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2007 CESGA ANNUAL ACTIVITY REPORT



CESGA



CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS





THE YEAR OF

FINISTERRAE

CESGA ANNUAL REPORT 2007

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message from the president



CESGA worked very intensely in the year 2007 as a consequence of the agreements reached with the Ministry of Education and Science and with the Spanish National Research Council (CSIC) to include CESGA in the Map of Singular Scientific Technological Installations and in order to promote it as a Centre of Excellence in Computational Science.

In addition to the daily activity, the centre carried out the important activity of remodeling the building and the technical infrastructures, which required considerable extra effort on the part of the totality of CESGA's personnel and an occasional inconvenience for users of the Centre. For these reasons we congratulate and we thank the personnel of CESGA for their cooperation and good will. We also beg the pardon of those users who were affected by the inconveniences of the project.

As a result of this work, the hardware and software of the supercomputer FINIS TERRAE were installed in December 2007. This initiated the tuning phase that was required before making it available to the research community, project to occur in March 2008.

In 2008, we look forward to new and important activities directed toward the increase of the quantity and quality of the services offered by CESGA and to the promotion and development, in a decided fashion, of research activity in Computational Science.

Salustiano Mato de la Iglesia

Director General for Research, Development and Innovation Regional Government of Galicia (Xunta de Galicia)

message from the vice-president



During its 15 year history, CESGA has been continually incrementing its research activity and its services, as well as permanently improving in accordance with Norm ISO 9001.

On the basis of CESGA's accumulated experience and the solid structure available, CESGA is initiating a program of research excellence in Computational Science, defining specific lines of collaboration with other centres of excellence that have already been established or that are in the process of being established in its nearby environment.

The joint project of the Government of Galicia and the Spanish National Research Council (CSIC) for the development of Computational Science was reaffirmed with the installation of the supercomputer, FINIS TERRAE, and the subsequent initiation of the construction of a new site for CESGA in which new research activities in Computational Science will be developed and which will provide important capacities for computing that are required by the scientific community.

José Manuel Fernández de Labastida y del Olmo

Vice-President for Scientific & Technical Research, Spanish National Research Council (CSIC)

highlights



» The most noteworthy activities and events that took place at CESGA during the year 2007 are summarized below.

CESGA FOUNDATION

- » The installation of the supercomputer Finis Terrae.
- » A 5- fold increase of the computing capacity, achieving close to 21 TFLOPS.
- » The Proposal of CESGA as a Centre of Excellence in Research in Computational Science (CESGA - Computational Science Research Centre).
- » The organization of the 1st Portuguese-Spanish IBERGRID Conference, the Iberian Grid Infrastructure.
- » The computing hours consumed increased by 29% with respect to the previous year, reaching 2,062,610 hours.
- » The Foundation participated in 19 RTD projects. Of these projects, 2 were financed by the European Commission, 8 by the Government of Spain, and 9 by the Government of Galicia. Likewise, the Foundation participates in 9 Thematic Networks and Technological Platforms.
- » The Foundation signed an Agreement of Collaboration with the Ministry of Education and Science for the construction of a new building for CESGA.

S.A.X. CESGA

- » S.A.X. CESGA renewed the Agreement of Collaboration with the Director General of Industrial Promotion and the Information Society for the support of the Initiative for Free Software in Galicia.
- » S.A.X. CESGA's building was reconfigured and adapted for the housing of the supercomputer, Finis Terrae.
- » S.A.X. CESGA participated in 20 RTD projects. Of these projects, 7 were financed by the European Commission, 2 by the Government of Spain and 11 by the Government of Galicia. Likewise, the Society participated in 5 thematic networks.

Javier García Tobío Managing Director

Mission Statements

mission statements

CESGA Foundation

Mission

To promote, disseminate and deliver high performance computing and communications services to the research communities of Galicia and CSIC as well as to those companies or organisms which request them, with the goal of increasing competitiveness by means of technological development and innovation.

Main functions

- » To manage the Science and Technology Network of Galicia.
- » To promote and develop cooperation among companies and institutions.

FUNCTIONAL AREAS, RESOURCES AND SERVICES OF BOTH ENTITIES

S.A.X. CESGA

Mission

To promote support services for research, development innovation in the field of Information Technologies and Communications both in Galicia and the scientific community of CSIC.

Thus, S.A.X. CESGA is dedicated to the innovation and improvement of its high performance computing and advanced communications services as well as to those activities designed to serve the knowledge society.

Main functions

- » To promote and disseminate the use of high performance computing technologies and advanced communications.
- » To promote and disseminate the use of technologies related to the knowledge society including e-Business, e-Learning, and Geographical Information Systems.

CESGA FOUNDATION

HPC, HTC AND GRID COMPUTING

HPC, HTC Servers, GRID Servers. Scientific Software Applications

Storage Servers

Code Optimization, Problem Definition. Parallelisation, User Support...

Critical Storage Systems

TRAINING

RTD PROJECTS

Viability Analysis,

Proposal Development,

Consortium Creation,

Project Negotiation,

Management...

Workshops and Training Courses for Users

S.A.X. CESGA

e-LEARNING					
RESOURCES	SERVICES				
e-Learning Room Network and e-Learning Platform, "AULA CESGA", Access Grid, Room Network	Analysis, Development, Implementation and Hosting of Solutions				

e-BUS	INESS
RESOURCES	SERVICES
Galicia's e-Business Leveraging Centre	Viability Analysis, Project writing, Partnerships Formation

COMMUNICATIONS

DATA STORAGE

RECETGA Science and Technology Network of Galicia

DNS, Hosting, Mail Servers, Mailing List, FTP. News. Mirrors. Multicast, Videoconference, MCU / Gateway, Proxycache, Network Management. Security Systems, Statistics...

(EDUCATION)

DISSEMINATION

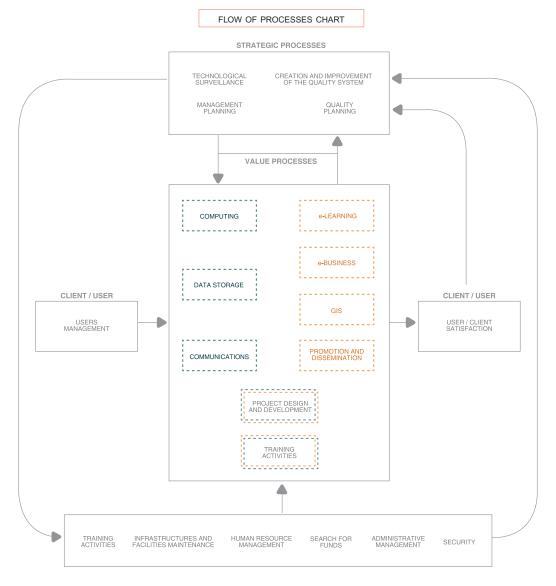
Web, Publications, Presentations, Seminars, Scientific Conferences...

GEOGRAPHIC INFORMATION SYSTEMS

Map Servers. Analysis, Geographical Development Data Bases Implantation and **Lodging Solutions**



quality of services





During 2007, the CESGA Foundation as well as S.A.X. CESGA renewed the certification of quality, **ISO 9001:2000**, that was obtained in December 2005. At this time CESGA became into the first supercomputing centre in Spain to receive this certification, now renewed.

The renovation of the certification was the culmination of intensive work related to the application of the norm as well as to the continued improvement of the internal processes and procedures of CESGA with the aim to increase the quality of the services offered to the users.

Quality, a map of processes

Only during this second year in which the certification was in force, 2 processes, 5 procedures, and 6 instructions have been

improved. CESGA was audited twice, both with successful results. One audit was internal but performed by external auditors and one was external for the renovation of the certification.

Additionally, in 2007, advances were made in the automating of all of the processes associated with quality control, with improvements in the monitoring systems of the Centre (users, systems, applications, etc.) and the installation of the new application for quality control was continued in accordance with the Norm ISO 9001: 2000.

Moreover, an audit was conducted and all personal data file management systems were reorganized in order to comply with the LOPD and the LSSI (Spanish law affecting personal data protection and information society issues).

Government Bodies

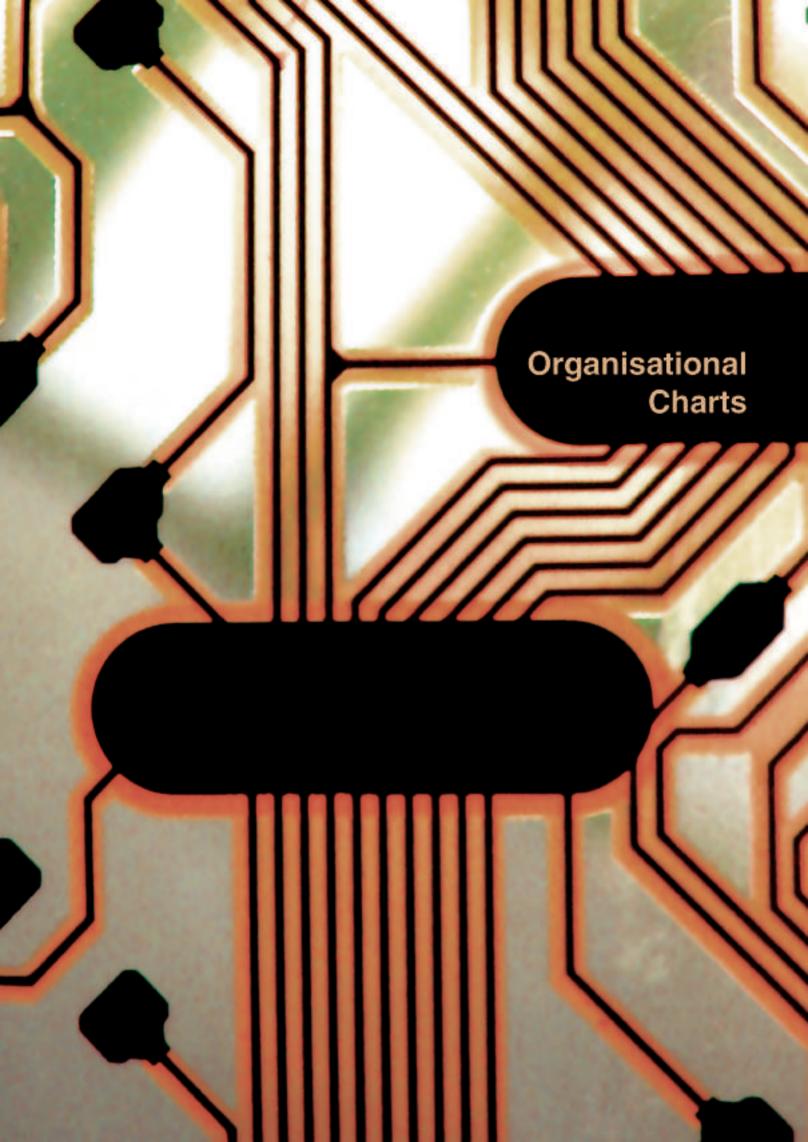
government bodies of the legal entities that constitute CESGA

S.A.X. CESGA

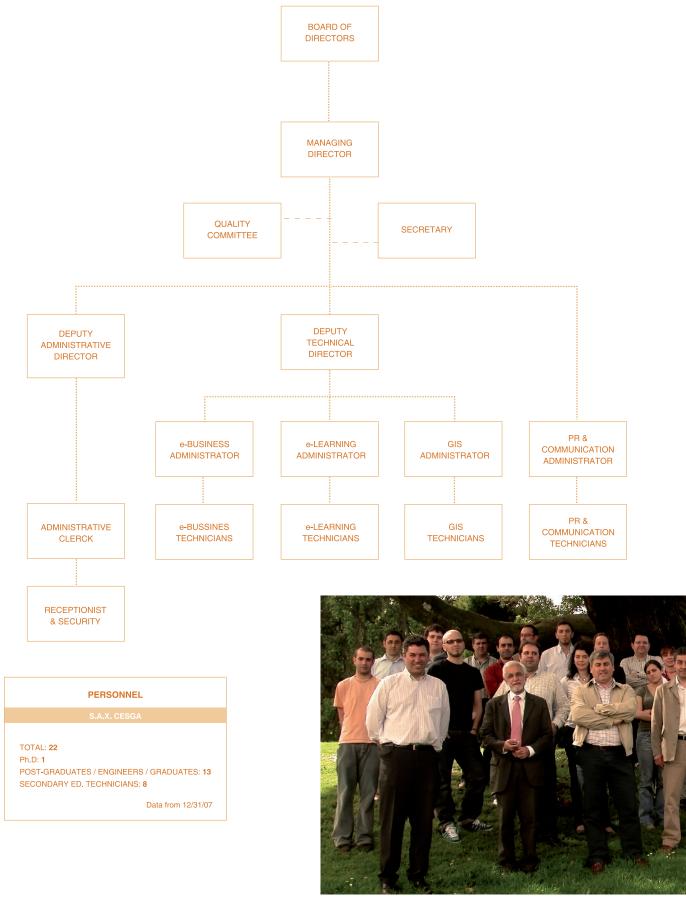
BOARD OF DIRECTORS S.A.X. CESGA						
	PRESIDENT	Salustiano Mato de la Iglesia	Director General for RTD Regional Ministry for Innovation and Industry			
	SECRETARY	José Carlos López Corral	Legal Adviser Regional Ministry for Innovation and Industry			
	MEMBER	Gonzalo Gómez Montaña	Director General of the Computing Centre for Tax Management, Finances and Accouting Regional Ministry of Finance			
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	MEMBER	Antonio Álvarez Alonso	Researcher Marine Research Institute			
UNIVERSITY OF A CORUÑA	MEMBER	Mª Concepción Herrero López	Vice-President for Research University of A Coruña			
UNIVERSITY OF SANTIAGO DE COMPOSTELA	MEMBER	Mª José Alonso Fernández	Vice-President for R&D University of Santiago de Compostela			
UNIVERSITY OF VIGO	MEMBER	Manuel Joaquín Reigosa Roger	Vice-President for Research University of Vigo			

CESGA FOUNDATION

FOUNDATION	Director General for RTD Regional Ministry for Innovation and Industry	Legal Adviser Regional Ministry for Innovation and Industry	Director General of the Computing Centre for Tax Management, Finances and Accounting Regional Ministry of Treasury	Director General for the Promotion of Industry and Information Society Regional Ministry for Innovation and Industry	Director General for the Promotion of Science and Technology in the Galician University System Regional Ministry of Education	Vice-president for Scientific and Technological Research Spanish National Research Counci (CSIC)	Institutional Coordinator Spanish National Research Council Galician Division
MEMBERS OF THE BOARD OF TRUSTEES OF CESGA FOUNDATION	Salustiano Mato de la Iglesia	José Carlos López Corral	Gonzalo Gómez Montaña	MP Elena Veiguela Martinaz	Rogelio Conde Pumpido	José Manuel Fdz, de le Bastida y del Olmo	Uxio Laberta Fernández
MEMBERS OF THE	PRESIDENT	SECRETARY	MEMBER	MEMBER	MEMBER	VICE-PRESIDENT	MEMBER
	REGIONAL	OF		SPANISH NATIONAL RESEARCH	COUNCIL		

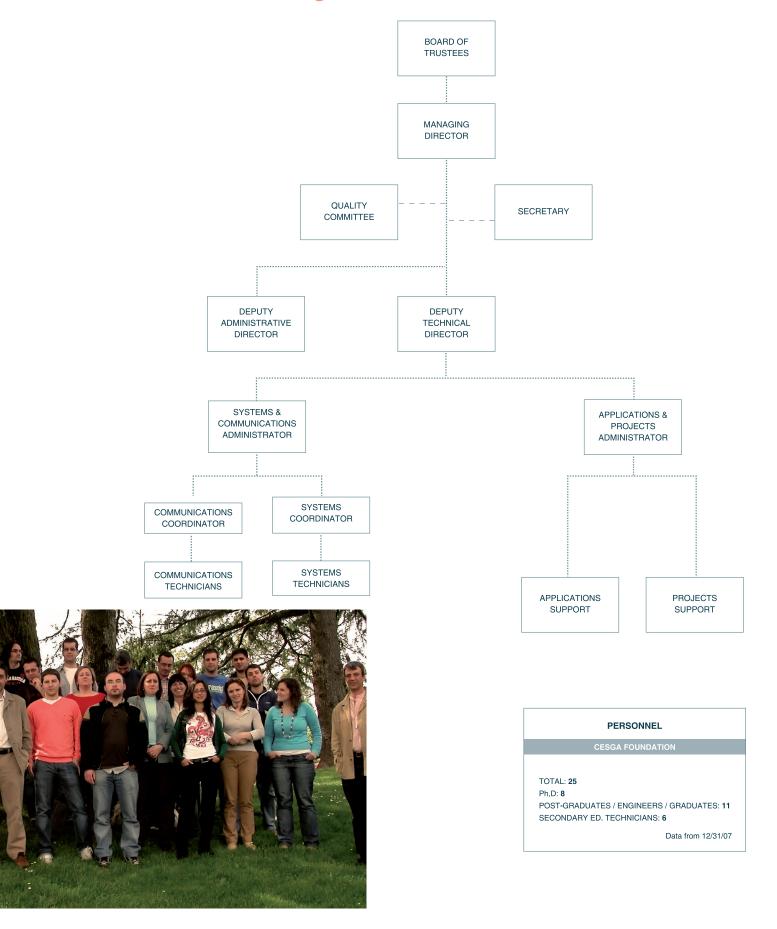


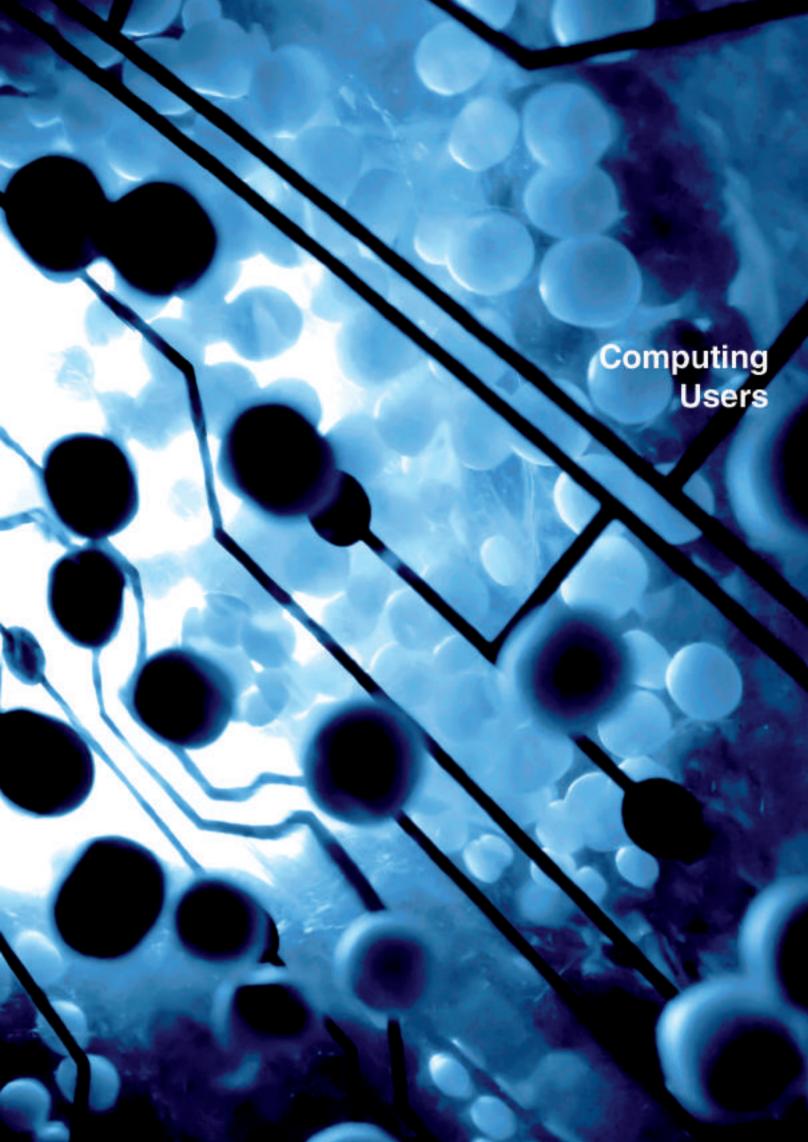
S.A.X. CESGA organisational chart



CESGA'S WORK FORCE, ITS MOST VALUABLE ASSET

CESGA Foundation organisational chart





most active users in 2007 by institution

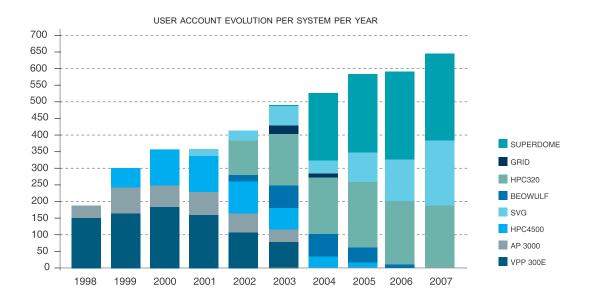
USER	DEPT. / CENTRE	HOURS USED
SANTIAGO DE COMPOSTELA U	JNIVERSITY (USC)	
Manuel Pereiro López	Applied Physics	99,450.6
Bernardo Adeva	Particle Physics	67,760.7
Jorge Botana Alcalde	Applied Physics	62,726.2
Jesús Ángel Varela Carrete	Organic Chemistry	59,932.0
Ricardo Vázquez López	Particle Physics	51,465.7
Rubén Meana Piñeda	Physical Chemistry	37,745.9
A CORUÑA UNIVERSITY (UDC		
Daniel Rivero Cebrián	Communications & Information Technologies	75,411.0
Luís Rodríguez Vázquez	Chemistry, Physics and Chemical Engineering I	47,582.5
Daniel Rodríguez Ramos	Chemistry, Physics and Chemical Engineering I	36,407.3
Olga Blanco Mosquera	Fundamental Chemistry	34,229.1
Eduardo Carro Rey	Chemistry, Physics and Chemical Engineering I	32,392.5
Vicente Ojea Cao	Fundamental Chemistry	30,600.4
VIGO UNIVERSITY (UVIGO) Laura Estévez Guiance	Physical Chemistry	41,098.2
Rosana Álvarez Rodríguez	Organic Chemistry	26,230.4
Ángel Rodríguez de Lera	Organic Chemistry	21,735.2
Manuel Martínez Piñeiro	Applied Physics	13,154.3
Cristina López Bravo	Telematics Engineering	11,413.2
Guilvaume Silvestre de Ferrón	Applied Physics	8,455.4
SPANISH NATIONAL RESEARC	H COUNCIL (CSIC)	
Fabrice Dayou	Dept. of Molecular and Infrared Astrophysics	26,700.1
Joaquim Ortega Castro	Earth Sciences & Environmental Chemistry	20,405.3
-	Theoretical Chemistry & Molecular Modelling	·
Noemí Hernández Haro	Earth Sciences & Environmental Chemistry	20,076.2
	Theoretical Chemistry & Molecular Modelling	
Gonzalo Jiménez Oses	Theoretical Chemistry & Molecular Modelling Chemistry Stereo-selective Organic Synthesis Group	19,087.7
Gonzalo Jiménez Oses Alejandro Valbuena Jiménez	Theoretical Chemistry & Molecular Modelling Chemistry Stereo-selective Organic Synthesis Group Developmental Neurobiology	19,087.7 16,680.9

computing users

Number of Active Accounts

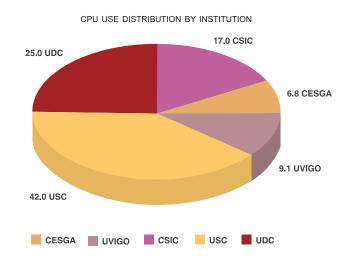
The Superdome was the system with the greatest number of active accounts (users with a significant consumption of hours during the year) with a total of 264 (8 more than in 2006). The HPC320 occupies the third position with 187 active accounts (2 less than in the prior year), in spite of the fact that this system will stop offering services during 2008. The SVG cluster experienced the greatest increase in active accounts, now

having 194 (67 more than in 2006), in addition to GRID projects users. In total, the number of active accounts grew from 572 in 2006 to 645 this year, which indicates an increase of 12% (in 2006, growth in the number of active accounts was only 2%). The growth was fundamentally motivated by the increase in the number of users in the SVG cluster, thanks to the technological updating of this cluster at the end of 2006.



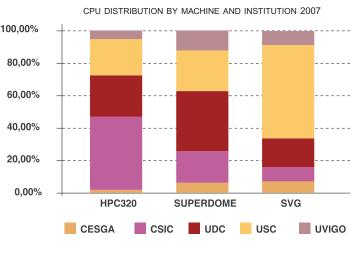
Distribution by Institutions of the CPU hours Consumed in all of the Systems

All of the institutions increased the number of hours consumed with respect to the previous year. By institution the greatest increase in the number of hours of computation was registered by the University of Santiago of Compostela with 42% of the hours (2.3% less than the previous year), followed by the University of A Coruña with 25% of total consumption (1.4% less than the past year). The three Galician universities together represent 76.1% of the consumption, and CSIC, 17% of the total (as compared to 13.7% in the prior year). The projects in which CESGA participates were responsible for 6.8% of the hours consumed.



