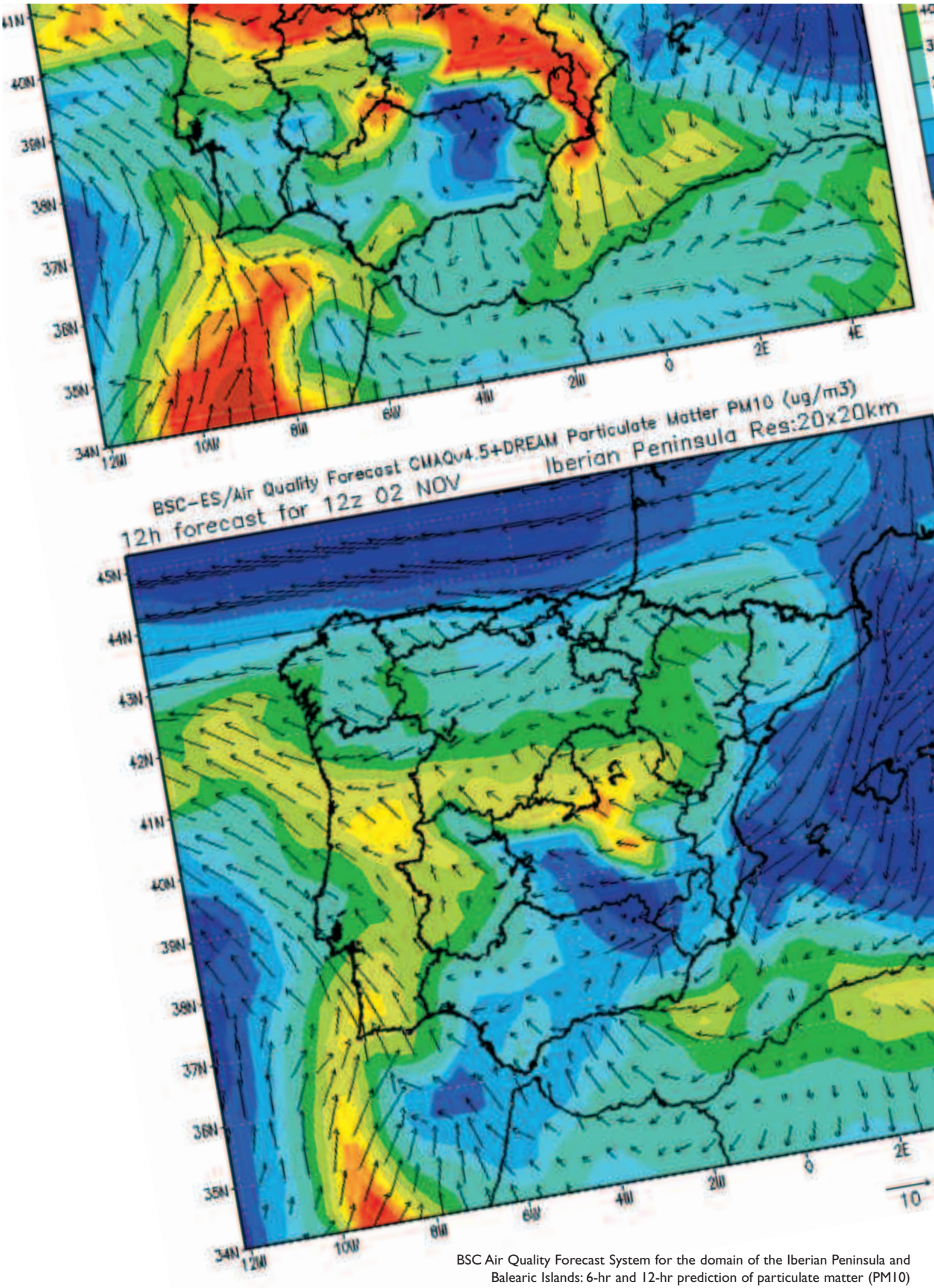

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