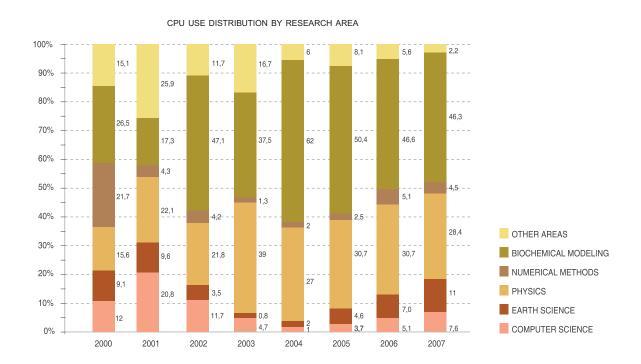
CPU Distribution by Research Area

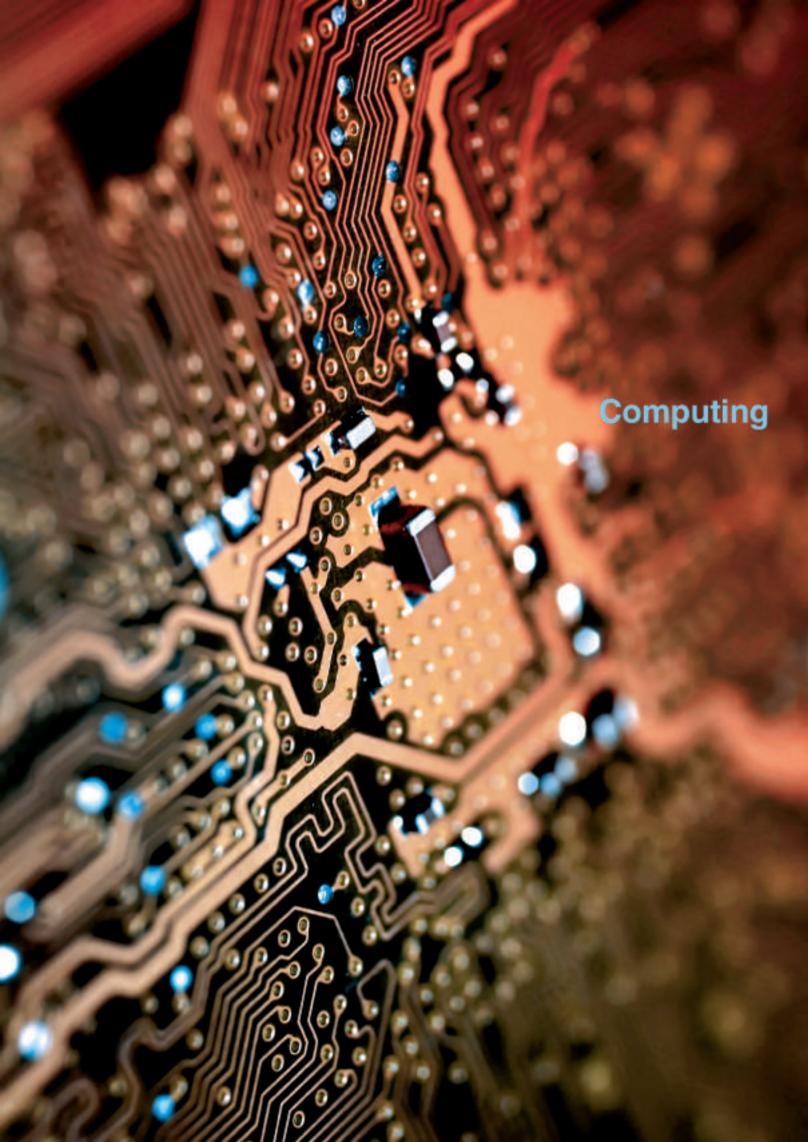
Organized by research areas, the computing related to biochemical 100,00% modelling consumed 46.3% of the computing hours during 2007 and 28.4% were dedicated to the study of physics. These two areas represent 74.7% of the total consumption of hours. Biochemical modeling is again, as it was in the previous year, the area with the highest computational demand, even though it decreased by 0.3%. The increase in the area of earth sciences is also noteworthy as it has grown from 4.6% in 2005 to 11% in 2007, while computing sciences grew from 3.7% in 2005 to 7.6% in 2007.



CPU Usage Distribution by Institution and Machine

In this graphic, we can see which systems are most in demand for each one of the institutions that use CESGA's computing services. As can be appreciated, the CSIC's researchers principally utilize the HPC320 server, with more than a third of the system's utilization, while the Superdome is divided principally between the investigators of the Universities of Santiago and A Coruña. The SVG is most used by researchers of the University of Santiago.





computing

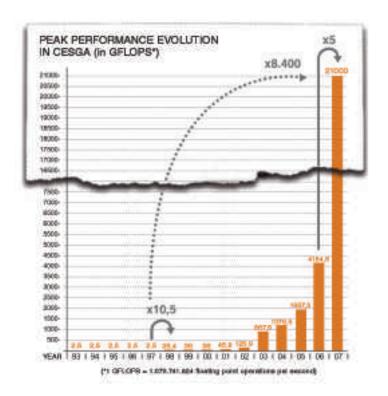
Different architectures of high-performance computing systems are available for CESGA's community of users. Depending upon the algorithms involved, users choose the computing architecture that is most appropriate.

Regarding the computing servers, the most relevant activities of 2007 are listed below.

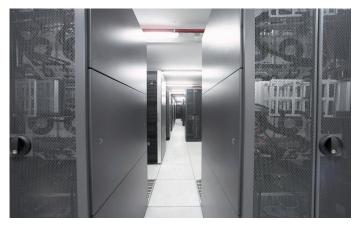
» Preparation of the support infrastructure of FINIS TERRAE

- » Enlargement of the Data Centre room. Relocation of the current servers to their new space within the Data Centre.
- » Installation of the FINIS TERRAE Supercomputer.

The most significant computing activities at CESGA are illustrated in the following graphs:

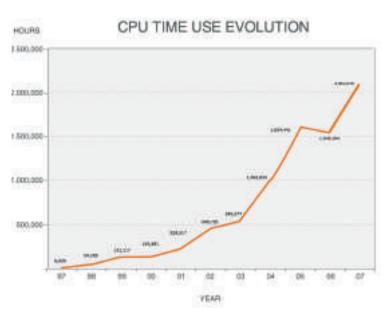






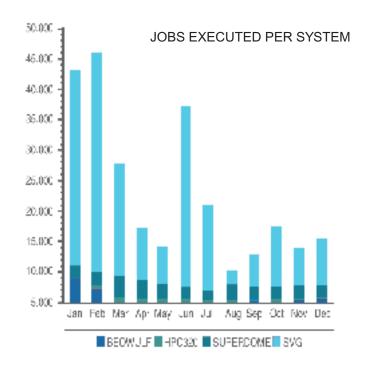
During 2007, the most utilized servers were the SVG cluster and the HP Integrity Superdome. During the same year, the amplification of the SVG cluster with GRID nodes was put into production which increased the consumption in this cluster (in addition to 200,433 CPU hours utilized in GRID projects that are not reflected in these graphics). Levels of occupation close to 100% were reached for all servers. In spite of diverse incidents with the Superdome computing server, such as stoppages due to work associated with the adaptation of the new Data Centre and

The electrical and air conditioning installations, the prioritization of parallel jobs (whose efficiency is inferior to that of sequential jobs) and the requirements for an increased quantity of memory, the number of consumed hours increased and surpassed 2 million (2,062,610 hours) as compared to 1,654,411 hours during the prior year, which represents 24% growth. During the entire year, the HPC320 server installed in 2002 and whose retirement from production is scheduled for 2008, also continued at a level of utilization of 71,2%.



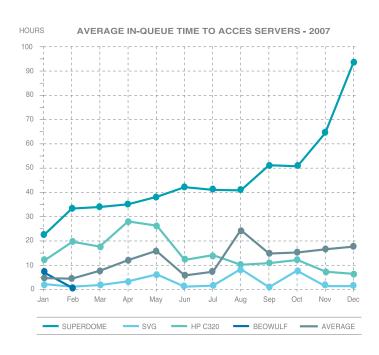
Number of jobs executed

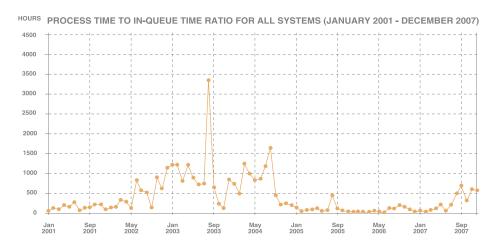
The number of jobs executed daily represents the quantity of simulations that the users performed with each of the computing servers. This value not only depends on the available computing capacity but also on the resources necessary for the execution of the simulations. The systems with the greatest number of jobs were the SVG and the HP Superdome, especially the first, given that it is a server that is oriented to productivity, that is to say, the performance of a large number of independent jobs with necessities for computing that are relatively low. In addition, relative to the servers that are dedicated to GRID projects, another 100,115 jobs were performed within the EGEE project and 26,534 for the int.eu.grid project.

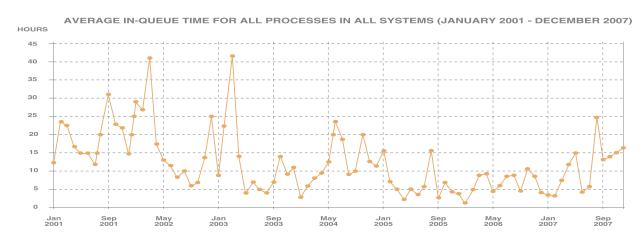


Average in-queue time

The average in-queue time represents the mean length of time that users should wait from the moment that they request CESGA resources until their simulations can begin to utilize those resources. These times vary in function of the quantity of simulations that are being performed and that ideally should be as close to zero as possible in order to limit the time that researchers have to wait until they obtain the results of the simulations. With all of this in mind, the higher the level of occupation of the computing systems, the more time it is necessary to wait until sufficient resources are available. As such, this measure is also a good indicator of the level of existing saturation of the computing resources. Normally, the waiting times decrease in the holiday periods of summer and Christmas and they increase significantly when new users are incorporated. In the graph, one can see that the systems with the longest in-queue times are the Superdome (more than 20 hours during the entire year and increasing to more than 50 in the last quarter of the year) and the HPC320, with shorter waiting times during the months of July and August. While the average in-queue time increased in the Superdome from 19 to 43 hours, it decreased from 19 to 15 hours in the HPC320, and it did not vary in the SVG cluster.







HPC: high performance computing servers

CESGA's users have different server architectures for High Performance Computing (HPC) at their disposal. This involves machines designed to solve a reduced number of problems, but of large dimensions, in a limited time. These architectures incorporate scalar high performance processors with access to large quantities of memory, utilizing internal networks with a low latency time and a high transfer capacity.

During 2007, the users had access to two different high performance systems.

HP Integrity Superdome

This SMP NUMA Cluster is formed by two nodes with a total of 128 Intel Itanium2 processors, 1500 MHz, 6 Mbytes cache, 384 GB of memory, and 4.6 Terabytes for temporary storage on

disc. An Infiniband network between the two nodes is available. For permanent data, the user has an HP EVA-3000 disc rack for massive storage with FiberChannel technology. This is the machine in which users perform the jobs with greatest computational demand. It is also a preferred option for the execution of parallel jobs.

COMPAQ HPC 320

This cluster is made up of 8 SMP machines with 4 Alpha EV68 processors of 1 GHz each and 80 GB of total memory. The nodes of this cluster are interconnected by means of a Memory Channel Dual Rail network.



HIGH PERFORMANCE COMPUTING SERVERS						
SERVERS	SERVERS YEAR INSTALLED ARCHITECTURE PROCESSORS, MEMORY, PEAK PERFORMANCE					
COMPAQ HPC320	2002	CLUSTER	32 CPU's, 80 GB MEMORY, 64 GFLOPS			

OPEN PLATFORMS FOR HPC

In 2006, CESGA was invited to become a member of Gelato. The Gelato Federation (www.gelato.org) is a work forum for the global technological community that is dedicated to the advancement of Linux over platforms based on Intel Itanium. CESGA contributes to the development and improvement of tools for the management of clusters and GRIDS, the management of memory, tools for the measurement of performance and resource use accounting, the adaptation and tuning of applications and libraries in Linux Itanium environments, among others.



HTC: high throughput computing & GRID servers



CESGA offers server architectures designed to solve a high number of problems of minimal computational complexity in a short period of time. The HTC servers, High Throughput Computing, incorporate a large quantity of scalar processors with rapid access to a local memory of limited size. These servers have an internal network of interconnection with medium-high latency.

This type of architecture is ideal for repetitive processes with low dependency between themselves, such as, genetic algorithms, massive processing of experimental data, the rendering of images, parametric calculus, etc. In 2006, CESGA acquired a DELL Blade Cluster with 292 processing cores, 148 GB of memory and a peak performance of 2,227 GFLOPS. This cluster was integrated in the Galicia Virtual Supercomputer (SVG). In 2007, 32 processors and 32 GB of memory were added.

SVG reflects the proposition that the Centre made in 1999 regarding low- cost cluster systems as an ideal solution for the increase of throughput jobs.

HTC systems, as well as other clusters, are increasingly more abundant in the laboratories and departments of research groups. These groups use the services of CESGA as a complement to their own, without the necessity to port their applications nor to learn new operating systems.

Due to their characteristics, the HTC servers installed at CESGA are used in GRID experiences and projects.

SIGNIFICANT GRID PROJECTS IN WHICH CESGA PARTICIPATES



















SPANISH THEMATIC NETWORK
IN GRID MIDDLEWARE

HIGH THROUGHPUT COMPUTING SERVERS INTEGRATED IN THE GALICIAN VIRTUAL SUPERCOMPUTER (SVG) YEAR INSTALLED ARCHITECTURE PROCESSORS, MEMORY, PEAK PERFORMANCE 50 CPU's, 0,5 -1 GB MEMORY CPU, 9,9 GFLOPS, 110 CPU, 300 GFLOPS (2004) svg 2001-2006 DISTRIBUTED PC CLUSTER COMPAQ BEOWULF **BEOWULF CLUSTER** 2002 16 CPU, 8 GB MEMORY, 16 GFLOPS **SVG DELL** 2004 **PC CLUSTER** 80 CPU, 80 GB MEMORY, 512 GFLOPS **SVG BLADES** 2006 **BLADE CLUSTER** 292 CORES, 148 GB MEMORY, 2.227 GFLOPS

housing of computing equipment

Meteogalicia

In CESGA's Data Centre, there is a SUN Microsystems computing server composed of two SMP nodes with a total of 20 CPUs, 40 GB of memory, and 48 GFLOPS of peak performance that was acquired by Meteogalicia in 2004. Since that date, the Centre has taken care of the housing and the administration of this equipment which is used in the development of meteorological research projects.

Since its creation, Meteogalicia has used CESGA's servers in order to produce daily meteorological predictions. In addition to this SUN machine, Meteogalicia regularly uses the following servers: HP Integrity Superdome, HPC 320, and the Galician Virtual Supercomputer (SVG).

LHCb-USC

Since 2002, the Experimental Group of High Energy Physics of the University of Santiago de Compostela (GAES) has a PC Cluster housed in CESGA's Data Centre. It participates as a Tier-2 Centre in the LHCb experiment coordinated by CERN. CESGA systems technicians have been responding to the necessities of equipment administration. This equipment is available for all users when it is not employed by the project. In 2007, 200 cores and 200 GB of memory were added to this cluster.



LHCb-USC	2002-2007	PC CLUSTER	339 CORES, 312 GB MEMORY, 1600 GFLOPS
METEOGALICIA	2004	2 SMP CLUSTERS	20 CPU, 40 GB MEMORY, 48 GFLOPS
SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
	SERVERS HOUSED AT CE	SGA	



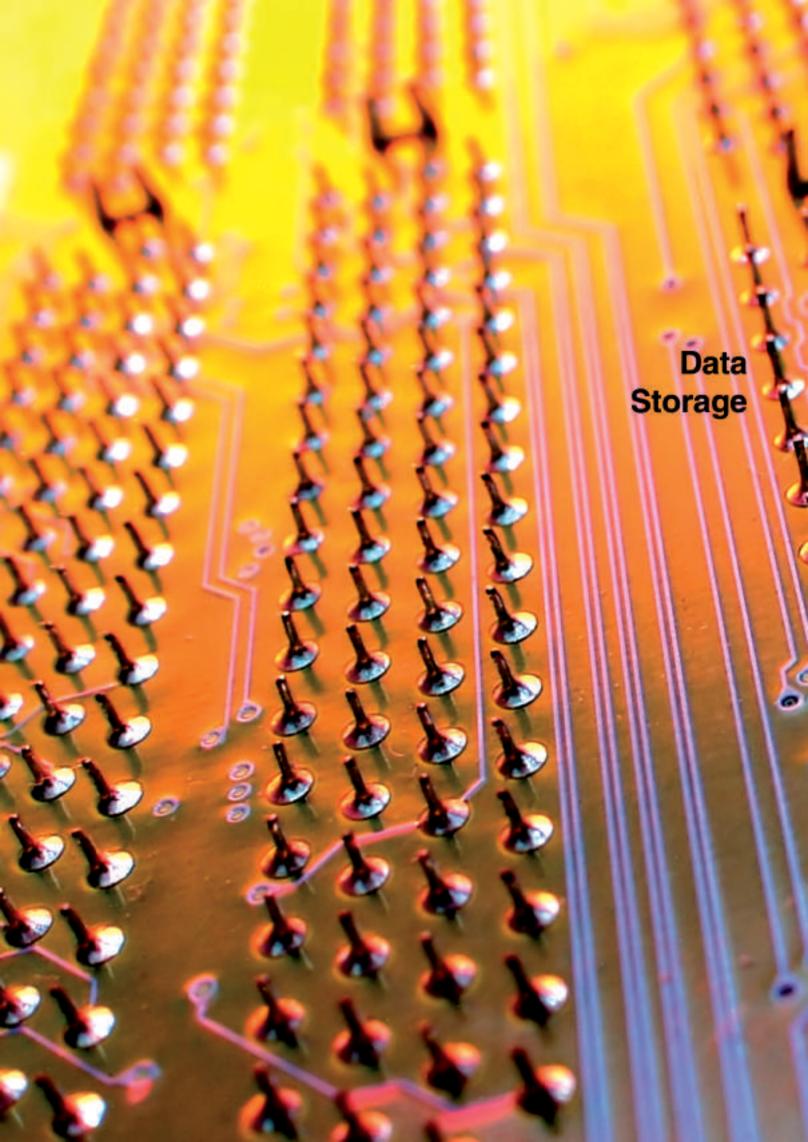








LHCb-USC CLUSTER



data storage

The total storage capacity that is available to the users of CESGA increased significantly in 2007 with the incorporation of Finis Terrae. Temporary storage capacity increased by 124 TB, parallel storage increased by 216 TB, and storage on tape increased by 160 TB with the incorporation of a new tape robot with a capacity of up to 1,400 cartridges of 1.6 TB each. The total storage available to users now is up to 642 Terabytes, which is an increase of 4.5 times more than the capacity of the prior year. The following Table shows the distribution of storage.

The storage of data is now organized according to a hierarchy of the type of data stored in order to assure the best quality of service in function of the information (criticalness of the data and speed of access). There were 49 users of the data storage service; 30 of those registered an increase in their user quota in the computing servers, 11 with massive data storage, and 8 with disc security copies (some users are subscribed to more than one service).

Storage service

Criteria for the classification of information

In 2007, the criteria introduced in 2004 regarding the classification of the types of data in the storage service was maintained.

This system permitted the accommodation of the distinctive services to the specific necessities of each group of information, responding in this manner to the growing demand for quantity and quality of service, such as the optimization of the different storage options available in the Centre. A description of the 5 types of information that are available in the service is presented below, in accordance with the classification previously defined.

Scratch has very low latency and maximum band width. It affects the computing production of the Centre. Average capacity (the data are only stored for the duration of the execution of the computing jobs). Availability may be low (they are temporary data) and it is not necessary to make back-ups.

Home Directories contain critical data that are susceptible to being analyzed and modified at any moment. The functioning of the computing services of the Centre depends on their availability. As such, they should have (maximum) availability as a priority as well as an ideal balance between capacity (average, in function of the number of users) and performance (average), of which back-ups are made on a daily basis.

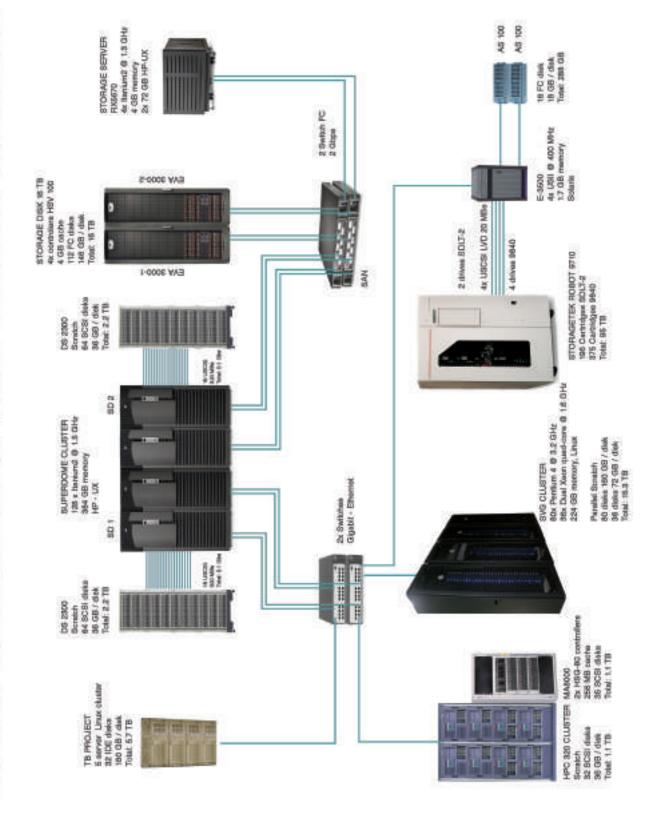
Massive data storage (MSS) is utilized to store data bases and research results; normally the content does not vary (they usually are of the WORM type) and the access velocity is usually not critical, although they require a high band width to access the servers. Back-ups can be made according to demand.

Back-ups to disk are the copies of the data that users make with their own servers or with their own PCs are stored in the CESGA's systems in order to keep a secure copy of their data. The availability of the service may be low. The service is offered by means of the network for which it is not necessary that the type of connection be one of high performance.

Scratch Parallel is very high performance (very low latency and maximum band width), similar to the first type with the addition that, in this case, the scratch data is shared between all of the nodes of the cluster and distributed among all of them). This permits an increase in both the access band width to the files and the total capacity of the scratch well above the local disc capacity. Its availability may be low due to the fact that it depends on many components that are not redundant. No back-ups of these data are made.

TYPE OF STORAGE	CAPACITY (Gbytes)
Temporary or Scratch	
Temporary Parallel	
Permanent Disc	
Таре	
TOTAL	642,822

CESGA'S DATA STORAGE RESOURCES 2007





scientific computing applications

Scientific applications

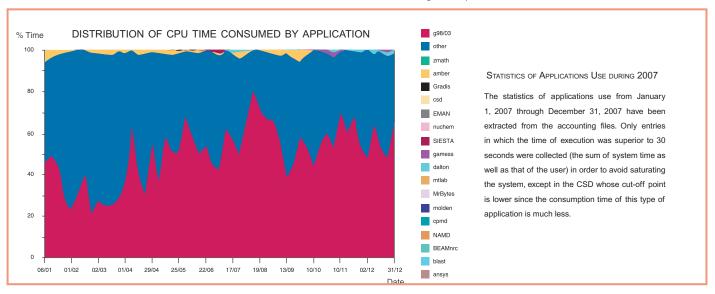
The activity in the area of applications included the following:

- » The elevated number of support activities performed during the year (123), which represents a yearly increase of 35%.
- » The portability of the applications that are most important for the future server, Finis Terrae. Such applications include:
 - AMBER version 9.0
 - · GAUSSIAN 03 versions C01, D.02 and E.01
 - · GROMACS versions 3.3.1 and 3.3.2
 - NAMD version 2.6b1
 - OCTOPUS version 2.1.0
 - GAMESS version 24 Mar 2007 (R1)
 - SIESTA version 2.0.1
 - CODE-ASTER version 9.1.0
 - · Libraries, such as:
 - FFTW version 3.1.2
 - GSL version 1.9
 - NETCDF versions 3.6.1 and 3.6.2
- » The organization of 6 training courses, internal and external:
 - For the i-MATH project, two computing courses: COMPUTATIONAL MATHEMATICS: Compilation, execution, and optimization of programs and Parallel programming utilizing OpenMP directives.
 - Globus 4
 - Programming with UPC
 - · AJAX, a practical focus
 - Seminar: Protection of Data of a Personal Character (LOPD).

- » The analysis of the new infrastructures of CESGA (Quad Core servers, the model of Finis Terrae, Finis Terrae) that generated a technical report related to the new Intel Quad-core processors.
- » At the same time, the use of the applications was facilitated to the users by means of its configuration via the utility "modules" that permit the dynamic configuration of a UNIX context for any number of software packages with their corresponding versions.
- » The elevated number of requests for new installations or updating (29) or for support for the compilation of user applications or with license of the user (17).
- » The analysis, in conjunction with mancomun.org and with the three Galician universities, of the free/libre software tools for CAD and numerical simulation in order to include them as support in CESGA.
- » The initiation of a collaboration project with CSCS (Swiss National Supercomputing Centre) in the area of chemical visualization by means of the COST GRIDCHEM network.

The activities listed above are summarized with the following figures:

- 55 applications or libraries of scientific computing in production
- 36 newly installed or operational applications.
- Parallelisation of 2 applications for users.
- · Development of an application.
- The publication of CESGA's Technical Report.
- The response to 123 requests for assistance.
- 1 management application put into production (quality management).



The catalogue of applications and libraries installed as of December 2007 on CESGA's computing servers with access for all users follows:

Area	Application	HPC 320	HP Superdome	SVGD	OTHERS
Scientific Analysis	ROOT	Х			
Scientific Data Bases	CSD				csd.cesga.es
	ZENTRALBLATT				zmath.cesga.e
Bioinformatics	BEAMnrc			Χ	
	Blast	X		Х	
	GlimmerM			Х	
	IM		Χ		
	Migrate	X		Х	
	MrBayes		X	Х	
	MSVAR		X		
	Phylip			Х	
	r8s		X	X	
Structural Calculus, Fluids and Magnetism	Ansys	X	X		
Molecular Simulation	Abinit			X	
Molecular dimulation	Aimpac	X			
	Amber	X	X	X	
	CPMD	X	X	X	
	Dalton	X	X	X	
	Gamess	X	X	X	
	Gaussian 03	X	X	X	
	Gaussian 98	X	X	X	
	Gromacs	X	X	X	
	LAMMPS		X		
	Molden	X	X		
	NAMD	X			
	NWChem	X	X		
	SIESTA		X	Χ	
	XPLOR-NIH			Χ	
Mathematical Libraries	ACML			Χ	
	ATLAS			Χ	
	BLAS	X	Χ		
	cernlib			Х	
	CLHEP			Х	
	FFTW	X	Χ	Х	
	GMP		X		
	LAPACK	Х	Χ		
	Numeric Python				
	ScaLAPACK		X		
	SUPERLU		X		
Simulation	Bsoft	Х		Х	
	EMAN			X	
	Geant			X	
	Matlab	X		X	
		X		X	
	SPIDER	^			
Oniontific Visualization and Automatics	Xmipp	· · · · · · · · · · · · · · · · · · ·		X	
Scientific Visualization and Animation	Ferret	X		X	
	Grace		.,	X	
	Grads	X	X	X	
	Ncarg	X	X	X	
	ncBrowse	X			
	ncl	X			
	Ncview	Х			
	NetCDF	Χ	Χ		
	udunits	X			
Software Management	CVS	X	Χ		

The new applications or libraries of utilities that were incorporated during 2007 at the request of the users, or for the incorporation of new versions, are listed below.

Application	Task			
Scientific Data Bases	ROOT			
CSD (New version installed)	Cambridge Structural Database is a data base that collects bibliographic, chemical, and crystallographic information of organic and organic-metallic compounds obtained by means of the diffraction of X-rays and the diffraction of neutrons.			
Molecular Simulation				
AMBER (new version in the SVG and	AMBER is a set of programs that permits the user to perform simulations of molecular			
Superdome / portal to Finis Terrae)	dynamics, fundamentally in bio-molecules, based in theories of force fields.			
EON (new installation in the SVG)	EON is a program for the comparison of electrostatic potentials in molecules of the Openeye package. It is a program that can be of great assistance in the design of libraries of compounds and in the processes of the design of pharmaceuticals by computer.			
GAMESS (new version in the SVG, HPC320 and Superdome / portal to Finis Terrae)	This is an analogue package to GAUSSIAN that incorporates "ab initio" methods, although it presents some specific solutions for the description of orbitals and other methods of optimization.			
GAUSSIAN 03 (new versions in the SVG and Superdome / portal to Finis Terrae)	GAUSSIAN 03 is one of the most used packages in computational Chemistry that permits the calculus of properties (energies, frequencies of vibration, optimum geometry, etc.) of molecules and intermedia of reaction, fundamentally by means of "ab initio" methods (theoretical).			
GOLD (new installation in the SVG)	GOLD is a program for the calculus of "docking" of small molecules in proteins. GOLD is highly considered within the community of molecular modeling because of its high precision and effectiveness.			
MATERIALS STUDIO (new installation in the SVG)	Materials Studio is a package of modeling and simulation that is easy to use for the study of chemical substances and materials including crystalline structures and processes of crystallization, polymers, catalysis, and structural activity.			
MOLPRO (new version in the Superdome)	MOLPRO is a complex system of "ab initio" programs for the calculus of the electronic structure in molecules. This package is specialized for highly precise calculus, with an intensive treatment of the problem of electronic correlation by means of CI multi-configuration methods, coupled-cluster, and likewise.			
NWCHEM (new version in the SVG, HPC320, and Superdome)	NWChem is a package for computational chemistry designed for execution in parallel high performance supercomputers as well as for clusters of conventional work stations. It is intended to be scalable in its capacity to deal with large problems in an efficient manner as well as in its use of available parallel computation resources.			
OMEGA (new installation in the SVG)	OMEGA is a program for the generation of data bases with structural conformers of the Openeye package that are necessary in the design processes of pharmaceuticals by computer.			
OPENBABEL (new installation in the SVG and in the Superdome)	OPEN BABEL is a set of tools designed for the speaking and understanding of the multi- ple languages that are actually used in chemical data. It is an open, collaborative project that permits the search, conversion, analysis, and storage of data in areas of molecular modeling, chemistry, materials, or biochemistry.			
Q5COST (new installation in the SVG and Superdome)	A library for the use of the standard formating of data in Quantum Chemistry Q5COST based on HDF5.			
QDYN (new installation in the SVG)	QDYN is a package for molecular dynamics for the calculus of free energy in bio-molecular systems.			

Application	Task
ROCS (new installation in the SVG)	ROCS is a program for the comparison of volumes and forms in molecules. It is part of the Openeye package used in the design processes of pharmaceuticals by computer.
SIESTA (new installation in the SVG and in the Superdome / portal to Finis Terrae)	SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and the implementation of a computer program used to carry out electronic structure calculus and simulations of "ab initio" molecular dynamics of molecules and solids.
TURBOMOLE (new installation in the SVG and in the Superdome)	TURBOMOLE is a package of specialized programs in Quantum Physics. Actually it is one of the most stable and rapid codes for standard methods in Quantum Physics (HF, DFT, MP2). Different from other codes in the area, its principal objective is to make possible the study of molecules of industrial relevance in a reasonable amount of time and with reasonable computational requirements.
WIEN2K (new installation in the SVG and in the Superdome / portal to Finis Terrae)	WIEN2k permits the calculus of electronic structures in solids using the theory of functional density (DFT).
XPLOR-NIH (new installation in the Superdome)	PLOR-NIH is a program for the determination of molecular structure that is constructed on the XPLOR program which includes additional tools.
Bioinformatics	
ALLEGRO (new installation in the SVG)	This application, with the basic functionality of Genehunter, provides a solution to problems of optimization that utilize the most advanced methodologies of genetic algorithms.
IM (new version in the Superdome)	The implementation of the MCMC method (Markov Chain Monte Carlo) for the analysis of genetic data by means of the model of the divergence of population, "Isolation with Migration".
MEGA2 (new installation in the SVG)	The utility of the conversion of data in projects related to the analysis of genetic relations ("linkage").
MERLIN (new installation in the SVG)	One of the most rapid software packages for the analysis of "pedigree" that is available today.
MSVAR (new installation in the Superdome)	A program for the detection of growths and declinations in population using "autosomal micro-satellite frequencies". This program is designed to aid the user in the exploration of demographic and genealogical histories that are most probably consistent with a set of chromosomes collected in one or more "loci". It is grounded in a simulation of the Markov Chain Monte Carlo (MCMC).
MULTIDIVTIME (new installation in the SVG)	A program for the study of velocities of molecular evolution and the estimation of divergence times.
PAML (new installation in the SVG)	PAML is a set of programs for the phylo-genetic analysis of DNA or of the sequences of proteins using algorithms of "maximum likelihood".
SIMWALK2 (new installation in the SVG)	SIMWALK2 is an application of genetic statistics for Haplotypes, "parametric linkage", "non-parametric linkage" (NPL), "identity by descent" (IBD) and "mistyping analyses on any size of pedigree". SimWalk2 uses Markov Chain Monte Carlo (MCMC) algorithms and "simulated annealing" in order to carry out these multipointed analyses.
Meteorological Simulation	
WRF/NMM (new installation in the SVG)	The Weather Research and Forecasting (WRF) model is a system of numerical meteorological prediction designed for operative predictions as well as for atmospheric research.

Application	Task
Electronic Microscopy Simulation	
EMAN (new version in the SVG)	EMAN is a complete software package for the construction of 3D models based on a set of images of particles that are randomly oriented. This technique is typically used in conjunction with individual molecules obtained using electronic cryomicroscopy.
XMIPP (new installation in the SVG) Optimisation	XMIPP, "X-Window-based Microscopy Image Processing Package", is a set of programs for the processing of images produced by means of electronic microscopy with the objective of the 3D reconstruction of individual particles.
Оринизации	
XPRESS-MP (new installation in the Superdome)	XPRESS-MP is a set of tools for the optimization and mathematical modeling that is used to solve problems of linearity, of wholes, of squares, of non-linearity, or of statistical programming.
Structural calculus, Fluids and Magnetism	
ANSYS (new installation in the SVG)	ANSYS is a package of finite elements that is initially oriented to the calculus of solid structures and thermal analysis which, in the past few years, has extended the field of application of finite elements to the mechanics of fluids and magnetism with the ANSYS Multiphysics package.
CODE-ASTER (new installation in the SVG)	CODE-ASTER is a software package for the analysis of finite elements and numerical simulation in structural mechanics.
SALOME (new installation in the SVG)	SALOME is software that approaches a genetic platform for pre- and post-pro- cessing in numerical simulation. It is based on an open and flexible architecture which is composed of reusable components that are available as open software.
OpenFOAM (new installation in the SVG)	OpenFOAM CFD Toolbox (Open Field Operation and Manipulation) permits the simulation of complex fluid flows that involve chemical reactions, turbulence, heat transfer, the dynamics of solids, and electromagnetism.
HEMCUVE (portal to Finis Terrae)	HEMCUVE is an electromagnetic user code that implements the Fast Multipole Method of parallel form.
Simulation	
AUGER (new installation in the SVG)	The Auger Observatory was designed for the detection and the study (with unprecedented quality and precision) of the cosmic energy rays that are close and above the limit of GZK, including energies of more than 1.019 eV. Within the limits of what is known today, there is no satisfactory explanation of the mechanisms of production in the universe of particles of such macroscopic energy. The Auger project is the only tool that the scientific community can offer with the objective of resolving a 30-year old astrophysical enigma.
MATHEMATICA (new installation in the SVG)	One of the most recognized mathematics software systems with thousands of original algorithms and a unified global design that can be applied to simple calculus operations and training demonstrations as well as to the development of large scale systems with high performance computing.
MATLAB (new version in the SVG)	A calculus package with multiple applications in the control of processes, the solution of equations, dynamic simulation, sign analysis, communications, etc. It permits the performance of very demanding computational tasks that necessitate much less development time than the traditional languages, such as, C, C TT, and Fortran.

Application	Task
Scientific Visualization and Animation	
NCVIEW (new version in the SVG, Superdome and HPC320)	NCVIEW is a graphic application for the representation of files with a netCDF format.
Libraries	
JASPER (new installation in the Superdome)	The JASPER Project is an open-source initiative that provides an implementation of reference for the code specified in the JPEG-2000 Part-1 (i.e., ISO/IEC 15444-1) standard.
LIBPNG (new installation in the HPC320)	LIBPNG is the official reference library for the PNG format. It practically supports all of the PNG specifications as it is extendable and has been amply tested for approximately 12 years.
ZLIB (new installation in the HPC320)	ZLIB is designed as a general library that is totally open-source and is used for the under standing of data and the use of virtually any hardware or operative system.
HDF5 (new installation in the SVG and Superdome)	HDF5 is software with a unique technology that makes possible the management of collections of data that are extremely large and complex.
Java	
JROCKIT (new installation in the SVG)	The BEA JRockit is designed for an optimal production of Java applications in large scale contexts. With it, Java developers do not need to know the internal programming of Java in order to achieve optimal production from their applications.



the science and technology network of galicia, RECETGA

The most relevant activities of RECETGA during the year 2007 are summarized below.

Network monitoring and management

The Science and Technology Network of Galicia reported a level of service availability of 99.604%. This percentage was affected in some Centres due to the non-availability of personnel during weekends. In said Centres, incidents such as cuts in electrical supply are not resolved until the next work day.

For the evolution and improvement of the network, the following activities were performed:

- » Change of the access equipment of the Hospital Xeral-Cíes in order to unify the addresses of the two hospitals, Xeral-Cíes and Meixoeiro, and to improve the management and the capacity of the first.
- » The following studies were performed with the objective of producing the plan of future investments.
 - A study of the evolution of the network and the design of the Plan of Evolution of RECETGA 2007-2013.
 - A study of the progressive substitution of ATM technology in RECETGA.



RECTEGA TECHNICAL SPECIFICATIONS

BACKBONE NETWORK

- · Based on Dark Fibre and SDH Radio Links
- · Gigabite and ATM Links
- JUNIPER M20, M10 & M10i Gigrouters
- FORE ATM SWitches

ACCESS NETWORK

- Based on Fibre Optics SDH Radio Links and other technologies such as WIFI, ISDN, ETC.
- Up to multiple Gigabit Ethernet as needed
- JUNIPER Gigarouters, FORE, CISCO and ENTERASYS Switches

NETWORK MANAGEMENT

Based Free / Libre Sofware and our own developments

CONNECTION TO RedIRIS

CESGA INTERNAL NETWORK

- Five links at 2.5 Gbps
- · Gigabit Ethernet Fast Ethernet ATM Network
- FORE ASX 200, ASX 1000 ATM Switches
- FORE ESX 4800 and 3COM
- FORE ESX 4800 AND 3COM

SERVICES AVAILABLE TO CONNECTED CENTRES

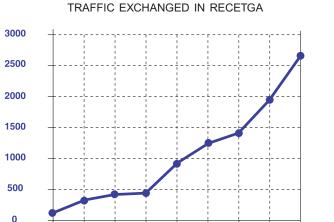
- DNS
- WEB HOSTING
- E-MAIL (with antivirus) AND ANTISPAM
- MAILING LISTS
- WEBMAIL
- USAGE STATISTICS
- FTP
- NEWS
- MIRRORS (contents of interest)
- REMOTE ACCESS SERVICES
- MULTICAST
- VIDEOCONFERENCE
- MCU / GATEWAY
- ILS
- EDUROAM
- NETWORK MANAGEMENT TOOLS
- SECURITY SERVICES (audits, incident management)

Noteworthy Projects

- » Participation in the call for projects, "A Distributed System for the Massive Synthesis of interactive TV channels using real time codification in Gpus", in collaboration with UDC.
- » Collaboration with RedIRIS in launching the test bed of the technologies of the PASITO network, a national platform of flexible testing in which 15 research centres participate.
- » Collaboration with RedIRIS in the launching of the node of the Military Unit of Emergencies (UME) in Galicia which coordinates all information relative to the prevention of catastrophes and the collaboration between public administrations within the national territory.
- » Continuation of the maintenance of the academic international roaming network, EDUROAM.
- » Integration of CESGA in the Network of Sensors of the Early Alert Centre for Virus and Information Security (CATA) of the National Institute of Communication Technologies (INTECO).

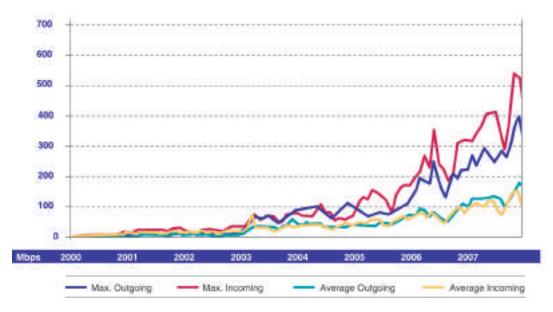
Adaptation of the infrastructures of CESGA for the housing of the Supercomputer Finis Terrae

Due to the arrival of the Finis Terrae system, CESGA had to adopt diverse measures in order to adequately accommodate the new infrastructure. These operations affected the area of communications, having to relocate the equipment within the Data Centre and to make changes in the supply of electricity.



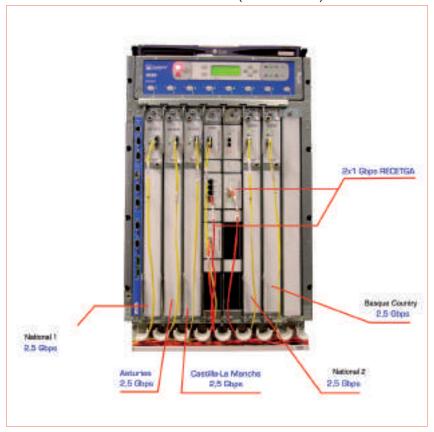
1999 2000 2001 2002 2003 2004 2005 2006 2007

RECETGA-REDIRIS EXCHANGED TRAFIC 2000-2007



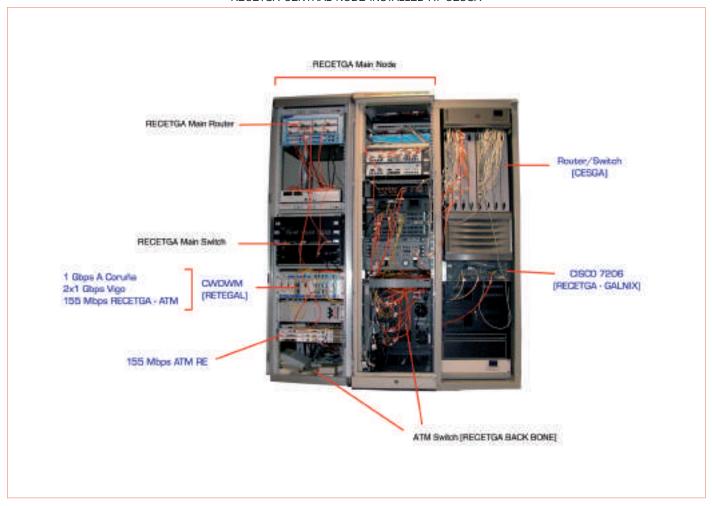
RedIRIS POP IN GALICIA (JUNIPER M40E)

EXTERNAL CONNECTIONS THROUGH



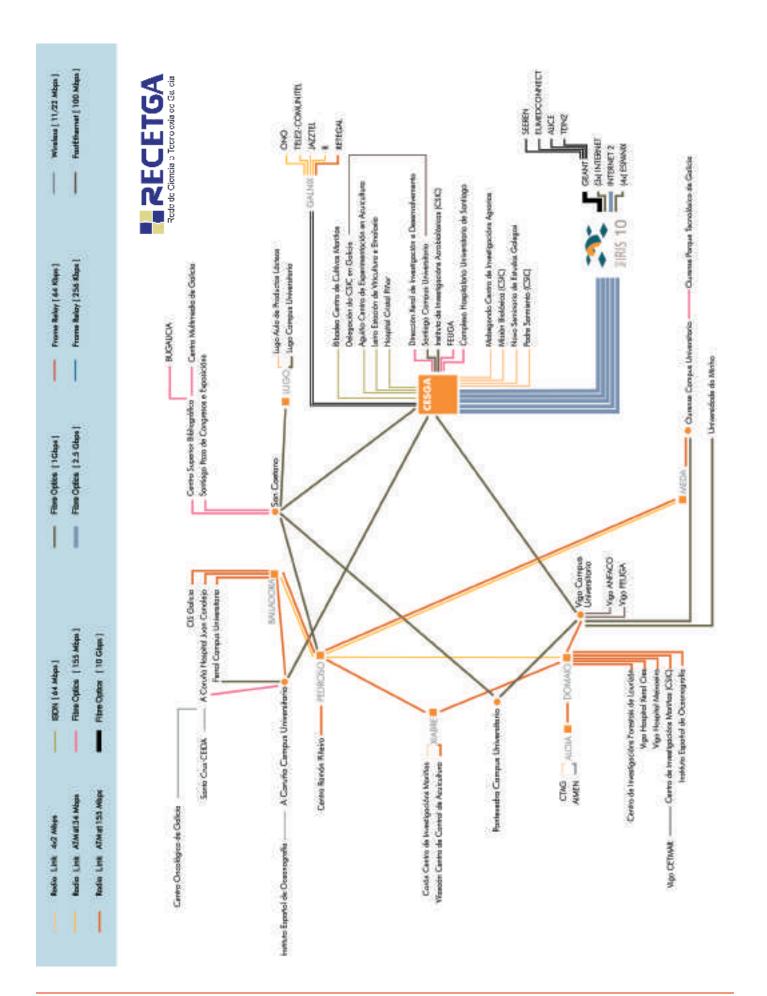


RECETGA CENTRAL NODE INSTALLED AT CESGA



centres connected to RECETGA

Centre	Link	Availability
A Coruña University Coruña Campus Ferrol Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155Mbps Fibre Optics (1Gbps) + ATM Radio Link at 155Mbps	99,986% 98,972%
Santiago de Compostela University Santiago Campus Lugo Campus	2 Fibre Optics (1Gbps) Fibre Optics (1Gbps)	99,929% 99,152%
Vigo University Vigo Campus Pontevedra Campus Ourense Campus	2 Fibre Optics (1Gbps) Fibre Optics (1Gbps) Fibre Optics (1Gbps)	99,988% 99,957% 99,984%
Minho University	Fibre Optics (155Mbps)	99,987%
BUGALICIA Consorcio de Bibliotecas Universitarias de Galicia	Fibre Optics (155Mbps)	98,945%
RTD Centres ANFACO - CECOPESCA (Vigo) Aula de Produtos Lácteos (USC - Lugo) Centro de Investigacións Forestais (Lourizán) Centro Superior Bibliográfico de Galicia Centro de Investigacións Lingüísticas "Ramón Piñeiro" Centro Tecnolóxico Armando Priegue AIMEN Estación de Viticultora e Enoloxía (Leiro) Centro de Cultivos Mariños (Ribadeo) Centro de Investigacións Agrarias de Mabegondo Centro de Investigacións Agrarias (Corón) Centro de Investigacións Mariñas (Corón) Centro de Supercomputación de Galicia Centro Tecnológico del Mar (CETMAR) Centro de Innovación e Servicios (Ferrol) Fundación Empresa - Universidade de Galicia (Vigo) Fundación Empresa - Universidade de Galicia (Santiago) CEIDA (Santa Cruz) Dirección Xeral de I+D+i Centro Tecnológico del Automóvil (CTAG) Hospitals Hospital Clínico Universitario de Santiago de Compostela Complexo Hospitalario "Xeral - Cíes" Complexo Hospitalario "Yeral - Cíes" Complexo Hospitalario Universitario "Juan Canalejo" Unidade de Investigación do Hospital do Meixoeiro Centro Oncológico de Galicia	FastEthernet (100Mbps) Radio Link 4x2 Mbps ATM Radio Link at 155 Mbps Fibre Optics (155Mbps) ATM Radio Link at 155 Mbps Radio Link 4x2 Mbps ISDN (64 Kbps) ISDN (64 Kbps) Radio Link 4x2 Mbps ATM Radio Link at 155 Mbps Radio Link 4x2 Mbps 2 Fibre Optics (16bps) Wireless (11/22 Mbps) ATM Radio Link at 155 Mbps + Wireless (11/22 Mbps) FastEthernet (100Mbps) Fibre Optics (155Mbps) Wireless (11/22 Mbps) FastEthernet (100Mbps) Fibre Optics (155Mbps) Wireless (11/22 Mbps) FastEthernet (100Mbps) FastEthernet (100Mbps) Radio Link 4x2 Mbps Fibre Optics (155Mbps) Radio Link 4x2 Mbps Fibre Optics (155Mbps) Radio Link ATM at 155 Mbps ATM Radio Link at 155 Mbps ATM Radio Link at 155 Mbps Wireless (11/22 Mbps)	99,168% 99,914% 99,997% 98,945% 99,997% 99,128% NA NA 98,936% 99,764% 99,591% 99,991% 99,916% 99,59 99,881% 99,002% 99,916%
IEO Instituto Español de Oceanografía - A Coruña Instituto Español de Oceanografía - Vigo	Wireless (11/22 Mbps) ATM Radio Link at 155 Mbps	99,916% 99,389%
CSIC Misión Biológica de Galicia Instituto de Investigaciones Agrobiológicas de Galicia Instituto de Investigaciones Marinas Instituto de Estudos Galegos "Padre Sarmiento" Delegación Institucional del CSIC en Galicia	Radio Link 4x2 Mbps Fibre Optics (1Gbps) Fibre Optics (155 Mbps) Radio Link 4x2 Mbps FastEthernet (100 Mbps)	99,403% 99,994% 98,032% 99,909% 99,997%
Other Centres Palacio de Exposicións e Congresos de Galicia Parque Tecnolóxico de Galicia Autopista Galega da Información Meteogalicia	Fibre Optics (155 Mbps) Fibre Optics (155 Mbps) Fibre Optics (155 Mbps) Fibre Optics (155 Mbps)	NA 99,731% 99,731% 99,731%
Exchange with other Networks GALNIX JAZZTEL RedIRIS RETEGAL SERGAS	2x100 Mbps 2 Mbps 5x2.5 Gbps 155 Mbps 155 Mbps	99,688% 2 Mbps 99,997% 99,731% 99,882%



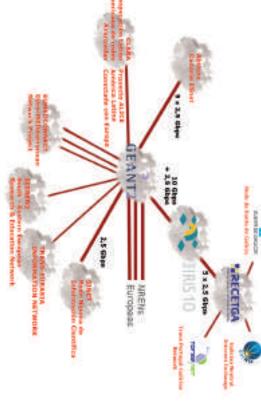
connections to research and academic networks

CONNECTIONS THROUGH GEANT

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RedIRIS TOPOLOGY

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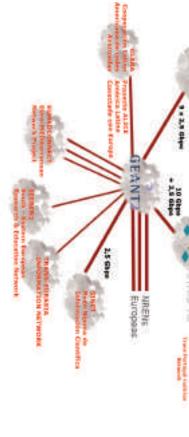
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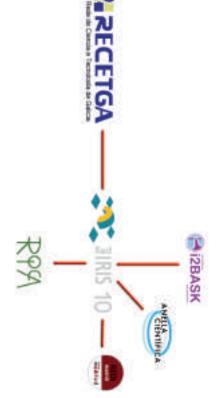
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CONNECTIONS THROUGH REGIONAL NETWORKS

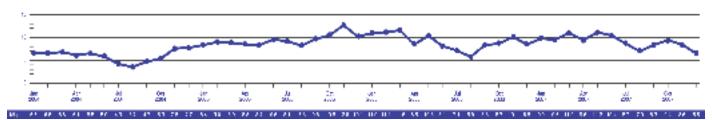


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GEANT TOPOLOGY

Galicia neutral internet exchange (GALNIX)

GALNIX MONTHLY TRAFFIC 2007



Since its creation in May of 2003, the Neutral Internet Exchange of Galicia, promoted and managed by CESGA, has locally routed the traffic that circulates in the Network of Science and Technology of Galicia (RECETGA) through the five telecommunications providers connected to it (Jazztel, ONO, R, RETEGAL, TELE2). With this activity, RECETGA facilitates the transit of information with an origin and destination within the Galician community.

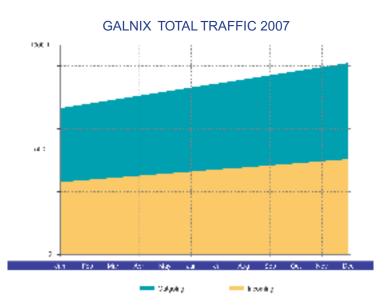
During the year 2007, GALNIX made possible the transmission of 221,249 TB of data.

May was the month of the year during which GALNIX registered the highest index of transmissions, with 11.2 Terabytes exchanged, followed by the months of March and June with 11.0 and 10.4, respectively. Nevertheless, similar activity can be appreciated in the exchange of data with indices that are very close to the monthly average (9.18 Terabytes), that only slightly decreases during the month of August, with 7.0 Terabytes exchanged.

Since its inauguration, the Galicia exchange has accumulated a total of 914,716 TB transmitted.

Since the technical and economic reasons that justified its establishment had been resolved, at the end of 200, the operators represented in GALNIX agreed in an extraordinary meeting of the Administrative Commission of December 14th 2007 that GALNIX will cease its activity at the beginning of 2008, leaving CESGA as a meeting point for the telecommunications companies.







new SMP-NUMA 2007 system



144 computing nodes:

- » 142 HP Integrity rx7640 nodes with 16 Itanium Montvale cores and 128 GB of memory each.
- » 1 HP Integrity Superdome node, with 128 Itanium Montvale cores and 1,024 GB of memory.
- » 1 HP Integrity Superdome node, with 128 Itanium 2 cores and 384 GB of memory.

A hierarchical storage system with:

- » 22 nodes for storage management with a total of 96 processing cores.
- » 390,000 GB on disk
- » 2,200,000 GB on tape (cartridge robot).

An interconnect Infiniband 4x DDR at 20 Gbps.

An external network at 10 Gbps.

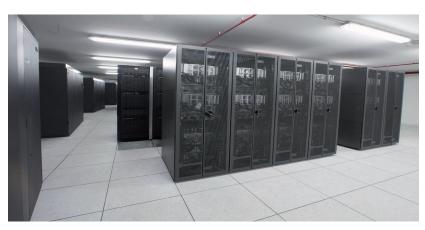
The system supports multiple operating systems concurrently as demanded by the research community, such as, Unix, Linux and Windows.

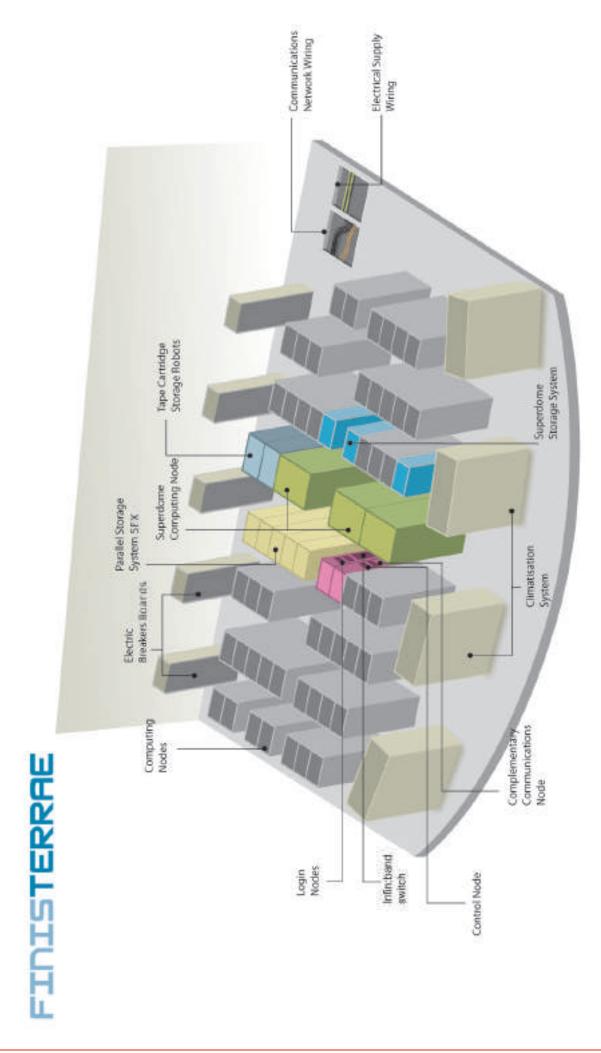
FINIS TERRAE includes open software such as, Linux, Lustre, Grid Engine, and Globus.

The system has the following compilers, libraries, and development tools: Intel C/C and Fortran, Intel MKL, Vtune, HP-MPI, and HP UPC.

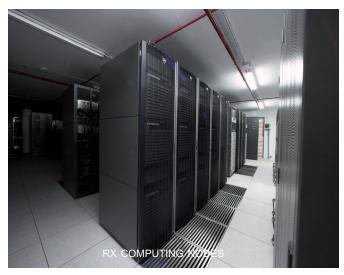
FINISTERRAE CLUS	TER SMP NUMA TECHNICAL SPECIFICATIO
COMPUTER	Integrity rx7640 / Superdome Itanium2 Cluster
APPLICATON AREAS	Computational Science Applied to: Nanotechnology, Health & Life Sciences, Ocean Sciences, Energy, HPC
MULTIPLE CONCURRENT O.S.	Unix, Linux, Windows
OPEN SOFTWARE	Linux, Lustre, Globus
COMPILERS, LIBRARIES & DEVELOPMENT TOOLS	Intel C/C++ and Fortran, Intel MKL, Vtune, HP-MPI and HP UPC
NODE INTERCONNECT	Infiniband 4x DDR at 20Gbps.
EXTERNAL NETWORK CONNECTION	10 Gbps.
PROCESSOR	Intel IA-64 Itanium2 Montvale Dual Core 1600 MHz (6,4 Gflops)
COMPUTING NODES	· 142 nodes, each with 16 cores & 128 GB memory · 1 node with 128 cores & 1.024 GB memory · 1 node with 128 cores & 8.104 GB memory · 1 node with 128 cores & 384 GB memory
PROCESSING CORES	2.528
MEMORY	19.670 GB
STORAGE NODES	22 nodes with 96 cores
HIERARCHICAL STORAGE	390.000 GB on disk & 2.200.000 GB on tape

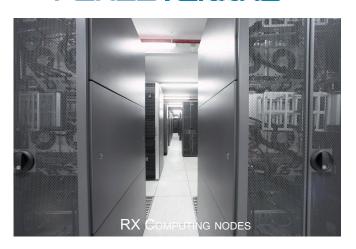


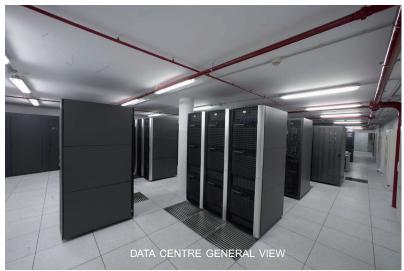




FINISTERRAE













adaptation of CESGA's facilities to house FINIS TERRAE

FINISTERRAE

During the year 2007, CESGA completed a series of renovation work in its building in order to receive the new computer with all of its technical requirements, as well as the increase of personnel scheduled to occur after the installation was accomplished. In spite of the complex apparatus and the continual nature of the work, it was attempted at all times to complete the works while creating the least possible impact on the services.

In order to support the increment in potential that the supercomputer required, a new line of 1.5 Mw was put down, 10 new electric circuit breakers as well as a 1,600 KVA transformer that is complementary to the now existing one with 180 KVA were installed. Two Systems of Uninterrupted Power Supply (UPS) of 400 KVA that complete the two now existing units of 180 KVA each were also installed.

In addition, an electricity generation group of 1,100 KVA and 8 tons of weight was installed, which meant a series of adaptations related to the fitting of the new equipment and the substitution of the previous one of 300 KVA. The new group permits all of the installation to be maintained in operation during prolonged cuts in electrical supply.

In order to dissipate the heat generated, two cooling plants of 580 KW each and 10 acclimatising units of 120 KW were also installed. Finally, a new system for the detection and extinction of fires based on HFC227 gas was installed.

The building itself suffered diverse modifications, such as the expansion from 220 m to 340 m of airconditioned technical surface space, the enlargement of the upper floor in order to accommodate new work stations, and the laborious and difficult jobs of excavation and reconstruction of exterior walls for the introduction of the power generator group and the cooling units.

EQUIPMENT	CHARACTERISTICS	
ELECTRICAL SUPPLY		
General Circuit Breaker Boards Remodeling	18 New circuit breaker boards (general distribution board, UPS distribution boards, 6 distribution boards in data centre)	
Transformer	1.600 KVA (complementing the previously existing one of 630 KWA)	
UPS	2x 400 KVA (complementing to the previous ones of 186 KVA)	
External Electrical Supply Line	1.5 Nw	
Power Generator	1.100 KVA	
CLIMATISATION		
Exterior Air Conditioners	2 x 580 KW	
In-Room Air Conditioning Units	10 units x 120 Kw	
DATA CENTER ROOM		
Technical Flooring Surface Area	From 220 m² to 340	
FIRE HAZARD CONTROL.		
Fire Datection & Extinction System	Based on HFC227 Gas	
OTHER		
Office Space Incresse	Offree Space Increased for 40 work stations	

support infrastructure

FINISTERRAE

Permanent Air-conditioning

Large computers generate an enormous amount of heat. In order to maintain optimal climatic conditions (22° and 50% of humidity), the building has two cooling units of 580 Kw each, with a total of 10 interior air-conditioning units.

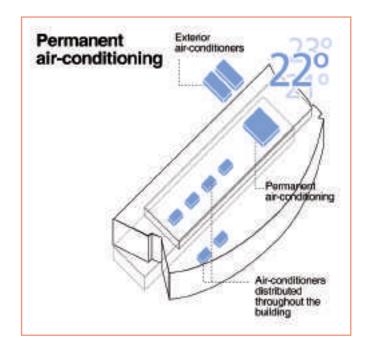
Exterior air-conditioners

Air-conditioning units room

Air-conditioners distributed throughout the building







Security - Electrical Power Supply

The Centre has a system of uninterrupted power supply (UPS) that guarantees continuity of power supply while external interruptions may exist. Additionally, a power generator assures the autonomy of the Centre indefinitely.

Transformer

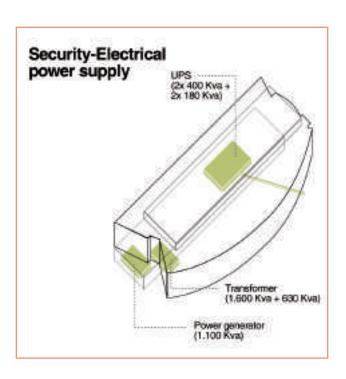
(1,600Kva+630 KVA)

Power generator (1,100 KVA)

LIDS

(2x400 KVA + 2x180 KVA)





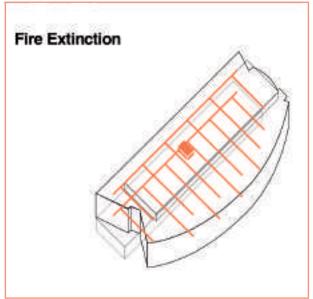
Fire Extinction

FINISTERRAE

A system of smoke detectors activates the alarm and initiates the gas (HFC227) extinction system when necessary. This gas rapidly displaces the oxygen in the rooms and impedes combustion.

UPS Extinction room Storage room Air-conditioning rooms Power generator room Electricity transformer centre (transformers)

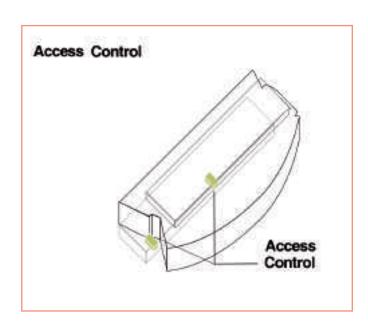


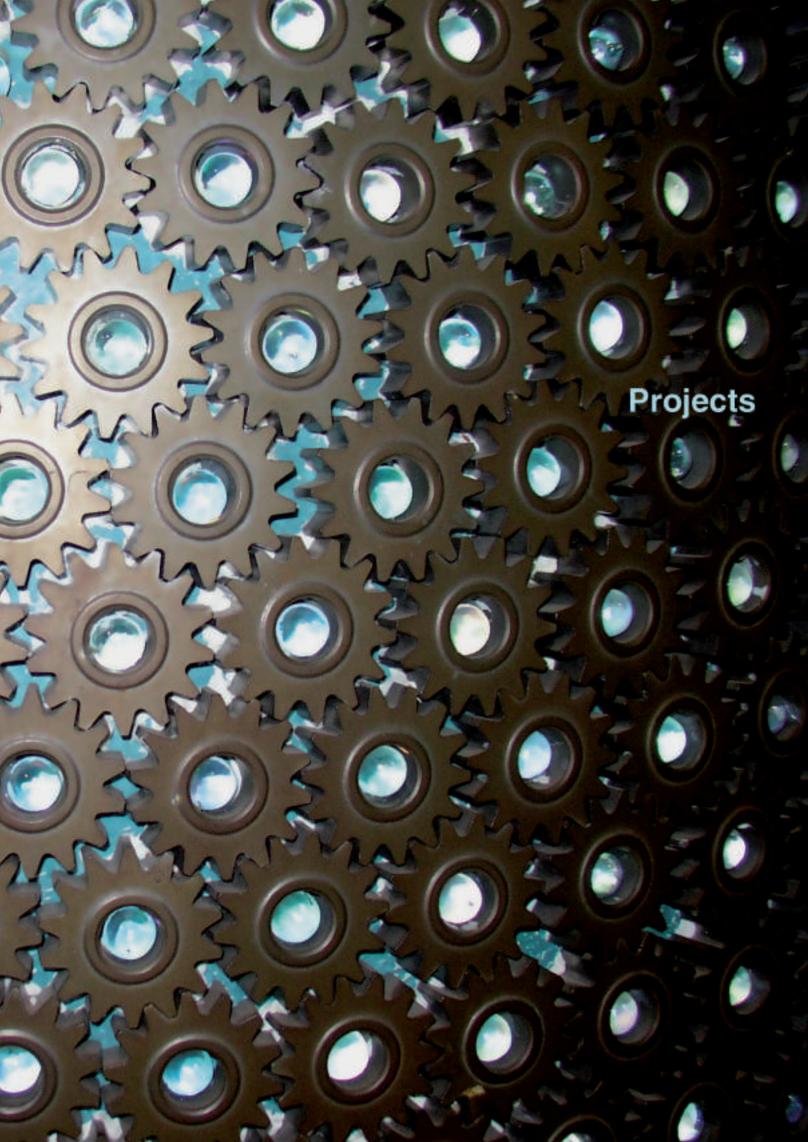


Access Control

Access to the computing and communications room is only available to authorized persons who are identified by means of an identification card and fingerprint control. All entries are recorded.







cesga foundation projects 2007

During 2007, the project activity of the CESGA Foundation was very intense and the results were notable. In all, the Foundation conducted or collaborated in more than 20 regional, national, or international project proposals. It is important to highlight the approval of two VII PM projects of the European Union and of a first project in the PROFIT program. Moreover, the index of success of resolved requests during the year was also very high (73%). All of the aforementioned was achieved while maintaining attention to the development of on-going projects, including landmarks such as EGEE, e-IMRT, or int.eu.grid. Of equal importance was the creation and the participation in regional, national, and international networks.

COMPUTING

Meteogalicia: Meteorological prediction models

Principal investigator: Ignacio López, CESGA

Funding Organism: The Director General of the Centre for

Information and Environmental Technology

Total funding: 72,121.45

Period: 2007

URL: www.meteogalicia.es

RETELAB: Virtual laboratory of the national network for oceanographic teledetection

Participants: University of Santiago de Compostela, AZTI, ICCM,

CESGA

Coordinator: José M. Cotos Yánez, USC

Principal Investigator: Ignacio López Cabido, CESGA

Funding Organism: The Ministry of Education and Science

(ESP2006-13778-CO4) Total funding: 242,726.00 CESGA funding: 114,950.00

Period: 2006-2009

Objectives: The development of a collaborative, distributed work environment that constitutes a virtual laboratory for the development of interdisciplinary research projects related to oceanographic tele-detection.

Ingenio Mathematica

Participants: UAL; UCA, UGR, UMA, UHU, UJaén, US, UNIOVI, UNIZAR, UIB, ULL, ULPGC, UCLM, UNILEON, UBU, USAL, UVA, ICREA (IB, UAB, UDL, UDG, UPC), UNEX, USC, UDC, UVigo, UPV/EHU, UAH, UC3M, UCM, UNED, UPM, URJC, UM, UNavarra, Unirioja, UA, UJI, UMH, UPV, UV, CSIC, INIA and CESGA (In total, more than 200 research groups in all of Spain.)

Coordinator: Enrique Zuazua, The Autonomous University of

Madrid

Principal Investigator: Andrés Gómez Tato, CESGA

Funding Organism: The Ministry of Education and Science

(CSD2006-00032) Funding: 7,500,000.00 Period: 2006-2011 URL: www.i-math.org

Objectives: "Proyecto Ingenio-Consolider" is designed to increment both quantitatively and qualitatively, the presence of Mathematics in science, technology, and research.

Formiga2007. Taking advantage of the continuous use of computer equipment by means of the integration and gridification of rooms

Principal Investigator: Ignacio López Cabido, CESGA

Funding Organism: Director General for RTD, the Regional

Government of Galicia Total funding: 184,621.00 CESGA funding: 104,121.00

Period: 2007-2009

Objectives: The project will integrate all of the available resources in the computer classrooms of the Galician universities employing GRID technology in order to facilitate their use by researchers for the solution of scientific problems.

g-Fluxo. A workflow tool in distributed environments: application to computational chemistry.

Participants: CESGA

Principal Investigator: Javier López Cacheiro, CESGA

Funding Organism: Directorate General for RTD. The Regional

Government of Galicia Total funding: 49,220.00 CESGA funding: 49,220.00

Period: 2007-2009

Objectives: The development of a workflow tool for distributed computation that permits the use of different applications and the computational resources that exist in CESGA or that are accessible by way of GRID as a unique environment.

IFEC. Qualified electronic signature infrastructure.

Participants: Aldaba Professional Services, Alaba Solutions and

Projects SL, University of Vigo, CESGA

Coordinator: José Antonio Castelao Boo, Aldaba Principal Investigator: Andrés Gómez Tato, CESGA

Funding Organism: Centre for the Technological and Industrial

Development, the Government of Galicia

Total funding: 263,067.60 CESGA funding: 19,978.70

Period: 2007-2008

Objectives: The study, design, and development of a qualified electronic signature infrastructure based in the infrastructure technology for the management of privileges (PMI) and an authority for the development of time (TSA) that, using existing free software, permits the easy inclusion of applications that require the control of authorisation as well as in the environment of the corporate management of authorisations.

EGEE II. Enabling Grids for EsciencE II

Participants: More than 100 institutions of Europe, Asia, and

America

Coordinator: Robert Jones, CERN

Principal Investigator: Ignacio López Cabido, CESGA

Funding Organism: European Union-VI Frame Program, the Go-

vernment of Galicia

Total funding: 36,971,360.00 CESGA funding: 182,530.00

Period: 2005-2008 URL: www.eu-egee.org

Objectives: The second phase of the establishment of a world-level GRID infrastructure that is available for researchers and businesses 24 hours a day. The objective is to give researchers

access to important computational resources independent of their geographical location.

Int.eu.grid. Interactive European Grid

Participants: IFCA, LIP (Portugal), Poznanskie Centrum Uperkomputerowo Sieciowe (Poland), Forschungszentrum Karlsruhe (Germany), UAB, CYFRONET AGH (Poland), GUP Linz (Austria), Trinity Collage (Ireland), II SAS (Slovakia), ICM

(Poland), BIFI (Spain), HLRS (Germany), and CESGA.

Coordinator: CSIC-IFCA

Principal Investigator: Carlos Fernández Sanchez, CESGA Funding Organism: European Union-VI Frame Program

Total funding: 1,986,000.00 CESGA funding: 114.000,00

Period: 2006-2008

URL: www.interactive-grid.eu

Objectives: The launching, maintenance, and operation of a quality GRID e-infrastructure in order to provide service to the communities of researchers with interactive applications that have a high computing demand.

e-IMRT

Participants: USC, UVigo, U. Wisconsin, CESGA Coordinator: Andrés Gomez Tato, CESGA

Principal Investigator: Andrés Gómez Tato, CESGA

Funding Organism: The Directorate General for RDT, The

Government of Galicia Total funding: 158.775,00 CESGA funding: 38.775,00

Period: 2005-2008

Objectives: The development of a distributed computational platform with access via web services for the optimised computation of radio-therapeutic treatments with accelerators and

their verification by means of simulation URL: http://eimrt.cesga.es

Folstein

Participants: UDC, UVigo, Televés, and CESGA Coordinator: Andrés Gómez Tato, CESGA

Principal Investigator: Andrés Gómez Tato, CESGA

Funding Organism: The Director General for RTD. The

Government of Galicia (PGIDIT05TIC00101CT)

Total funding: 280.352,00 CESGA funding: 49.500,00

Period: 2005-2008

 $\label{lem:condition} Objectives: The \ development \ of \ a \ \ platform \ for \ geriatric \ attention$

at home.

Partículas III

Participants: USC, CESGA

Coordinator: Juan José Saborido Silva, USC

Principal Investigator: Carlos Fernández Sanchez, CESGA Funding Organism: Ministry of Education and Science

Total funding: 174.500,00 CESGA funding: 11.550,6

Period: 2005-2007

Objectives: The launching of a GRID infrastructure for the LHCb

experiment of CERN.

Partículas IV

Participants: USC, CESGA

Coordinator: Juan José Saborido Silva, USC

Principal Investigator: Carlos Fernández Sanchez, CESGA Funding Organism: Ministry of Education and Science

Total funding: 305.525,01 CESGA funding: 13.797,00

Period: 2006-2010

Objectives: The launching of a GRID infrastructure for the LHCb

experiment of CERN.

COMMUNICATIONS NETWORKS

"Opera Oberta" (Open Opera)

Participants: USC, Uvigo, UDC, Uminho, and CESGA

Coordinator: Liceu of Barcelona

Principal Investigator: Ministry of Education and Science

Period: Indefinite

Objectives: The direct retransmission of operas from the Liceu of Barcelona to the participating universities in order to be utilized as teaching resources.

URL: www.opera-oberta.org

GALNIX. Galician Neutral Internet Exchange

Participant: AGI, CESGA

Principal Investigator: J. García Tobío, CESGA

Funding Organisms: The Regional Government of Galicia,

Comunitel, Jazztel, R, (ONO) and RETEGAL

Period: 2002-2007

Objectives: The maintenance of the neutral point of Internet traffic exchange in Galicia, galNIX.

Distributed system for the massive synthesis of interactive television channels using real time coding in Gpus

Participants: UDC, CESGA

Coordinator: Victor Manuel Gulías Fernández, UDC Principal Investigator: Ignacio López Cabido, CESGA

Funding Organism: The Directorate General for RTD. The

Government of Galicia (PGIDIT07TIC005105PR).

Funding: 96.002,00 Period: 2007-2010

Objectives: The utilisation of the processing capacities of graphic cards in order to codify multiple streams of video for

their retransmission in the network.

PASITO

Participants: CESCA, CICA, EHU, I2BASK, I2CAT, IMDEA, UAM, UC3M, UGR, UMU, UPC, UPM, UPV, UVIGO, RedIRIS

Coordinator: RedIRIS

Principal Investigator: Ignacio López, CESGA

Funding Organism: Ministry of Industry, Tourism, and

Commerce

Total funding: 705.000,00 Period: 2008 – 2009

Objectives: The launching of a national communications network

for the testing of new services.

THEMATIC NETWORKS & TECHOLOGICAL PLATFORMS

Name: e-Science of Spain

Coordinator: Vicente Hernández, The Polytechnic University of

Valencia

Finance: Ministry of Education and Science

Members: 68 groups and almost 700 researchers in the areas of applications, middleware, and GRID infrastructure and high performance computing in Spain.

URL: www.e-ciencia.es

Objectives: The national network of e-Science continues to coordinate and promote the development of scientific activity in Spain by means of the collaborative use of geographically distributed resources that are connected via Internet.

Acronym: CyTED-Grid

Name: CyTED-Grid. GRID technology as the regional engine of development.

Coordinator: Francisco Tirado Fernández. Universidad Complutense de Madrid U.C.M, Spain

Members: 21 Universities of Argentina, Spain, Venezuela, Portugal, Colombia, Chile, Paraguay, Uruguay, Brasil, Peru and Mexico

URL: www.cytedgrid.org

Objectives: The creation of a human and technological infrastructure among diverse Latin American groups who are potential users of GRID technology and who are dedicated to the field of computation and have experience in the area of scientific applications. The construction of a GRID network as a support for different applications to analyse to what point the available solutions are valid and the proposal of new developments that will provide the necessary functionality.

Acronym: CAPAP-H

Name: Network of High Performance Computing of Heterogeneous Parallel Architectures

Coordinator: Enrique S. Quintana Ortiz, Universidad Jaume I

Funding: Ministry of Education and Science

Members: 16 research groups of diverse Spanish universities

and CESGA

Acronym: RED-GHPC

Name: Galician Network of High Performance Computing

Coordinator: Ramón Doallo Biempica

Funding:

Members: Computer Architecture (GAC-UDC), Computer Architectures (GAC-USC), the Systems Laboratory (LDS-USC), Numerical Resolution of partially derived equations and numerical simulation in Engineering (MAP-USC), Numerical Models and Methods in Engineering and Applied Sciences (MAP-UDC), the Centre for Environmental Research and Information (CINAM), Integrated Engineering (ING-UDC), Theoretical and Computational Chemistry (QTC-USC), Antennas (ANT-UVI), Non-linear Physics (FNL-USC), the Centre of High Performance Computing (CESGA).

Acronym: I-Math

Name: MATHEMATICA CONSULTING & COMPUTING DE GALICIA

Funding: Director General for the Promotion of Science and Technology in the Galician University System, The Government of Galicia.

Members: Statistical Modeling and Applications (code USC: GI-1914), the Numerical Resolution of Partially Derived Equations and Numerical Simulation in Engineering (code USC: GI-1563), Mathematical Models and Numerical Simulation in Solid Mechanics (code USC: GI-1564), Modeling of Hydrodynamic Flows (code USC: GI-1566), Computer Architecture (code USC: GI-1638), the Differential Equations and Numerical Simulation Group (code UVIGO: MA1), Optimisation, Control and Numerical Modelling (code UVIGO: MA8), Statistical Inference (code UVIGO: IO1), Numerical Models and Methods in Engineering and Applied Sciences (code UDC: G000272), Modeling and Inferential Statistics, MODES, Computer Architecture (code UDC: G000265), CESGA.

Members: Biofarma-USC, the Centre of High -Performance Computing of Galicia (CESGA), the Complex Systems Research Group-USC, the Population Genetics and Cyto-Genetic-UVI Group, Imedir-RNAsa- UDC, Mathbioinfo-USC, Genomic Medicine-USC.

URL: http://mathematica.nodo.cesga.es

Acronym: RGB

Name: The Galician Network of Bio-information

Coordinator: Alejandro Pazos Sierra, Rnasa-IMEDIR, UDC Funding: Director General for the Promotion of Science and Technology in the Galician University System, the Government

of Galicia

Members: Genomic Medicine-USC, the Population Genetics and Cyto-Genetics Group-UVIGO, the Complex Systems Research Group-USC, the Bio-pharmacy Group-USC, the MathBioinfo Group-USC, Rnasa-IMEDIR Group-UDC, CESGA.

URL: http://rgb.cesga.es

Objectives: The structuring and integration of research and teaching activities in Bio-information that are performed in Galicia.

Acronym: GRIDCHEM

Name: Grid Computing in Chemistry

Funding: COST

Members: Entities of 18 European countries URL: http://www.cost.esf.org/index.php?id=1119

Objectives: The enabling and the acceleration of the transition of researchers to the infrastructure of computational science of the 21st century that will make European computational chemistry more competitive.

Acronym: INES

Name: Spanish Initiative for Software and Services

Coordination: INES is a platform that is open to any legal Spanish entity with interest and experience in software and service technologies.

Financing: Ministery of Industry, Tourism, and Commerce

Members: 136 Spanish businesses and institutions (TIC businesses, large business, SMEs or businesses associations, *Public Research Organisms and Technological Centres - TIC* (Universities, Research Centres and Public Institutions) and *industrial users*

URL: www.ines.org.es

Objectives: To define a strategic research program adapted to Spanish necessities and capacities that include the proposals of singular, strategic scientific-technological projects, such as tagging projects of high priority, with medium and long-term objectives.

Acronym: eMOV

Name: Spanish Platform of Wireless Communications Coordination: This was a 2005 initiative of the industrial sector, supported by the Ministry of Industry, Tourism, and Commerce, the Ministry of Education and Science, and the CDTI. It has a European technological platform of reference, eMOBILITY (the Mobile and Wireless Communications Technology Platform).

Financing: Ministry of Industry, Tourism, and Commerce, Ministry of Education and Science, and the CDTI

Members: 136 Spanish organisations

URL: www.aetic.es/emov

Objectives: The objective of the Spanish Platform of Wireless Communications (eMOV) is to contribute to the strengthening of the agents that play a part in the development of mobile and wireless systems and services. In the end, this should have the effect of improving the economic position of the sector in terms of the creation of employment and the generation of wealth as well as that of the impact that the adoption of these types of systems and services have on other sectors and on the Spanish society in general in terms of productivity and well-being.

S.A.X. cesga projects 2007

The activity of SAX CESGA during 2007 was unmatched in some departments. It is important to highlight the approval of the first projects financed by the Ministry of Education and Science in the area of Promotion and Communication, the successful completion of the first phase of the "Mancomún" project, and the activity in international projects of the department of electronic learning. On the other hand, the GIS department has evolved more discretely. Highlights include the presentation of a project with more than 10 Galician business participants to guarantee the quality of software (VG-CMMI-SPICE) and the CAPITA project; both are of great strategic importance.

Objectives: The development of a Geographic Information System for the study of possible areas of impact related to environmental risks.

GIS-SIFI

Participants: CIS Madera, CESGA

Coordinator: Xosé Francisco Pedras Saavedra, CIS Madera Principal Investigator: Francisco Landeira Vega, CESGA Funding Organism: The General Administration of RDI, the

regional Government of Galicia Total funding: 100.000,00 CESGA funding: 28.750,00

Period: 2005-2009

Objective: A map of the industrial forest sector of Galicia

GEOGRAHIC INFORMATION SYSTEMS AREA (GIS)

GIS-patrim07

Participants: General Administration of Patrimony, CESGA

Coordinator: Francisco Landeira, CESGA

Principal Investigator: Francisco Landeira, CESGA

Funding Organism: the General Administration of Patrimony,

The regional Government of Galicia

Total funding: 10.930,00 CESGA funding: 10.930,00

Period: 2007

Objectives: The development of tools and technical assistance for GIS material at the Archaeological Services of the General Administration of Patrimony.

GIS-Environmental Risks

Participants: CIS Design and Technology-USC, Escuela

Politécnica Superior de Lugo, CESGA

Coordinator: Juan Aneiros, CIS

Principal Investigator: F. Landeira Vega, CESGA

Funding Organism: the General Administration of RDI, the

regional Government of Galicia Total funding: 345.609,00

CESGA funding: 51.260,00

Period: 2005-2007

E-LEARNING

Aula Molina

Participants: USC, Universidad de La Molina (Perú), CESGA Coordinator: María José Rodríguez Malmierca, CESGA Principal Investigator: Javier García Tobío, CESGA

Funding Organism: Director General for Exterior Cooperation,

the Regional Government of Galicia

Total funding 93.852,00 CESGA funding: 60.000,00

Period: 2006-2007

Objectives: The pilot analysis, implementation, and evaluation of an e-learning model at the National Agrarian University of La Molina by means of open code tools in order to support access to the formation of collectives with limited possibilities for participation in on-site training.

e-Hospital. E-learning opportunities for adult patients during hospitalization in health care institutions

Participants: Die Berater (Austria), Danube University Krems (Austria), ORT (France), Training Centre of the Saxonian Economy (Germany), Academy of Humanities and Economics (Poland), USC, CESGA

Coordinator: Holger Bienzle, Die Berater

Principal Investigator: María J. Rodríguez Malmierca, CESGA Funding Organism: the European Commission: Socrates-

Grundtvig Program Total funding: 416.498,00 CESGA funding: 42.415,00

Period: 2005-2008

Objectives: The analysis of the application of e-learning techniques to hospitalised adults during long periods of time and the production of manuals and tools for teachers who work in this context.

EFELCREN. Flexible and creative educational environments

Participants: USC, Trinity College (Ireland), Centre of Information Technology (Lithuania), Ca'Foscarti University of Venice (Italy), Haslev Seminarium (Denmark), Euneos Corporation (Finland), CESGA

Coordinator: Beatriz Cebreiro López, USC

Principal Investigator: María J. Rodríguez Malmierca, CESGA Funding Organism: the European Commission: Socrates-

Comenius Program Total funding: 449.754,00 CESGA funding: 54.625,00

Period: 2005-2008

Objectives: The analysis and development of training proposals for flexible and creative educational contexts in primary and secondary education by means of the use of new information technologies and the identification of new teaching strategies. The project also takes into consideration the creation and the availability of these e-learning materials to teachers.

IEPTL. Integrating European Projects into Teaching and Learning

Participants: USC, CESGA

Coordinator: Beatriz Cebreiro López y Carmen Fernández

Morante, USC

Principal Investigator: María J. Rodríguez Malmierca, CESGA Funding Organism: the European Commission: Socrates-

Comenius Program
Total funding: 98.498,00

CESGA funding: 9.660,00

Period: 2006-2007

Objectives: The identification of best practices and the demonstration of the impact of the Socrates programs in education.

e-Intervention. The study and analysis of the impact of new technologies utilisation applied to the assistance of handicapped persons and their families: quality of life and self-management

Participants: UDC, CESGA

Coordinator: Mª José Rodríguez Malmierca, CESGA

Principal Investigator: Mª José Rodríguez Malmierca, CESGA Funding Organism: Director General for RTD, the regional

Government of Galicia Total funding: 120.000,00 CESGA funding: 70.000,00

Period: 2006-2009

Objectives: The study and analysis of the impact of the use of new information technologies as applied to attending to handicapped persons and their families.

SUMA

Participants: Eleven Spanish businesses in the sector and three

Spanish universities

Coordinator: Pedro Artiga Calvo, Tecsidel S.A.

Principal Investigator: Mª José Rodríguez Malmierca, CESGA Funding Organism: Ministry of Industry, Tourism, and Commerce:

Plan Avanza

Total funding: 1.417.164,00 CESGA funding: 13.313,00

Period: 2007

Objectives: A strategic project of the e-learning work group of the INES technological platform that is dedicated to the integration of e-learning services based on standards.

T-Maestro. Multimedia Adaptive Educational System based on Reassembling TV Objects.

Participants: UVIGO, CESGA

Coordinator: Mª José Rodríguez Malmierca, CESGA

Principal Investigator: Mª José Rodríguez Malmierca, CESGA

Funding Organism: Director General for RTD, the regional

Government of Galicia Total funding: 182.804,00 CESGA funding: 108.054,00

Period: 2007-2010

Objectives: An intelligent tutor for the creation of personalised and adaptable learning contents in T-learning and M-learning

about MHP and DVB-H.

Parents

Participants: Academy of Management (Poland), University of Oradea (Rumania), Die Berater (Austria), Training 2000 (Italy),

Associació Baobab (Spain) and CESGA Coordinator: Academy of Management (Poland)

Principal Investigator: Mª José Rodríguez Malmierca, CESGA Funding Organism: the European Commission: Socrates-

Leonardo Program Total funding: 298.530,00 CESGA funding: 39.681,00 Period: 2007 – 2009

Objectives: The application of a specific TIC methodology and tools in order to provide support to parents in their role as guides regarding the work and the studies of their children.

YES

Participants: Die Berater (Austria), Local Mission Agenais and Albret (France), Glotta Nova (Slovenia), Further Training Centre for the Saxon Economy (Germany), Transfer (Slovakia), Reflexion Foundation (Holland), Meter Silesia (Czech Republic) and CESGA.

Coordinator: Die Berater

Principal Investigator: Mª José Rodríguez Malmierca, CESGA Funding Organism: the European Commission: the Socrates-

Leonardo Program
Total funding: 393.739,00
CESGA funding: 29.248,00
Period: 2007 – 2009

Objectives: The design and distribution of a support system based on TIC as well as specific e-learning training to SMEs in

order to try to improve the incorporation of youth who have not completed their studies into positions of employment. This will include the analysis and evaluation of e-learning models as well as the adaptation of the TIC to this context.

RedLeche

Participants: USC, FEPALE, andy CESGA Coordinator: Juan Mendez Dónega, USC

Principal Investigator: Mª José Rodríguez Malmierca, CESGA Funding Organism: Director General for Exterior Cooperation,

the regional Government of Galicia

Total funding: 167.874,00 CESGA funding: 5.514,00 Period: 2007 – 2008

Objectives: On-line training for the Latin American milk industry in the web.

INFORMATION SOCIETY

ICHNOS. Innovation and change. Network of one-stop shops

Participants: Ancitel Sardegna (Italy), The Vysocina Region (the

Chech Republic), CESGA

Coordinator: J Deckmyn, Ancitel Sardegna Principal Investigator: Ramón Basanta

Funding Organism: the European Union - INTERREG IIIC

Program

Total funding: 1.108.670,00 CESGA funding: 406.000,00

Period: 2005-2007

Objectives: The initiation of windows and unique points of biness access with the premise that, in many regions, they will represent a key tool for the promotion of local development.

CIC-Commerce

Participants: the Foundation for the Promotion of Industrial Quality and Technological Development in Galicia, IDITE Minho,

EGANET, CESGA, and 10 small- and medium-size Spanish and

Portuguese businesses.

Coordinator: Juan José Gómez Romero Principal Investigator: Ramón Basanta, CESGA

Funding Organism: Director General for RTD, the regional

Government of Galicia, and the European Union: Spanish-

Portuguese INTERREG IIA Program

Total funding: 1.000.000,00 CESGA funding: 150.000,00

Period: 2004-2007

Objectives: The articulation of activities dedicated to the raising of awareness inmicro-SMEs in Galicia and the north of Portugal that are facing processes of innovation. The goal is to present the information in a way that proves to them that the incorporation of new technologies implies the advancement and optimisation of management processes. Other objectives include the creation of a communication channel between the participating businesses in order to establish contact with manufacturers, points of sale, professional and the Administration, and the creation of a B2B platform of concrete services between businesses.

FREE/ LIBRE SOFTWARE

Mancomun.org, Galician Initiative for Free/Libre Software

Participants: UDC, USC, UVigo, EGANET, IGALIA, Alfa21,

CESGA and 10 other institutions Coordinator: Ramón Basanta, CESGA

Principal Investigator: Javier García Tobío, CESGA

Funding Organism: Directorate General for Industrial Promotion and the Information Society, the Regional Government of

Galicia

Funding: 1.172.000,00 CESGA funding: 1.172.000,00

Period: 2005 - 2007

Objectives: The promotion of free software in Galicia with the launching of Mancomun.org, a meeting point of the different initiatives concerning free software that are developed in different contexts (business, educational, volunteer).

CoopTIC

Participants: The Galician Association of Agrarian Cooperati-

ves, Computer-3

Coordinator: Computer-3 S.L.

Principal Investigator: Ramón Basanta, CESGA

Funding Organism: Directorate General for RTD, the regional

Government of Galicia Total funding: 117.701,00 CESGA funding: 20.650,00

Period: 2006 - 2009

Objectives: To conduct an investigation that will determine the optimum design of the architecture of a system that permits the tracing of origin for agricultural and market garden cooperatives.

VG-CMMI-SPICE

Participants: CESGA, SUMMA, Servicios de Ingeniería y Consultores, S.A., Brújula Telecom, S.A., AT4.Net Internet and Comunicación, S.L., ALTIA Consultores, S.L., BAHIA Software, S.L., IGALIA, S.L., ALDABA Servicios Profesionales, LAMBDASTREAM, S.L., SATDATA Telecom, S.L., 2MARES DEMIL, S.L., SHYLEX Telecomunicaciones, S.L., OPTARE Solutions, S.L., Factoría de Software e Multimedia, S.L.

Coordinator: Ramón Basanta, CESGA

Principal Investigator: Ramón Basanta, CESGA

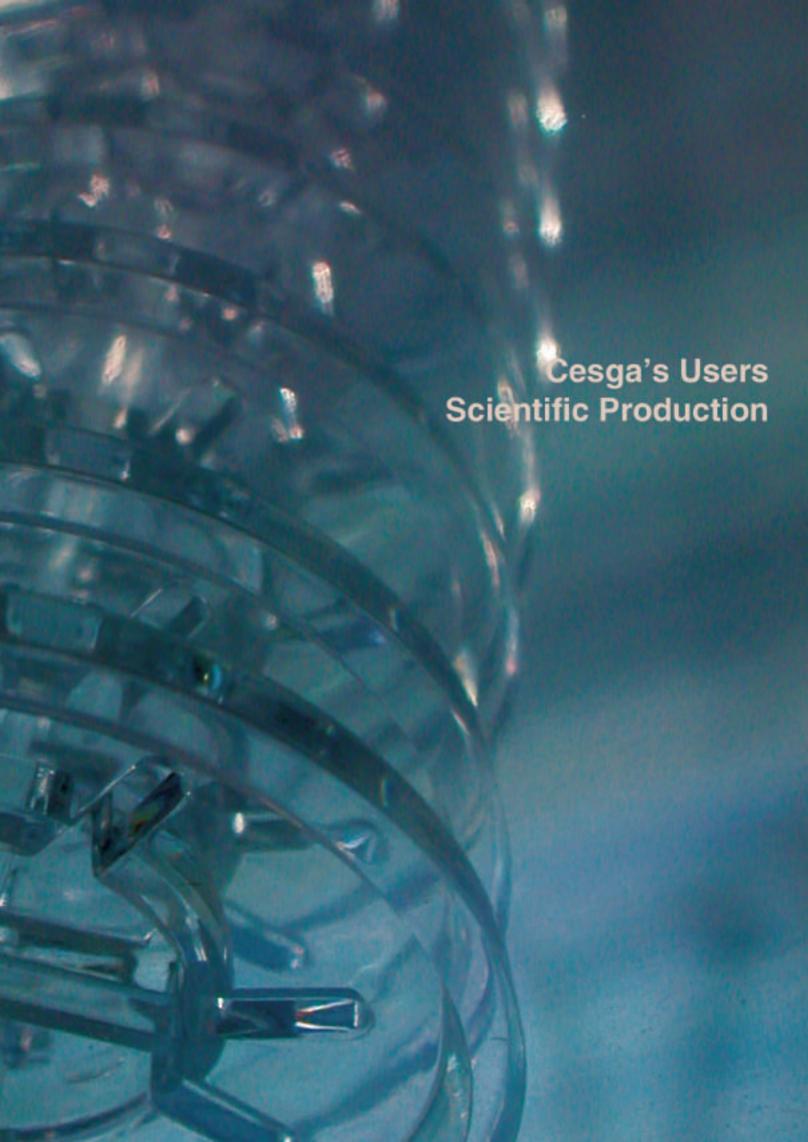
Funding Organism: Ministry of Industry, Tourism, and

Commerce

Total funding: 670.754 ,00 CESGA funding: 62.802,00

Period: 2007 - 2009

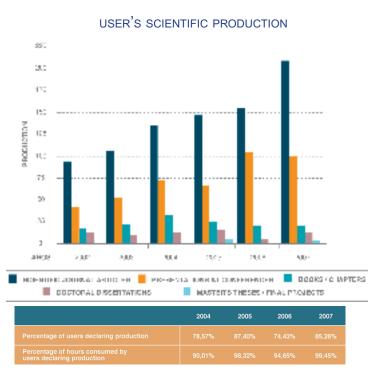
Objectives: Strategic associative activity regarding the orientation to technological excellence in the development of software by means of the establishment of models of quality certification (CMMI, SPICE).



scientific production reported by CESGA's users

This year it is important to emphasize the increment in the number of scientific articles declared (close to 30%). The increase in this number can be partially explained by the change in the methodology of measurement. This is the first time that publications were requested from user that, although they did not make use of the supercomputers in 2007, they did make use of them in 2006 and they were preparing, or were at the point of presenting, a publication not yet presented or "in press".

On the other hand, there was a small decrease in the number of presentations reported to congresses, while, in accordance with information provided by the users themselves, they maintained the rhythm of doctoral theses, presented an defended. In summary, the entrance into production of the Supermode in 2004 and the permanent updating of the SVG in computing capacity has been fruitful in terms of the scientific production of the users, doubling the publication of sicentific articles in the last 5 years from 107 in 2003 to 208 in 2007. the good results obtained in such a short period of time demonstrate the necessity for a supercomputing infrastructure with permanent updating capacity



DISTRIBUTION OF SCIENTIFIC PRODUCTION PER YEAR

PRODUCT	2002	2003	2004	2005	2006	2007
SCIENTIFIC ARTICLES	93	107	134*	147	154	208
ACCEPTED	4	8	20	16	26	19
SUBMITTED	16	29	26	27	23	24
PUBLISHED	73	70	91	104	105	165
NTATIONS IN CONFERENCES	42	52	72*	65	105	101
PRESENTATIONS	33	40	53	37	53	46
POSTERS	9	12	35	28	52	47
DOCTORAL THESES	17	21	32	24	18	18
DEFENDED	9	4	5	9	10	11
PRESENTED	0	0	0	0	3	5
IN PROCESS	8	17	27	15	5	2
MASTERS THESES GRADUATE PROJECTS	12		12	14		10
DEFENDED	6	4	5	13	3	8
IN PROCESS	6	5	7	1	2	2
BOOKS / CHAPTERS	NA	NA	NA			
ACCEPTED / IN PRESS	NA	NA	NA	4	1	1
SUBMITTED	NA	NA	NA	1	0	2
PUBLISHED	NA	NA	NA	0	3	0
TOTAL	169	194	256	260	301	351

DISTRIBUTION OF SCIENTIFIC PRODUCTION DECLARED

					2
SCIENTIFIC ARTICLES	ଚତ	28	63	51	208
A11111111	co	m	7	4	49
SUBMITTED	11	5	4	4	74
PUBLISHED	33	ผ	궑	43	Ð
PRESENTATIONS IN CONFERENCES	36	10	96	19	101
1981 SENTATIONS	N	7	O).	63	45
FOSTERS	14	3	19	11	47
INPREPARATION	-		7		
DOCTORAL THESES	4	4		9	18
DILBOTT	1	n	4	м	#
PRESENTED	2	1	2		ю
IN PROCESS	-		÷		N
MASTERSTHESES/ GRADUATE PROJECTS	-	2	6	4	10
D-I ENDED	-	5	۲	4	8
IN PROJECT 835			2		R
BOOKS / CHAPITHS	F			2	es
ACCEPTED	1				1
PUBLISHED				N	N
OTHERS	-		10		7
SUDMITTED			1		
PUB_ISHED			O		
IN TRUCK BEE	-				
TOTAL	109	44	119	62	351

scientific production reported by CESGA's users

SPANISH NATIONAL RESEARCH COUNCIL (CSIC)



Scientific Articles Published

FDayou; M.I.Hernández; J.Campos Martinez and R. Hernández Lamoneda. 1-Spin-orbit coupling in O2(v)+O2 collisions. II. Quantum scattering calculations on dimer states involving the X 3Sg+, a 1Dg, and b1Sb+ states of O2 Journal of Chemical Physics. 126. 194309. 2007

M.Villa; M.L.Senent and R.Dominguez-Gómez. ZPVE correction to the FIR Spectrum to the propanal isotopomers, Chemical Physics Letters. 436. 15-18. 2007.

B.García; S.Gonzalez; F.J.Hoyuelos; S.Ibeas; J.M.Leal; M.L.Senent; T.Biver; F.Secco and M.Venturin. Thermodynamics and kinetics of the Nickel II- Salicylhydroxamic Acid system. Phenol rotation induced by metal ion binding. Inorganic Chemistry. 46. 3680-3687. 2007.

A.Spielfiedel; N.Feautrier; C.Balanca; F.Dayou, F.Lique and M.L.Senent. 3) Molecules as Diagnostic Tools in the Interstellar Medium. Molecular Physics. 105 (9). 1263-1269. 2007.

FLique; M.L.Senent; A.Spielfiedel and N.Feautrier. 4) Rotationally inelastic collisions of SO (X3 -) with H2: potential energy surface and first results with para-H2. Journal of Chemical Physics. 126. 164312. 2007.

H. Massó; V. Veryazov; P. Malmqvist; B.O. Roos and M.L.Senent. 5) Ab initio characterization of the C5. Journal of Chemical Physics. 127 (15). 154318. 2007.

B.García; F.Secco; S.Ibeas; A. Muñoz; F. J. Hoyuelos; J.M. Lea;, M.L. Senent and M.Venturini. 6) Structural NMR and ab initio study of Salicylhydroxamic and p-Hydroxybenzohydroxamic acids: Evidence for an extended aggregation. Journal of Organic Chemistry. 72 (21). 7832-7840. 2007.

M.L.Senent H. Massó and M.Hochlaf. 7) An harmonic spectroscopic study of the ground electronic state of various C4 radical isotopomers, The Astrophysical Journal. 670. 1510. 2007.

Rivera-Calzada; Spagnolo L; Pearl LH; Llorca O. Structural model of full-length human Ku70-Ku80 heterodimer and its recognition of DNA and DNA-PKcs. EMBO Reports. January 8, 2007,(1):56-62. Epub Dec 8, 2006.

Alex Mansergas; Josep M. Anglada; Santiago Olivella; Manuel F. Ruiz-López and Marilia Martins-Costa. On the nature of the unusually long OO bond in HO3 and HO4 radicals. Physical Chemistry Chemical Physics. 9. 5865. 2007.

Enrique Marcos; Ramon Crehuet; and Josep M. Anglada. Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. Journal of Chemical Theory and Computation. Published on the Web, December, 2007.

Martinez-Cruz B; Godoy JA; Genetic evidence for a recent divergence and subsequent gene flow between Spanish and Eastern imperial eagles. Bmc Evolutionary Biology 7, 2007.

A. García-Vela i. Intramolecular vibrational redistribution in Ne-Br_2: The signature of intermediate resonances in the excitation spectrum. Journal of Chemical Physics. 126. 124306. 2007.

S. López López; R. Prosmit; and A. García Vela. Nonadiabatic photodissociation dynamics in (HI)_2 induced by intracluster collisions. Journal of Chemical Physics. 126. 161102. 2007.

S. López López; R. Prosmit and A. García Vela. Modeling the (HI)_2 photodissociation dynamics through a nonadiabatic wave packet study of the I*-HI complexa. Journal of Chemical Physics. 126. 184307. 2007.

E. Carmona-Novillo, M. Bartolomei, M. I. Hernandez, J. Campos-Martinez, Quasiclassical trajectory study of reactive and dissociative processes in H_2 + H_2: Comparison with quantum mechanical calculations, Journal of Chemical Physics. { f 126} 124315-1:124315-11. 2007.

F. Dayou; M. I. Hernández; J. Campos Martínez; R. Hernández Lamoneda. Spin-orbit coupling in O2(v)+O2 collisions. II. Quantum scattering calculations on dimer states involving the X 3Sg+, a 1Dg, and b1Sb+ states of O2 Journal of Chemical Physics. 126. 194309. 2007.

J. Campos Martínez; M. Bartolomei; E. Carmona Novillo; Marta I. Hernández; R. Hernández Lamoneda; F. Dayou. Interactions and collision dynamics in \$O_2+O_2\$. Progress in Theoretical Chemistry and Physics, 2007.

Lopez Lopez S.; Prosmiti R.; Garcia Vela A.; Nonadiabatic photodissociation dynamics in (HI)(2) induced by intracluster collisions. Journal of Chemical Physics 126 (16): Art. No. 161102. April 28, 2007.

Valdes A.; Prosmiti R.; Villarreal P.; Ab initio potential energy surface and spectrum of the B((3)Pi) state of the Hel2 complex. Journal of Chemical Physics 126 (20) 204301. May 28, 2007.

Valdes A.; Prosmiti R.; Villarreal P.; et al. Ab initio vibrational predissociation dynamics of He-I-2(B) complex. Journal of Chemical Physics 126 (24): Art. No. 244314. June 28, 2007.

Villarreal P; De Lara Castells MP; Prosmiti R.; et al. Spectral simulations of polar diatomic molecules immersed in He clusters: application to the ICI (X) molecule. Physica Scripta 76 (3): C96-C103. September, 2007.

Diez Pardos C.; Valdes A.; Prosmiti R.; et al. Additive intermolecular potentials from ab initio calculations: trends in Rg(2)-dihalogen van der Waals trimers. Theoretical Chemistry Accounts 118 (3): 511-517. September, 2007.

Diez Pardos C.; Valdes A.; Prosmiti R.; et al. Additive intermolecular potentials from ab initio calculations: trends in Rg(2)-dihalogen van der Waals trimers. Theoretical Chemistry Accounts 118 (3): 511-517. September, 2007.

Roncero O.; De Tudela RP; De Lara Castells MP; et al. Exact and quantum Chemlstry-like calculations in helium doped clusters: The He2Br2(I) example. International Journal of Quantum Chemistry 107 (14): 2756-2762. November, 2007.

Lopez Lopez S.; Prosmiti R.; Garcia Vela A. Modeling the (HI) (2) photodissociation dynamics through a nonadiabatic wave packet study of the I-*-HI complex. Journal of Chemical Physics 127 (18): Art. No. 184307. November, 2007.

Delgado Barrio G.; Lopez Duran D.; Valdes A.; et al. Potential energy surfaces and dynamics of HeNBr2 van der Waals complexes. 10th European Workshop on Quantum Systems in Chemistry and Physics. Topics in the Theory of Chemical and Physical Systems. 193-202, 2007. September, 2005.

Delgado Barrio G.; Valdes A.; Lopez Duran D.; et al. Dynamics and potential energy surfaces for small to medium size Hendihalogen clusters. 8th International Symposium on Frontiers of Fundamental Physics. Frontiers of Fundamental Physics. 48-49, October, 2007.

Alonso M.; and Herradon B.; Neural networks as a tool to classify compounds according to aromaticity criteria. Chemistry –A European Journal 13, 3913-3923. 2007.

L. Barrio; J. M. Campos Martin; J. L. G. Fierro. A spectroscopic and DFT study of tungstic acid peroxocomplexes. Journal of Physical Chemistry A, 111, 2166, 2007.

M. C. Navarro; A. M. Mancho; H. Herrero. Instabilities in buoyant flows under localized heating. Chaos. 17, 2, 023105-1- 023105-10, 2007.

J. M. Martín García; R. Portugal and L. Manssur. The Invar tensor package. Computer Physics Communications. 177, 640-648. 2007.

Mohammad Solimannejad; Ibon Alkorta and Jose Elguero. Stabilities and properties of O3-HOCl complexes. A

computational study. Chemical Physics Letters. 23–27. 449. 2007.

Oscar Picazo; Ibon Alkorta; José Elguero; Markku R. Sundberg and Jaana Valo. Bonding Properties Related with Chiral Discrimination in Dinuclear Metal Complexes of Group 10 Eur. Journal of Inorganic Chemistry. 324–332. 2007.

Ibon Alkorta; Jose Elguero and Krzysztof Zborowski. Chiral Recognition in Diaziridine Clusters and the Problem of Racemization Waves. Journal of Physical Chemistry. 111. 1096-1103. A 2007.

Ibon Alkorta; Jose Elguero and Janet E. Del Bene. HCP and H3C-CP as Proton Acceptors in Protonated Complexes containing Two Phosphorus Bases: Structures, Binding Energies, and Spin-Spin Coupling Constants. Journal of Physical Chemistry. 111. 9924-9930. A 2007.

K. Zborowski; I. Alkorta and J. Elguero. A Theoretical Study of Chiral Recognition in Bis[amino(phenyl)methanol]chromium(0) Complexes Polish. J. Chem. 81. 621–629. 2007.

Krzysztof Zborowski; Ibon Alkorta and Jose Elguero. Enantiodifferentiation in protonation processes. A theoretical study. Journal of Molecular Structure: THEOCHEM. 811, 37–44. 2007.

Corzana, F; Cuesta, I; Freire, F. The pattern of distribution of amino groups modulates the structure and dynamics of natural aminoglycosides: Implications for RNA recognition. Journal of The American Chemical Society. 129. 2849-2865. March 14, 2007.

Freire, F; Cuesta, I and Corzana, F. A simple NMR analysis of the protonation equilibrium that accompanies aminoglycoside recognition: Dramatic alterations in the neomycin-B protonation state upon binding to a 23-mer RNA aptamer. Chemical Communications, 174-176, 2007.

Corzana, F; Busto, JH and Jimenez Oses, G. Serine versus threonine glycosylation: The methyl group causes a drastic

alteration on the carbohydrate orientation and on the surrounding water shell . Journal of the American Chemical Society. 9458-9467. 2007.

Victor L. Cruz; Sonia Martínez; Javier Martínez Salazar and José Sancho. Proposed Polymerization Termination Mechanism for 3-R-Indenyl ansa-Zirconocenes (R = n-Alkyl) based on DFT Calculations and Experimental Observations. Macromolecules. 40. 7413–7415. 2007.

Victor L. Cruz; Jorge Martinez; Javier Martínez Salazar; Javier Ramos; Manuel L. Reyes; Alejandro Toro-Labbe and Soledad Gutierrez. QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer. 48(26). 7672-7678. 2007.

V.L. Cruz; S. Martinez; J. Martinez Salazar; D. Polo-Cerón; S. Gómez-Ruiz; M. Fajardo and S. Prashar. 3D-QSAR study of ansa-metallocene catalytic behavior in ethylene polymerization. Polymer. Volume 48. Issue 16. 4663-4674. July 27, 2007.

Francisco Corzana; Jesús H. Busto; Gonzalo Jiménez Osés; Marisa García de Luis; Juan L. Asensio; Jesús Jiménez Barbero; Jesús M. Peregrina and Alberto Avenoza. Serine versus threonine glycosylation. The methyl group causes a drastic alteration on the carbohydrate orientation and on the surrounding water shell. Journal of the American Chemical Society. 129. 9458-9467. 2007.

Gonzalo Jiménez Osés; Carlos Aydillo; Jesús H. Busto; María M. Zurbano; Jesús M. Peregrina and Alberto Avenoza. The role of the countercation in diastereoselective alkylations of pyramidalized bicyclic serine enolates. An easy approach to alfa-benzylserine. The Journal of Organic Chemistry. 72. 5399-5402. 2007.

Alberto Avenoza; Jesús H. Busto; Noelia Canal; José I. García; Gonzalo Jiménez Osés; Jesús M. Peregrina and Marta Pérez Fernández. Mechanistic study of the ring-size modulation in Michael–Dieckmann type reactions of 2-acylaminoacrylates with ketene diethyl acetal. New Journal of Chemistry. 31. 224-229. 2007.

José I. García; Gonzalo Jiménez-Osés; Víctor Martínez Merino; José A. Mayoral; Elísabet Pires and Isabel Villalba. QM/MM modeling of enantioselective pybox-ruthenium and box-coppercatalyzed cyclopropanation reactions. Scope, performance and applications to ligand design. Chemistry – A European Journal. 13. 4064-4073. 2007.

Manzano H and Ayuela A. Dolado JS. On the formation of cementitious C-S-H nanoparticles. Journal of Computer-Aided Material Design. 14 (1). 45-51. April, 2007.

Manzano H.; Dolado JS. and Guerrero A. Mechanical properties of crystalline calcium-silicate-hydrates: comparison with cementitious C-S-H gels Physica Status Solidi. A-Applications and Materials Science 204 (6). 1775-1780. June, 2007.

Scientific articles in-press

N. Inostroza; J. R. Letelier; P. Fuentealba and M.L.Senen. 1-Theoretical ro-vibrational spectrum of CF+. Spectrochimica Acta A.

S. López López; R. Prosmiti and A. García Vela. Effect of the Excitation Energy on the (HI)_2 Nonadiabatic Photodissociation Dynamics. Journal of Physical Chemistry A.

Alonso, M.; Casado, S.; Miranda, C.; Tarazona, J. V.; Navas, J. M.; Herradón, B. Decabromobiphenyl (PBB-209) activates the aryl hydrocarbon receptor while decachlorobiphenyl (PCB-209) is inactive. Experimental evidences and computational rationalization of the different behavior of some halogenated biphenyls. Chemical Research in Toxicology. 2008.

D. Díaz; M. C. Fernández Alonso; G. Cuevas; F. J. Cañada and J. Jiménez Barbero. On the role of aromatic-sugar interactions in the molecular recognition of carbohydrates. A 3D view by using NMR. Pure and Applied Chemistry.

Presentations at Congresses/Conferences

M.Villa; M.L.Senent and R.Hidalgo. Ethane C-H stretching vibrational spectra coupling. Molecular Spectroscopy Conference. Ohio State University. 2007.

F.J. Melendez; M.C. Sicilia; C. Muñoz-Caro; A. Niño and M. L Senent. Estudio teórico del comportamiento energético y estructural del catión C3H+. XXXIII Congreso Internacional de Químicos Teóricos de Expresión Latina. La Habana, Cuba. 2007.

M.L.Senent; M.Hochlaf; H.Massó and R.Letelier. Química teórica aplicada a la astrofísica molecular: cadenas carbonadas Tipo Cn. XXVII Jornadas Chilenas de Química, Termas de Chillán Chile. November, 2007.

N.Inostroza; M.L.Senent; M.Hochlaf and R.Letelier. Caracterización de especies de interés astrofísico mediante métodos ab initio: SiC3 lineal. XXVII Jornadas Chilenas de Química, Termas de Chillán. Chile. November, 2007.

R. Letelier; N. Hinostroza; M. L. Senent. Autovalores del oscilador anarmónico tridimensional. Aplicación a la rotación-vibración de un trompo esférico. XXVII Jornadas Chilenas de Química, Termas de Chillán. Chile. November, 2007.

Angel Rivera-Calzada; Laura Spagnolo; Laurence H. Pearl and Oscar Llorca. 3D structure of the Non-Homologous End-Joining (NHEJ) machinery. CNIO cancer conferences. Links between Cancer, Replication Stress and Genomic Integrity. Madrid. Nov. 5-7,2007.

MA. Recuero-Checa; A. Dore; A. Rivera-Calzada; LH. Pearl and Oscar Llorca. Estudios estructurales mediante microscopía electrónica del complejo xrcc4-dna ligasa iv implicado en la reparación de roturas de adn. XXIII Bienal de la Sociedad de Microscopía de España. Bilbao, July 3-6, 2007.

Recuero-Checa MA; Arias-Palomo E; Dore AS; Rivera-Calzada A; Pearl LH; Llorca O. Estudios estructurales mediante microscopía electrónica del complejo xrcc4-dna ligasa iv

implicado en la reparacion de roturas de ADN. XXIII Bienal de la Sociedad de Microscopía de España. Bilbao, July 3-6, 2007.

A. García Vela. Nonadiabatic photodissociation dynamics in (HI)_2 induced by intracluster collisions. COMET XX, International Conference on Molecular Energy Transfer, Arcachon, France, 2007.

M. Alonso; B. Herradón; Towards a quantitative scale of aromaticity. XXXI Reunión Bienal de la Real Sociedad Española de Química, Toledo, September 9-14, 2007.

Marisa García; Francisco Corzana; Jesús H. Busto; Gonzalo Jiménez Osés Luis; Juan L. Asensio; Jesús Jiménez Barbero; Jesús M. Peregrina and Alberto Avenoza. alfa-O-Glicosidación de serina versus treonina: efecto en la orientación del carbohidrato y en la primera esfera de hidratación. XXXI Reunión Bienal de la RSEQ. Toledo. September, 2007.

- J.S. Dolado; H. Manzano; A. Porro; A. Ayuela; J. Hamaekers and M. Griebel. On the formation of cementitious C-S-H nanoparticles: A computational bottom-up approach. 12th International Congress on the Chemistry of Cement. Montreal, Canada. July 8-13 2007.
- J. S. Dolado. On the formation of cementitious C-S-H nanoparticles: A computational bottom-up approach. Trends in Nanotechnology. San Sebastián, Spain. September 3-7, 2007.

V Timon; N. Hernandez Haro; A Hernandez Laguna and C.I. Sainz-Diaz. Estudio teórico de la adsorción de películas de agua en superficies de mica. Encuentro internacional de HIELOCRIS (proyecto frontera del CSIC). Menorca, Spain. April 25 – 28, 2007.

E. Molina Montes; D. Donadio; A. Hernández Laguna; C.I. Sainz-Díaz and M. Parinello. First principles molecular dynamic of the dehydroxylation reaction of pyrophyllite. EUROCLAY 2007 Aveiro, Portugal. July 22-27, 2007.

N. Hernández Haro; V. Timón; C.I. Sainz Díaz and A. Hernández Laguna. Theoretical study of ice like films adsorbed on muscovite surface. EUROCLAY 2007. Aveiro, Portugal. July 22-27, 2007.

V.Timón; N. Hernández Haro; C.I. Sainz Díaz and A. Hernández Laguna. Estudio dinámico de la formación de estructuras tipo hielo adsorbidas sobre la superficie de los filosilicatos laminares 2:1 dioctaédricos. XXXI Reunión Bienal de la Real Sociedad Española de Física / 17 Encuentro Ibérico para la enseñanza de la Física. Libro de Resumenes 232. Granada, Spain. September 10-14, 2007.

E. Molina Montes; D. Donadio; M. Parinello; A. Hernández Laguna and C. I. Sainz Díaz. Dinámica molecular ab initio de las reacciones de deshidroxilación de los minerales de la arcilla. XXXI Reunión Bienal de la Real Sociedad Española de Física / 17 Encuentro Ibérico para la enseñanza de la Física. Libro de Resumenes 232. Granada, Spain. September 10-14, 2007.

N. Hernández Haro; V.Timón; C.I. Sainz Díaz and A. Hernández Laguna. Estudio DFT de películas de agua adsorbidas sobre modelos de superficie de mica. XXXI Reunión Bienal de la Real Sociedad Española de Física / 17 Encuentro Ibérico para la enseñanza de la Física. Libro de Resumenes 232. Granada, Spain. September 10-14, 2007.

V.Timón; N. Hernández Haro; C.I. Sainz Díaz and A. Hernández Laguna. Estudio DFT de la influencia de la presión sobre el volumen de la pirofilita. XXXI Reunión Bienal de la Real Sociedad Española de Física / 17 Encuentro Ibérico para la enseñanza de la Física. Libro de Resumenes 232. Granada, Spain. September 10-14, 2007

Posters at congresses/conferences

A. García Vela. Intramolecular vibrational redistribution in Ne-Br_2:The signature of intermediate resonances in the excitation spectrum. COMET XX, International Conference on Molecular Energy Transfer, Arcachon, France. 2007.

S. López-López; R. Prosmiti and A. García-Vela. Nonadiabatic photodissociation dynamics in (HI)_2 induced by intracluster collisions. ECAMP 2007. Trento, Italy. 2007.

A. García Vela. Intramolecular vibrational redistribution in Ne-Br_2:The signature of intermediate resonances in the excitation spectrum. ECAMP 2007. Trento, Italy. 2007.

R. Prosmiti; A. Valdes; C. Diez Pardos; P. Villarreal and G. Delgado-Barrio. Ab initio intermolecular potentials: structure and dynamics of Rg\$_2\$-dihalogen van der Waals clusters. Quantum Systems in Chemistry and Physics-XII London,UK. 2007.

V. Alemán; G. Delgado; B. González; J.S. Medina; R. Prosmit; P. Villarreal and G. Winter. Viscosidades del agua líquida pura. XXXI Reunión Bienal de Física. Granada. 2007.

V. Alemán; G. Delgado; B. González; J.S. Medina; R. Prosmit; P. Villarreal and G. Winter. Viscosidades del agua líquida pura. XXXI Reunión Bienal de Física. Granada. 2007.

R. Prosmiti; A. Valdes; P. Villarreal; G. Delgado-Barrio; D. Lemoine and B. Lepetit. Vibrational predissociation dynamics of He-I\$_2\$(B) cluster. COMET-XX. International Conference on Molecular Energy Transfer, Arcachon, France. 2007.

S. Lopez Lopez; R. Prosmiti; and A. Garcia Vela. Nonadiabatic photodissociation dynamics in HI\$_2\$ induced by intracluster collisions. ECAMP-9. Crete, Greece. 2007.

Jorge Martínez; Víctor L. Cruz; Javier Martínez Salazar and Alejandro Toro-Labbe. Iron based post-metallocene catalyst for ethylene polymerization: Establishing the Nature of the Active Species. European Polymer Congress. Portoroz, Slovenia. July, 2007.

Carlos Aydillo; Gonzalo Jiménez Osés; Jesús H. Busto; Jesús M. Peregrina; María M. Zurbano and Alberto Avenoza. Síntesis de alfa-alquilserinas mediante alquilación diastereoselectiva de N,O-acetales bicíclicos. XXXI Reunión Bienal de la RSEQ. Toledo, Spain. September, 2007.

J. Ortega Castro;, C.I. Sainz Díaz and A. Hernández Laguna. Theoretical high pressure study of substituted 2:1 dioctahedral phyllosilicates. EUROCLAY 2007. Aveiro, Portugal. July 22-27, 2007.

E. Molina Montes; V. Timón; C.I. Sainz Díaz and A. Hernández Laguna. Ab initio study of the mechanism for the dehydroxylation process in models of 2:1 dioctahedral phyllosilicates. EUROCLAY 2007. Aveiro, Portugal. July 22-27, 2007.

J. Ortega Castro; C.I. Sainz Díaz and A. Hernández Laguna. DFT elastic constants of 2:1 dioctahedral phyllosilicates. EUROCLAY 2007. Aveiro, Portugal. July 22-27, 2007.

N. Hernández Haro; M. Pruneda; A. Hernández-Laguna and C.I. Sainz-Díaz. Vibrational absorbance of hydrixyl groups in 2:1 dioctahedral phyllosilicates. EUROCLAY 2007. Aveiro Portugal. July 22-27, 2007.

PhD Thesis (Defended)

PhD: D. Sergio López López; Director: A. García Vela. Fotodisociación UV de agregados de van der Waals con enlaces de hidrógeno. Universidad Complutense de Madrid, Facultad de Física, 2007.

PhD Thesis (Presented)

Helena Massó Gonzalez. Director: María Luisa Senent. Estudio ab initio espectroscopico de las cadenas carbonadas C4, C5 y C6 de interés astrofísico. Universidad Autónoma de Madrid, 2007

D. Joaquín Ortega Castro. Investigación mecano-cuántica del orden/desorden catiónico y propiedades elásticas de filosilicatos 2:1 dioctaédricos. Universidad de Granada, July 28, 2007.

UNIVERSITY OF A CORUÑA, UDC



Scientific Articles Published

D. Andrade, B. B. Fraguela, R. Doallo. Precise Automatable Analytical Modeling of the Cache Behavior of Codes with Indirections. ACM Transactions on Architecture and Code Optimization (TACO) 4(3) September 16, 2007.

D. Andrade; M. Arenaz; B.B. Fraguela; J. Touriño; R. Doallo. Automated and Accurate Cache Behavior Analysis for Codes with Irregular Access Patterns. Concurrency and Computation: Practice and Experience. 19(18), 2407-2423. December, 2007.

Emilio J. Padrón; Margarita Amor; Montserrat Bóo; Ramón Doallo. Proc. of the 15th Euromicro Conference on Parallel, Distributed and Network Based Processing (PDP 2007) 134-138, 2007.

Lea Vaiana; Carlos Platas-Iglesias; David Esteban-Gómez; Fernando Avecilla; Andrés de Blas and Teresa Rodríguez-Blas. Receptor versus Counterion: Capability of N,N -bis(2-aminobenzyl)-diazacrowns for Giving Endo and/or Exocyclic Coordination of Zn(II). European Journal of Inorganic Chemistry,1874-1883. 2007.

David Esteban-Gómez; Carlos Platas-Iglesias; Fernando Avecilla; Andrés de Blas and Teresa Rodríguez-Blas. Effect of Protonation and Interaction with Anions on a Lead(II) Complex with a Lateral Macrobicycle Containing a Phenol Schiff-base Spacer. European Journal of Inorganic Chemistry, 1635-1643. 2007.

Martín Regueiro-Figueroa; David Esteban-Gómez; Carlos Platas-Iglesias; Andrés de Blas and Teresa Rodríguez-Blas. Metal ion Complementarity: Effect of the Ring Size Variation on the Conformation and Stability of Lead(II) and Cadmium(II) Complexes with Pendant-armed Crowns. European Journal of Inorganic Chemistry, 2198-2207. 2007.

Bertha Guijarro Berdiñas; Oscar Fontenla Romero; Beatriz Pérez Sánchez; Paula Fraguela. A Fast Semi-Linear Backpropagation Learning Algorithm. 17th International Conference on Artificial Neural Networks, ICANN. Lecture Notes in Computer Science. ISSN: 0302-9743, Vol. 4668, 190-198. 2007.

Marcos Chas; Dolores Abella; Víctor Blanco; Elena Pía; Gerardo Blanc;, Antonio Fernández; Carlos Platas-Iglesias; Carlos Peinador and José M. Quintela. Synthesis of New Selfassembled Pd(II) and Pt(II) Rectangular Metallomacrocycles. A Comparative Study of their Inclusion Complexes Chemistry – A. European Journal. 13, 8572-8582. 2007.

Esteban-Gomez D; Platas-Iglesias C; Avecilla F; et al. Effect of protonation and interaction with anions on a lead(II) complex with a lateral macrobicycle containing a phenol Schiff-base spacer. European Journal of Inorganic Chemistry Issue:12. 1635-1643. 2007.

Miriam Rega; Paloma Candal; Carlos Jiménez and Jaime Rodríguez. Mycothiazole: Synthesis of the C8–C18 Subunit and Further Evidence of the (Z)-∆14 Double Bond Configuration, European Journal of Organic Chemistry. 934–942. 2007

Javier Poza; Miriam Rega; Vanessa Paz; Beatriz Alonso; Jaime Rodríguez; Nélida Salvador; Antonio Fernández and Carlos Jiménez. Synthesis and evaluation of new 6-hydroximinosteroid analogs as cytotoxic agents. Bioorganic & Medicinal Chemistry 15, 4722–4740. 2007.

Raquel G. Soengas; Cristina Anta; Alfonso Espada; Rosa M. Nieto; Marta Larrosa; Jaime Rodrígueza and Carlos Jiménez. Vanchrobactin: absolute configuration and total synthesis. Tetrahedron Letters 48. 3021–3024. 2007.

Miriam Rega; Carlos Jiménez; Jaime Rodríguez. 6E-Hydroximinosteroid homodimerization by cross-metathesis processes. Steroids. 72, 729–735. 2007.

Leonardo Castellanos; Carmenza Duque; a Jaime Rodríguez and Carlos Jiménez. Stereoselective synthesis of (–)-4-epiaxinyssamine. Tetrahedron 63, 1544–1552. 2007.

Daniel Rivero; Juan Rabuñal; Julián Dorado; Alejandro Pazos. Automatic Design of ANNs by Means of GP for Data Mining Tasks: Iris Flower Classification Problem. Lecture Notes in Computer Science. Vol. 4431, 500-507. 2007.

Daniel Rivero; Julián Dorado; Juan Rabuñal; Marcos Gestal. A comparison between ANN generation and training methods and their development by means of graph evolution: 2 sample problems. Lecture Notes in Computer Science. Vol. 4507, 94-101. 2007.

Scientific Articles in-press

D. R. Ramos; M. V. García; M. Canle L; J. A. Santaballa; P. G. Furtmüller; C. Obinger. Myeloperoxidase-catalyzed chlorination: the quest for the active species. Journal of Inorganic Biochemistry.

Presentations at Congresses/Conferences

D. Rodríguez Ramos; M. Canle-López; J.A. Santaballa; P. G. Furtmüller; C. Obinger. Human Myeloperoxidase: the quest for the chlorinating species. 5th International Meeting on Human Peroxidases. Akaroa, New Zeeland. February 20-23. 2007.

M. Canle L.; M. I. Fernández P.; M. V. García; J.A. Santaballa. Mechanisms of oxidation of biologically relevant substrates by N-chloro-taurine. XXXI Reunión Bienal de la Real Sociedad Española de Química Lugar. Toledo, Spain. September 9-14, 2007.

Jaime Rodriguez. Heteronuclear coupling constants studies for the relative stereochemistry determination in 1,2 and 1,3 acyclic nitrogen chiral centers. Euromar 2007 Magnetic Resonance Conference. Tarragona, Spain. July 1-5, 2007. M. I. Fernández; Josep M. Oliva; M. Canle L. and J.A. Santaballa. Radical Species Derived from s-Triazine Pesticides: Geometry, Thermodynamics and Kinetics. XI European Symposium in Organic Chemistry (ESOR XI) Faro, Portugal. July 1-6, 2007.

Jaime Rodriguez. J-Based Analysis and DFT-NMR Assignations to Natural Complex Molecules: Application to 7-Hydroxy-5,6-epoxycholestanes. 2nd Spanish-Moroccan Symposium on Organic Chemistry and the 5th Andalusian-Moroccan Meeting on Natural Products Chemistry Torremolinos-Málaga, Spain. October 15-17, 2007.

Posters at congresses/conferences.

E.Carro; M. Canle; L. M. Fernández González; J. A. Santaballa. Oxidation of Pyrimidine Bases: Mechanism of Thymine Chlorination. XI European Symposium in Organic Chemistry (ESOR XI). Faro, Portugal. July 1-6, 2007.

D. R. Ramos; MV. García; M. Canle L.; J.A. Santaballa. Modeling the active site of Myeloperoxidases. XI European Symposium in Organic Chemistry (ESOR XI) Faro, Portugal. July 1-6, 2007.

E.Carro; M. Canle L.; J. A. Santaballa. Oxidation of Pyrimidine Bases: mechanism of Uracil Chlorination. XXXI Reunión Bienal de la Real Sociedad Española de Química. Toledo, Spain. September 9-14, 2007.

PhD Thesis (defended)

Antonio Freire Corbacho. Directores: M. Canle López e J. Arturo Santaballa L. Degradación de contaminantes orgánicos persistentes: estudio teórico - experimental del mecanismo de hidrólisis y de la fotofísica del asulam. December 17, 2007. School of Sciences, the University of A Coruña.

Daniel Rivero. Desarrollo y Simplificación de Redes de Neuronas Artificiales mediante el uso de técnicas de Computación Evolutiva. The University of A Coruña.

PhD Thesis (presented)

José París López. Directores: Manuel Casteleiro, Ignasi Colominas. Restricciones en tensión y minimización del peso: Una metodología general para la optimización topológica de estructuras. The University of A Coruña. December 2007.

Diego Andrade Canosa. Systematic Analysis of the Cache Behavior of Irregular Codes. Departament of Electronic and istems. The University of A Coruña April, 2007.

Master's Thesis. Defended Projects.

Paula Fraguela. Un nuevo algoritmo de aprendizaje neuronal basado en gradiente descendente y mínimos cuadrados. September, 2007.

Félix Manuel; Carballal Fortes. Análisis de algoritmos de aprendizaje máquina para la detección de intrusos en redes de ordenadores. school of Information, The University of A Coruña. September, 2006.

UNIVERSITY OF SANTIAGO DE COMPOSTELA, USC.

Scientific Articles Published.



Quinteiro, Javier; Rodríguez-Castro, J.; Rey-Méndez, Manuel. Population genetic structure of the stalked barnacle Pollicipes pollicipes (Gmelin, 1789) in the north-eastern Atlantic: influence of coastal currents and mesoscale hydrographic structures. Marine Biology, 153(1): 47-60, 2007.

Lorenzo Freire, S.; Alonso Meijide, J. M.; Casas Méndez, B. and Fiestras Janeiro, M. G. Characterizations of the Deegan-Packel and Johnston power indice. European Journal of Operational Research, 177, 1, 431-444, Ed. Elsevier Science, 2007.

Lorenzo Freire, S.; Alonso Meijide, J. M.; Casas Méndez, B. y Hendrickx, R. Balanced contributions for multi-issue allocation situations. Center Discussion Paper 2005-93, Tilburg University, Tilburg, The Netherlands. ISSN: 0924-7815, 2007.

Lorenzo Freire, S.; Alonso Meijide, J. M.; Casas Méndez, B. y Hendrickx, R. Balanced contributions for TU games with awards and applications. European Journal of Operational Research. 182, 2, 958-964, Ed. Elsevier Science. 2007.

Bergantiños Cid, G.; Casas Méndez, B.; Fiestras Janeiro, M. G. and Vidal Puga, J. A solution for bargaining problems with coalition structure. Working Paper Series 11-05. Mathematical Social Sciences. 54, 35-58. 2007.

J.A.Lorenzo and J.L.Albín and D.E.Singh and T.F.Pena and F.F.Rivera An inspector/executor based strategy to efficiently parallelize N-Body simulation programs on shared memory systems. Parallel and distributed computing; proceedings. International Symposium on Parallel and Distributed Computing. 45-52. Hagenberg, Austria, ISBN 978-0-7695-2917-2. 2007.

M.Aldegunde; A.J.García Loureiro; K.Kalna; A.Asenov. Study of fluctuations in advanced MOSFETs using a 3D finite element parallel simulator. Journal of Computational Electronics, vol. 5, issue 4, 311-314, 2006.

M. Rodríguez-Damián; E. Cernadas; A. Formella; M. Fernández-Delgado and P. Sá-Otero. Automatic detection and classification of grains of pollen based on shape and texture. IEEE Transactions on Systems, Man and Cybernetics, Part C, Vol 36.No 4, 531-542, 2006.

D. Gomes; M. Fernández-Delgado and S. Barro. Polytope ARTMAP: pattern classification without vigilance based on

general geometry categories. IEEE Transactions on Neural Networks, Vol. 18, No 5, 1306-1325, Septiembre 2007.

N.Seoane; A.J.García Loureiro; K.Kalna, A.Asenov. Impact of intrinsic parameter fluctuations on the performance of HEMTs studied with a 3D parallel drift-diffusion simulator. Solid-State Electronics, vol. 51, 481-488. 2007.

G. Rodríguez; P. González; M. Martín; J. Touriño. Enhancing Fault-Tolerance of Large-Scale MPI Scientific Applications. Parallel Computing Technologies, volumen 4671 de Lecture Notes in Computer Science. ISBN: 3-540-73939-4. 2007.

J.C. Mouriño; M.J. Martín; P. González and R. Doallo. Fault Tolerant Solutions for a MPI Compute Intensive Application. Proceedings 15th Euromicro Conference on Parallel, Distributed and Network-based Processing. Napoles, Italy. February, 2007.

Ángel Piñeiro; Xavier Banquy; Silvia Pérez-Casas; Édgar Tovar; Abel García; Alessandra Villa; Alfredo Amigo; Alan E. Mark; Miguel Costas. On the Characterization of Host-Guest Complexes: Surface Tension, Calorimetry, and Molecular Dynamics of Cyclodextrins with a Non-ionic Surfactant. The Journal of Physical Chemistry B. 111, 4383-4392. 2007.

Jorge Hernández-Pascacio; Cristina Garza; Xavier Banquy; Norma Díaz-Vergara; Alfredo Amigo; Salvador Ramos; Rolando Castillo; Miguel Costas; Ángel Piñeiro. Cyclodextrin-Based Self-Assembled Nanotubes at the Water/Air Interface. The Journal of Physical Chemistry B. 111, 12625-12630. 2007.

V.Pardo; P.Blaha; M.Iglesias; K.Schwarz; D.Baldomir; J.E.Arias. Erratum:Magnetic structure and orbital ordering in BaCoO3 from first principles calculations [Phys.Rev.B70,144422(2004)] Physical Review B. Volume A: 059902 – 059902. 2007. ISBN: 0163-1829.

S.Blanco-Canosa; F.Rivadulla; V.Pardo; D.Baldomir; J.-S. Zhou; M.Garcia Hernandez; M.A.Lopez- Quintela; J.Rivas; J.B.Goodenough. Enhanced Pressure Dependence of Magnetic Exchange in A2+[V2]O4 Spinels Approaching the Itinerant

Electron Limit. Physical Review Letters A, 99 Pag. 187201 - 187201-4. ISBN: 0031-9007. 2007.

V. Pardo; P. Blaha; R. Laskowski; D. Baldomir; J. Castro; K. Schwarz; J. E. Arias. Ising-type behavior in the antiferromagnetic phase of BaCoO3 from first principles. Physical Review B. Volume A. 165120 - 16512-6. ISBN: 0163-1829. 2007.

M. Pereiro; D. Baldomir; S. V. Mankovsky; K. Warda; J. E. Arias; L. Wojtczak and J. Botana. Calculations of giant magnetoresistance in Fe/Cr trilayers using layer potentials determined from ab initio methods. Journal of Physics - Condensed Matter. Volume A. 106210-1 - 106210-14. 2007.

K. Warda; L. Wojtczak; M. Pereiro; D. Baldomir and J. Arias. GMR via temperature-dependent layered potential distribution. Journal of Magnetism and E306Magnetic Materials. Volume A: 316. e320 - e322. ISBN: 0304-8853/01. 2007.

D. Baldomir; J. Rivas; D. Serantes; M. Pereiro; J.E. Arias; M.C. Bujan-Nuñez; C. Vazquez-Vazquez. Magnetocaloric effects in magnetic nanoparticle systems: A Monte Carlo study. Journal of Non-Crystalline Solids. Volume A: 353, 790 – 792. ISBN: 0022-3093. 2007.

D. Baldomir; J. Rivas; D. Serantes; M. Pereiro; J.E. Arias; M.C. Bujan-Nuñez; C. Vazquez-Vazquez. Magnetic field dependence of the magnetocaloric effect in magnetic nanoparticle systems: A Monte Carlo simulation. Journal of Non-Crystalline Solids Clave: A ,Volume 353, 793 – 795. 2007. ISBN: 0022-3093

M. Pereiro and D. Baldomir. Structure of small silver clusters and static response to an external electric field. Physical Review. Volume A: 75, 033202-1 - 033202-10. 2007. ISBN: 1050-2947

V. Pardo; D. Baldomir; J. Castro; M. Iglesias and J.E. Arias. Ising-type anisotropy and spin state transitions in GdBaCo2O5.5 from first-principles calculations. Journal of Magnetism and Magnetic Materials. Volume A: 316, e656 - e658. ISBN: 0304-8853. 2007.

P.M. Botta; V. Pardo; C. de la Calle; D. Baldomir; J.A. Alonso and J. Rivas. Ferromagnetic clusters in polycrystalline BaCoO3. Journal of Magnetism and Magnetic Materials. Volume A: 316. e670 - e673. ISBN: 0304-8853. 2007.

J. Botana; M. Pereiro; D. Baldomir; J.E. Arias; K. Warda and L. Wojtczak. Electronic configuration of nFe/3Cr/nFe (n=1 - 6) trilayers in FM state. Journal of Magnetism and Magnetic Materials. Volume A: 316. e360 - e364. ISBN: 0304-8853. 2007.

Jorge Botana; 1 Manuel Pereiro; Daniel Baldomir; Juan Enrique Arias; 2 Krzysztof Warda and Leszek Wojtczak. Magnetic-dependent structure in eight-atom gold clusters. Journal of Applied Physics. Volume A: 103. 07B716-1 - 07B716-3 ISBN: 0021-8978. 2007.

B. Hernando; J. L. Sanchez Llamazares; J. D. Santos; Ll. Escoda; J.J. Suñol; R. Varga; D. Baldomir and D. Serantes. Thermal and magnetic field-induced martensite-austenite transition in Ni50.3Mn35.3Sn14.4 ribbons. Applied Physiscs Letters. Volume A: 92. 042504-1 - 042504-4. ISBN: 0003-6951, 2007.

M.Pereiro; D.Baldomir and J.E.Arias. Unespected Magnetism of Small Silver Clusters. Physical Review A. A Volume: 75. 063204-1 - 063204-6 ISBN: 1050-2947. 2007.

M.M.G. Alemany; R.C. Longo; L.J. Gallego; D.J. González, L.E. González; Murilo L. Tiago and James R. Chelikowsky. Ab initio molecular dynamics simulations of the static, dynamic, and electronic properties of liquid Pb using real-space pseudopotentials. Physical Review B 76, 214203. 2007.

M.M.G. Alemany; Xiangyang Huang; Murilo L.Tiago; L.J. Gallego and James R. Chelikowsky. The Role of Quantum Confinement in P-Type doped Indium Phosphide Nanowires. Nano Letters 7, 1878. 2007.

M.M.G. Alemany, Manish Jain, Murilo L. Tiago, Yunkai Zhou, Yousef Saad, and James R. Chelikowsky. Efficient first-principles calculations of the electronic structure of periodic systems. Computer Physics Communications 117, 339. 2007.

Alemany, M. M. G.; Longo, R. C.; Gallego, L. J.; González, D. J.; González, L. E.; Tiago, Murilo L.; Chelikowsky, James R. Ab initio molecular dynamics simulations of the static, dynamic, and electronic properties of liquid Pb using real-space pseudopotentials. Physical Review B, vol. 76, 214203. 2007.

J. Alvarez-Muniz (Santiago de Compostela U.) , P. Brogueira (Lisbon, IST) , R. Conceicao (LIP, Coimbra) , J. Dias de Deus (Lisbon, CENTRA & Lisbon, IST) , M.C. Espirito Santo, M. Pimenta (LIP, Coimbra & Lisbon, IST) Percolation and high energy cosmic rays above 10**17 eV. Astropart.Phys.27:271-277, e-Print: hep-ph/0608050. 2007.

Penabad, E. et al. Comparative analysis between operational weather prediction models and QuikSCAT wind data near the Galician coast, Journal of Marine Systems. doi:10.1016/j. jmarsys. 07.008. 2007.

Martorell L; Costas J; Valero J; Gutierrez-Zotes A; Phillips C, Torres M; Brunet A; Garrido G; Carracedo A; Guillamat R; Vallès V; Guitart M; Labad A; Vilella E. Analyses of variants located in estrogen metabolism genes (ESR1, ESR2, COMT and APOE) and schizophrenia. Schizophrenia Research. [Epub ahead of print] PMID: 18164902. December 28, 2007.

Vilella E; Costas J; Sanjuan J; Guitart M; De Diego Y; Carracedo A; Martorell L, Valero J; Labad A; De Frutos R; Nájera C; Moltó MD; Toirac I; Guillamat R; Brunet A; Vallès V; Pérez L; Leon M; de Fonseca FR; Phillips C; Torres M. Association of schizophrenia with DTNBP1 but not with DAO, DAOA, NRG1 and RGS4 nor their genetic interaction. Journal of Psychiatric Research. [Epub ahead of print] PMID: 17408693. April 2, 2007.

Fernandez-Ramos, A.; Martinez-Nunez, E.; Vazquez, S. A.; Rios, M. A.; Estevez, C. M.; Merchan, M.; Serrano-Andres, L. Journal of Physical Chemistry A. 111, 5907. Hydrogen Transfer vs Proton Transfer in 7-Hydroxy-quinoline (NH3)3: A CASSCFCASPT2 Study. 2007.

Mousavipour, S. H.; Fernandez-Ramos, A.; Meana-Paneda, R.; Martinez-Nunez, E.; Vazquez, S.A.; Rios, M.A. Direct-Dynamics VTST Study of the [1,7] Hydrogen Shift in 7-Methylocta-

1,3(Z),5(Z)-triene. A Model System for the Hydrogen Transfer Reaction in Previtamin D3. Journal of Physical Chemistry A 111,719.2007.

Ramilowski JA; Mikosz AA; Farrelly D. Rotational structure of small He-4 clusters seeded with HF, HCl, and HBr molecules. Journal of Physical Chemistry. 111. 49. 12275-12288. 2007.

Calvo, P.; Crugeiras, J.; Rios, A.; Rios, M. A. Nucleophilic Substitution Reactions of N-Chloramines: Evidence for a Change in Mechanism with Increasing Nucleophile Reactivity. Journal of Organic Chemistry, 72(9), 3171-3178, 2007.

Peña-Gallego,Ángeles; Rodríguez-Otero, Jesús; Cabaleiro-Lago, Enrique M. A theoretical study of the influence of BF3 on the reaction path of the [4 + 2] cycloaddition of vinylketene with formaldimin. Tetrahedron. A. 63 11617-11621. ISBN: 0040-4020. 2007.

Rodríguez-Otero, Jesús; Cabaleiro-Lago, Enrique M; Peña-Gallego, Angeles. Theoretical study of the walk rearrangement in perfluorotetramethyl (Dewar thiophene) exo-S-oxid. Tetrahedron. A. 63.2191-2198. ISBN: 0040-4020, 2007.

Montero-Campillo, M.; Merced Rodríguez-Otero, Jesús; Cabaleiro-Lago. Ab initio and DFT study of the aromaticity of some Fulvalenes derived from Methylidenecyclopropabenzen. Journal of Molecular Modeling. A 13. 919-926. ISBN: 0948-5023. 2007.

Pena-Gallego, Angeles; Rodriguez-Otero, Jesus; Cabaleiro-Lago, Enrique M. A DFT study of the [4+2] cycloadditions of conjugated ketenes (vinylketene, imidoylketene and formylketene) with formaldimine. The pericyclic or pseudopericyclic character from magnetic properties. Tetrahedron A. Volume: 63. 4937-4943. ISBN: 0040-4020.2007.

Cabaleiro-Lago, Enrique M.; Rodriguez-Otero, Jesus; Pena-Gallego, Angeles. A computational study of the electrocyclization of o-divinylbenzene and derivatives. Journal of Molecular Structure-Theochem A. 811. 141-151. ISBN: 0166-1280. 2007.

Pena-Gallego, A.; Rodriguez-Otero, J.; Cabaleiro-Lago, E. M. A ComparativeTheoretical Study of the Pericyclic-pseudopericyclic Character in a Group of Cyclizations of Dienylketenes to Cyclohexadienones. Journal of Physical Chemistry A. 111. 2935-2940. ISBN: 1089-5639. 2007.

Pena-Gallego, A.; Rodriguez-Otero, J.; Cabaleiro-Lago, E. M. A ComparativeTheoretical Study of the Pericyclic-pseudopericyclic Character in a Group of Cyclizations of Dienylketenes to Cyclohexadienones. Journal of Physical Chemistry A. 111. 2935-2940. ISBN: 1089-5639. 2007.

Hosein Mousavipour, S; Fernández Ramos, Antonio; Meana Pañeda, Rubén; Martínez Núñez, Emilio; Vázquez, Saulo A.; Ríos, Miguel A. Direct-Dynamics VTST Study of the [1,7] Hydrogen Shift in 7-Methylocta-1,3(Z),5(Z)-triene. A Model System for the Hydrogen Transfer Reaction in Previtamin D3. J. Physical Chemistry A. 111 (4). 719 -725. 2007.

Fernandez-Ramos, Antonio; Emilio Martínez-Nunez, Emilio; Vazquez, Saulo A.; Ríos, Miguel A.; Estevez, Carlos M.; Merchan, Manuela; Serrano-Andres, Luis. Hydrogen Transfer vs Proton Transfer in 7-Hydroxy-quinoline (NH3)3: A CASSCF/CASPT2 Study. Journal of Physical Chemistry. A. 111, 5907-5912. 2007.

Harmata, Michael; Zheng, Pinguan; Schreiner, Peter R.; Navarro-Vazquez, Armando. Diastereoselectivity in an electrocyclization reaction of cyclopentadienones. Tetrahedron Letters. 48 (33). 5919-5922. ISSN: 0040-4039. 2007.

Navarro-Vazquez, A; Rodriguez, D; Martinez-Esperon, MF; Garcia, A; Saa, C.; Dominguez, D. Acid-catalyzed cyclization of acyliminium ions derived from allenamides. A new entry to protoberberines. Tetrahedron Letters. 48 (15). 2741-2743. ISSN: 0040-4039. 2007.

Freire, Félix; Seco, José Manuel; Quiñoá, Emilio; Riguera, Ricardo. Challenging the absence of observable hydrogens in the assignment of absolute configurations by NMR: Application to chiral primary alcohols. Chemical Communications. 1456-8. 2007.

Freire, Félix; Calderón, Félix; Seco, José Manuel; Quiñoá, Emilio; Riguera, Ricardo. The Relative and Absolute Stereochemistry of Secondary/Secondary Diols: The Low Temperature 1H NMR of Their bis-MPA esters. Journal of Organic Chemistry. 72. 2297-2301. 2007.

Porto, Silvia; Seco, José Manuel; Ortiz, Aurelio; Quiñoá, Emilio; Riguera, Ricardo. Chiral thiols: the assignment of their absolute configuration by 1H. NMR REVISTA: Org. (24), 5015 - 5018, 2007.

Rebeca García Fandiño, Rebeca; Gulías, Moisés; Castedo, Luís; Granja, Juán R.; Mascareñas, José L.; Cárdenas, Diego J. Palladium-Catalysed [3+2] Cycloaddition ofAlk-5-ynylidenecyclop ropanes to Alkynes: A Mechanistic DFT Study. Chemistry - A European Journal. 14, 272 – 281. 2008.

Riveros, R; Rumbo, A; Sarandeses, LS; Mouriño, A. Synthesis and Conformational Analysis of 17r,21-Cyclo-22-Unsaturated Analogues of Calcitriol. Journal of Organic Chemistry. 72, 5477-5485. 2007.

Scientific articles in press

Alonso Meijide, J. M.; Casas Méndez, B.; Holler, M. J.; and Lorenzo Freire, S. (2007), Computing Power Indices: Multilinear extensions and new characterization. Discussion Paper 153. Sozialökonomisches Seminar der Universität Hamburg. Germany. European Journal of Operational Research.

Carpente Rodríguez, L.; Casas Méndez, B.; García Jurado, I. and Van den Nouweland, A. (2007). Coalitional interval games for strategic games in which players cooperate. Working Paper 2005-16, University of Oregon. Economics Department. Theory and Decision.

Longo Pazos, Roberto. A density-functional study of the possibility of noncollinear magnetism in small Mn clusters

using SIESTA and the generalized gradient approximation to exchange and correlation. Journal of Chemical Physics. 2008.

D. Díaz; X. C. Pardo; M. Martín; P. González; G. Rodríguez. CPPC-G: Fault-Tolerant Applications on the Grid. Lecture Notes in Computer Science.

Nestor Armesto; Leticia Cunqueiro; Carlos A.Salgado and W.C.Xiang. Medium-evolved fragmentation functions. Journal of High Energy Physics. arXiv:0710.3073.

Pilar Salgado Rodriguez. A finite element method for the magnetostatic problem in terms of scalar potentials. SIAM Journal on Numerical Analysis.

Varela, J. A.; Rubín, S. G.; Castedo, L.; Saá, C. J. "Formal" and Standard Ruthenium-Catalyzed [2 + 2 + 2]. Cycloaddition Reaction of 1,6-Diynes to Alkenes: A Mechanistic Density Functional Study". Org. Chem. 2008.

Clemente, José C.; Robbins, Arthur; Graña, Paula; Paleo, M. Rita; Correa, Juan F.; Villaverde, M.; Sardina, F. Javier; Govindasamy, Lakshmanan; Agbandje-McKenna, Mavis; McKenna, Robert; M. Dunn, Ben; Sussman, Fredy. Design, synthesis, evaluation and crystallographic based structural studies of HIV-1 protease inhibitors with reduced response to the V82A mutation. Journal of Medicinal Chemistry, 51, 0000, 2008.

Presentations at Congresses/Conferences

J.C. Mouriño; A.Gómez; C. Fernández; F. J. González; D.A. Rodríguez; J. Pena; F. Gómez; D. González and M. Pombar. The eIMRT project: Planning and Verification of IMRT treatments on GRID. IBERGRID: 1st Iberian Grid Infrastructure. pp. 341--352. Santiago de Compostela, May 2007.

A. Gómez; C. Fernández; J.c. Mouriño; J. López; F.J. G. Castaño; D. Rodríguez; L. Domínguez; D. González; J. Pena; F. Gómez; D. G. Castaño and M. Pombar. Monte Carlo Verification of IMRT

treatment plans on Grid. HealthGrid 2007. 105-114. Ginebra, Switzerland. 2007.

M.Aldegunde; A.J.García Loureiro; K.Kalna. 3D Parallel Finite Element Monte Carlo Simulation of nano-MOSFETs. 6th International Conference on Large-Scale Scientific Computations. 2007.

N.Seoane; A.J.García Loureiro. Análisis del rendimiento de la simulación 3D paralela de dispositivos semiconductores utilizando el resolutor BiCGSTABJ. CEDI 2007. XVIII Jornadas de Paralelismo, vol. II, Zaragoza, Spain, Thomsom, 619-627, September 11, 2007.

B. Gómez; E. Penabad; C. F. Balseiro; V. Pérez-Muñuzuri. PEIXE, An application for verification of forecast time series. Third international Workshop on verification methods. ECMWF, Reading, UK. 2007.

Gomez, B.; Balseiro, C. F.; Penabad, E.; Perez-Muñuzuri, V. Improvements on a limited area parameterization ensemble forecasting system. From one to several boundary conditions. 7th EMS Annual Meeting. San Lorenzo de El Escorial, Spain. 2007.

Miguez-Macho, G.; Fernadez-Diaz, I.; Malvesada, M. L.; Gomez-Hombre, B. X.; Balseiro, C. F.; Penabad, E. Numerical study of the fall 2006 flooding events in Galicia with WRF-NMM: the role of the warm sea surface temperature anomaly. 7th EMS Annual Meeting. 2007.

Alfredo Bermúdez; Pilar Salgado. A finite element method for the magnetostatic problem in terms of scalar potentials. The Second Chilean Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE 2007), Concepción, Chile, January 16-19, 2007.

Mascareñas, J.L.; Granja, J.R.; Castedo, L.; García Fandiño, Rebeca. Palladium-Catalyzed [3+2] Cycloaddition of ALK-5-Ynylidenecyclopranes to Alkynes and Alkenes. A mechanistic DFT study. Chemistry - A European Journal. 2007.

Posters in Congresses/Conferences

J.C. Mouriño; A. Gómez; C. Fernández; J. López; F.J. González Castaño; D.A. Rodríguez; J. Pena; F. Gómez; D. González Castaño and M. Pombar. El proyecto elMRT: Planificación y Verificación de tratamientos IMRT en GRID. XVI Congreso Nacional de Física Médica. Granada, Spain, 2007.

Carpente, L.; Casas, B.; Fiestras, G.; García Jurado, I.; Jácome, C. and Puerto, J. A model and heuristic algorithms for solving a time optimization problem in an agricultural cooperative. VIII Congreso Galego de Estatística e Investigación de Operacións, 179-184. ISBN: 978-84-690-9136-4. 2007.

M.Aldegunde; A.J.García Loureiro; A.Martinez; K.Kalna. Parallel 3D Monte Carlo Simulation of MOSFETs Using Tetrahedral Finite Elements. 12th International Workshop on Computational Electronics. 2007.

N.Seoane; K.Kalna; A.García Loureiro; A.Asenov. Threshold voltage variability in nanoscaled In0.75Ga0.25As implant free MOSFET. 12th International Workshop on Computational Electronics. Amherst, USA, October 8, 2007.

N.Seoane; A.J.García Loureiro; K.Kalna; A.Asenov. Analysis of the impact of intrinsic parameter fluctuations in a 50 nm InP HEMT. 6ª Conferencia de Dispositivos Electrónicos. El Escorial, Spain. 2007.

P.Brocos; N. Díaz-Vergara; A. Villa; A. E. Mark; Á. Piñeiro. Potential of mean force calculations by MD simulation for cyclodextrin + octyl-b-D-glucopyranoside complexes. Thermodynamics 2007, Rueil-Malmaison, France. September 26-28, 2007.

Lucía Gestal Souto and Gonzalo Míguez Macho. A high resolution calculation of the equilibrium water table depth and the equilibrium soil moisture profile for the Iberian Peninsula. Preprint volume of the 7th EMS Annual Meeting. 2007.

Pre-operational WRF validation in Galicia: a comparison with MM5. M. Malvesada; E. Penabad; B.Gómez; C.F. Balseiro; G. Míguez-Macho; I. Fernández; Grupo de Física No Lineal. University of Santiago de Compostela. (2) MeteoGalicia. Regional Ministry for Environment and Sustainable Development. Regional Government of Galicia. (maria@fmares.usc.es). 2007.

M.N. Lorenzo; J.J. Taboada and I. Iglesias. 7th EMS Annual Meeting / 8th ECAM. Thermohaline circulation as an example of nonlinear-processes in the climate system.

M.N. Lorenzo; J.J. Taboada and I. Iglesias. Transitions of the thermohaline circulation induced by noise in an earth model of the intermediate complexity. Second International Conference on Earth System Modelling (ICESM)

Malvesada, M.; Penabad, E.; Gómez, B.; Balseiro, C.F.; Míguez-Macho, G.; Fernández, I. Pre-operational WRF validation in Galicia: a comparison with MM5. 7th EMS Annual Meeting. San Lorenzo de El Escorial, Spain.

Saavedra, S.; Méndez, M.R.; Souto, J.A.; Bermídez, J.L.; Vellón, M.; Costoya, M. Regional transport of tropospheric ozone: a case study in the northwest coast of Iberian Peninsula. 29th NATO/SPS International Technical Meeting on Air Pollution Modelling and its Application. Aveiro, Portugal. September 2007.

Docobo, J. A.; Tamazian, V. S.; Andrade, M.; Ling, J. F.; Balega, Y. Y.; Lahulla, J. F.; Maximov, A.; Gonzalez-Romay, J. R. Affiliation: AA(Observatorio Astronómico Ramón María Aller, Santiago de Compostela, Spain), AB(Observatorio Astronómico Ramón María Aller, Santiago de Compostela, Spain), AC(Observatorio Astronómico Ramón María Aller, Santiago de Compostela, Spain), AD(Observatorio Astronómico Ramón María Aller, Santiago de Compostela, Spain), AE(Special Astrophysical Observatory, Karachai-Cherkessia, Russia), AF(Observatorio Astronómico Nacional, Madrid, Spain), AG(Special Astrophysical Observatory, Karachai-Cherkessia, Russia), AH(Observatorio Astronómico Ramón María Aller, Santiago de Compostela, Spain) Title: Double Stars Speckle Interferometry With The 3.5 m Telescope At Calar Alto (Almeria, Spain). Binary Stars as Critical Tools and Tests in Contemporary Astrophysics, International Astronomical Union. Symposium no. 240, held 22-25 August, 2006 in Prague, Czech Republic, S240, p. 62 Publication Date: 08/2007 Origin: IAU Bibliographic Code: 2007IAUS..240...62D

Cabaleiro Lago, Enrique M.; Rodríguez Otero, Jesús; Merced Montero, M.; Angeles Peña Gallego, Angeles. Características de la interacción en complejos C10H8 (H2X)1,2; X= O, S. XXXIII Congreso de Químicos Teóricos de Expresión Latina. La Habana (Cuba). September 17-21, 2007.

Rodríguez Otero, Jesús; Cabaleiro Lago, Enrique M.; M. Merced Montero Campillo, M. Merced; Peña Gallego, Angeles. Interacciones catión-p y anión-p: efecto de la formación del complejo sobre la aromaticidad. XXXIII Congreso de Químicos Teóricos de Expresión Latina. La Habana, Cuba. 2007.

Montero, M. Merced; Rodríguez Otero, Jesús; Cabaleiro Lago, Enrique M.; Peña Gallego, Angeles. Estudio teórico del mecanismo de la cicloadición [2+2+2+1] de monóxido de carbono y enediinos catalizada por rodio. XXXIII Congreso de Químicos Teóricos de Expresión Latina. La Habana, Cuba. 2007.

Rodríguez-Otero, Jesús; Cabaleiro Lago, Enrique M.; Peña-Gallego, Angeles; Montero Campillo, M. Merced. Cation-pi and anion-pi interactions. Changes in aromaticity upon complexation. 11th International Electronic Conference on Synthetic Organic Chemistry. 3-906980-19-7. Lugo, Spain. 2007.

Montero-Campillo, M. Merced; Cabaleiro Lago, Enrique M.; Rodríguez-Otero, Jesús. M.Merced Montero-Campillo Enrique M. Cabaleiro-Lago Jesús Rodríguez-Otero. 11th International Electronic Conference on Synthetic Organic Chemistry. 3-906980-19-7. Lugo, Spain. November 1-30, 2007.

Meana Pañeda, Rubén. Direct Dynamics calculations of the CH3OH + H hydrogen abstraction reaction in gas phase and aqueous solution. ISOTOPES. Benicassim, Spain. 2007.

Saá, Carlos; Varela, Jesús A.; Rubín, Silvia G.; Carlos González Rodríguez, Carlos; Varela Fernández, Alejandro; Castedo, Luis. Cicloadiciones formales catalizadas por rutenio entre 1,6-diinos y arenos vinílicos. XXXI Reunión Bienal de la Real Sociedad Española de Química. Toledo, spain. 2007.

PhD Thesis (Defended)

Dinani Gomes Amorim. Directores: Manuel Fernández Delgado e Senén Barro Ameneiro. Redes ART con categorías internas de geometría irregular. Departamento: Electrónica e Computación. Universidade de Santiago de Compostela.

Natalia Seoane Iglesias. Optimización de un simulador 3D paralelo aplicado al estudio de fluctuaciones de parámetros intrínsecos en dispositivos HEMT. Departamento: Electrónica e Computación. Universidade de Santiago de Compostela.

Daniel Vazquez Martinez. Reconstruccion tomografica de gradientes de indice con simetria rotacional: Aplicaciones a cristalinos. Universidade de Santiago de Compostela.

Cezar Rodrigues, Luis. Diseño, síntesis y actividad biológica de un nuevo ligando superagonista (AMCR277A) del receptor buclear de la vitamina D. 2007. Universidade de Santiago de Compostela.

PhD Thesis (Presented)

Romero Vidal. Precision Determination of the S-wave pipi Isospin Scattering Length Difference |a0-a2| in the DIRAC experiment.

Carballido Reboredo, María Raquel; Director(es): Julio A. Seijas Vázquez, Julio A; Vázquez Tato, M. Pilar. Síntesis asistida por microondas de compuestos de interés biológico e industrial: haloarenos, fulvenos, tricloropirrolidonas, azoles y flavonoides. Modelado de espectros de absorción electrónica de flavonoides. Universidade de Santiago de Compostela.

Others

B. Adeva, A. Romero; O. Vázquez Doce; C. Mariñas and J. L. Fungueiriño Pazos. K+K- and Kp production in DIRAC using time-of-flight measurements. Study of Kpi. Nota interna de DIRAC 2007-02.

A. Romero; B. Adeva; J. L. Fungueiriño Pazos and O. Vázquez Doce. Final results for pionium lifetime measurement with 2001 data. Nota interna de DIRAC 2007-07.

A. Romero; B. Adeva; J. L. Fungueiriño Pazos and O. Vázquez Doce. Pionium lifetime and |a0-a2| measurement with the full DIRAC Ni data sample. Nota interna de DIRAC 2007-14.

A. Romero; B. Adeva; J. L. Fungueiriño Pazos and O. Vázquez. Doce Pionium lifetime measurement with DIRAC 2002 and 2003 Ni data. Nota interna de DIRAC 2007-15.

Andrade, M. New orbit for WDS 16198+2646. IAU Commision 26. (Double Stars) Information Circular Publication. 10/2006 Origin: IAUDS Bibliographic Code: 2006IAUDS.160....2a

Docobo, J. A.; Ling, J. F. New orbits for WDS 14138+3059, WDS 20311+3333 Publication: IAU Commision 26. (Double Stars) Information Circular Publication. 10/2006 Origin: IAUDS Bibliographic Code: 2006IAUDS.160....2D

Docobo, J. A.; Tamazian , V. New orbitS for WDS 16450+2928, WDS 18044+0337. Publication: IAU Commision 26. (Double Stars) Information Circular Publication. 02/2007 Origin: IAUDS Bibliographic Code: 2007IAUDS.161S...1D

UNIVERSITY OF VIGO, UVIGO.



Scientific Articles Published

Fernández, José Luis; Fernández Doval, Angel; Trillo, Cristina; Deán, J. Luis; López, José Carlos. Video Ultrasonics by Pulsed TV Holography: A New Capability for Non-Destructive Testing of Shell Structures. International Journal of Optomechatronics, 1, 122-53, 2007, ISSN: 1559-9620 (on-line) 1559-9612 (paper).

Pineiro, Manuel M.; Galindo, Amparo; Parry, Andrew O. Surface ordering and capillary phenomena of confined hard cut-sphere particles. SOFT MATTER 3 (6). 768-778, 2007.

Hermida Ramón, J.M; Graña, A.M. Blue-Shifting Hydrogen Bond in the Benzene-Benzene and Benzene-Naphthalene Complexes. Journal of Computational Chemistry. 28, 540, 2007.

Hermida Ramón, J.M; Graña, A.M; Estévez, C. Structural Study of Methane Hydrate. Journal of Structural Chemistry. 18(5) 649-652. 2007.

Hermida Ramón, José M.; Estévez, Carlos M. Towards the Design of Neutral Molecular Tweezers for Anion Recognition. Chemistry - A European Journal. 13(17) 4743 - 4749. 2007

Fernández-Ramos, Antonio, Martínez Núñez, Emilio; Vázquez, Saulo A.; Ríos, Miguel A.; Estévez, Carlos M.; Merchán, Manuela; Serrano Andrés, Luís. Hydrogen Transfer vs Proton Transfer in 7-Hydroxy-quinolineâ (NH3)3: A CASSCF/CASPT2 Study. Journal of Physical Chemistry. A, 111 (26), 5907-5912. 2007.

Hermida Ramón, José M; Graña, Ana M.; M. Estévez, Carlos M. Structural Study of Methane Hydrate. Structural Chemistry Issue. 18, 5, 649-652. 2007.

Sardinha, Joao; Guieu, Samuel; Deleuze, Aurélie; Fernández Alonso, Carmen M.; Pilar Rauter, Amelia; Sinay, Pierre; Marrot, Jerome; Jime´nez-Barberoc, Jesús; Sollogouba, Matthieu. gem-Difluoro-carbasugars, the cases of mannopyranose and galactopyranose. Carbohydrate Research. 342, , 1689-1703. 2007.

Hermida Ramón, José M.; Graña, Ana M. Blue-Shifting Hydrogen Bond in the Benzene–Benzene and Benzene–Naphthalene Complexes. Journal of Computational Chemistry, 28, 540-546. 2007.

Rodríguez Otero, Jesús; Hermida Ramón, José M.; Cabaleiro-Lago, Enrique M. Analysis of the Nucleophilic Addition of Water to Ketenes. A DFT Study. European Journal of Organic Chemistry. 14, 2344-2351. 2007.

Hermida-Ramón, José M.; Estévez, Carlos M. Towards the Design of Neutral Molecular Tweezers for Anion Recognition. Chemistry - A European Journal. 13, 4743-4749. 2007.

Hermida-Ramón, José M.; Graña, Ana M.; Estévez, Carlos M. "Structural Study of the Methane Hydrate". Structural Chemistry, 18(5), 649-652. 2007.

Alvarez, Rosana; Nieto Faza, Olalla; De Lera, Angel R.; Cárdenas, Diego J. A Density Functional Theory Study of the Stille Cross-Coupling via Associative Transmetalation. The Role of Ligands and Coordinating Solvents. Wiley-VCH Verlag GmbH&Co. KGaA. www.asc.wiley-vch.de. 2007.

Silva López, Carlos; Nieto Faza, Olalla; Alvarez, Rosana; De Lera, Angel R. Pseudopericyclic Design Drives Antara-Antara [1,5] Methylene Sigmatropic Shifts from a Stepwise to a Concerted Mechanism. Journal of Computational Chemistry 28: 1411–1416. 2007.

Alvarez, Rosana; De Lera, Angel R.; Aurrecoechea M.; Durana, Aritz. Bimetallic Intermediates in the Formation of Nucleophilic Allenylzincs from Allenylpalladiums: A DFT Study. American Chemical Society. Publication on Web. 2007.

Silva López, Carlos; Nieto Faza, Olalla; Feldman, K.S.; Iyer M.R.; Hester, D.K. Cyclization cascade of allenyl azides: A dual mechanism. Journal of the American Chemical Society. 129 (24), 7638-7646. 2007.

Silva López, Carlos; Nieto Faza, Olalla; Souto, José A.; Alvarez, R.; De Lera, Angel R. Pseudopericyclic design drives antaraantara [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism. Journal of Computational Chemistry, 28 (8), 1411-1416. 2007.

Nieto Faza, Olalla.; Silva López, Carlos; De Lera, Angel R. "Sulfoxide-induced stereoselection in [1,5]-sigmatropic hydrogen shifts of vinylallenes. A computational study". Journal of Organic Chemistry. 72 (7), 2617-2624. 2007.

Alvarez, S.; Germain, P.; Alvarez, R.; Rodríguez Barrios, F.; Gronemeyer, H.; de Lera Angel R. Structure, Function and Modulation of Retinoic Acid Receptor beta, a Tumor Supresor. International Journal of Biochemistry & Cell Biology. 39(7-8):1406-1415.2007.

Nahoum, V.; Perez, E.; Germain, P.; Rodriguez-Barrios, F.; Manzo, F.; Kammerer, S.; Lemaire, G.; Hirsch, O.; Royer, C.A.; Gronemeyer, H.; de Lera, Angel R.; Bourguet, W. Modulators of the structural dynamics of the retinoid X receptor to reveal receptor function. Proceedings of the National Academy of Sciences of the United States of America. 104 (44): 17323-17328. 2007.

Silva López, Carlos; Nieto Faza, Olalla; De Lera, Angel R.; "Electrocyclic ring opening of cis-bicyclo[m.n.0] alkenes: The anti-woodward-hoffmann quest". Chemistry - A European Journal. 13 (17), pp. 5009-5017. 2007.

López Silva, Carlos; Nieto Faza, Olalla; Feldman, K.S.; Iyer, M.R.; Hester, D.K. Cyclization cascade of allenyl azides: A dual mechanism. Journal of the American Chemical Society. 129 (24), 7638-7646. 2007.

López Silva, Carlos; Nieto Faza, Olalla; De Lera, Angel.R. Electrocyclic ring opening of cis-bicyclo[m.n.0]alkenes:The anti-woodward-hoffmann quest. Chemistry - A European Journal. 13 (17), 5009-5017. 2007.

López Silva, Carlos; Nieto Faza, Olalla; Souto, José A.; Alvarez, R.; De Lera, Angel R. Pseudopericyclic design drives antaraantara [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism. Journal of Computational Chemistry. 28 (8), 1411-1416. 2007.

Nieto Faza, Olalla ; López Silva, Carlos ; De Lera, Angel R. Sulfoxide-induced stereoselection in [1,5]-sigmatropic hydrogen shifts of vinylallenes. A computational study. Journal of Organic Chemistry. 72 (7), 2617-2624. 2007.

Alvarez, R.; Nieto Faza, Olalla; De Lera, Angel R.; Cárdenas, D.J. A density functional theory study of the stille cross-coupling via associative transmetalation. the role of ligands and coordinating

solvents. Advanced Synthesis and Catalysis. 349 (6), 887-906. 2007.

Álvarez, Rosana; Nieto Faza, Olalla; De Lera, Angel R.; Cárdenas, Diego J. A DFT Study of the Stille Cross-Coupling via Associative Transmetalation. The Role of Ligands and Coordinating Solvents. www.asc.wiley-vch.de. Web. 2007.

Silva López, Carlos; Nieto Faza, Olalla; Souto, José A.; Alvarez, Rosana; De Lera, Angel R. Pseudopericyclic design drives [1a,5a] methylene sigmatropic shifts from a stepwise to a concerted mechanism. Journal of Computational Chemistry. 28: 1411–1416. 2007.

Alvarez, Rosana; De Lera, Angel R.; Aurrecoechea, Jose M.; Durana, Aritz. Bimetallic Intermediates in the Formation of Nucleophilic Allenylzincs from Allenylpalladiums: A DFT Study. American Chemical Society. Organometallics. 26, 2799-2802. 2007.

Vila, A; Mosquera, R.A. Atoms in Molecules Interpretation of the Anomeric Effect in the O C O Unit. Journal of Computational Chemistry. 28. 1516. 2007.

A. Vila, A; R. A. Mosquera, R.A. QTAIM explanation of the anomeric effect in the O–C–O unit II: 2-Methoxyoxane and 2,2-dimethoxypropane. Chemical Physics. 443, 22. 2007.

Eskandari, K.; Vila, A.; Mosquera, R. A. Interpretation of Anomeric Effect in the N-C-N Unit with the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry. 111, 8491. 2007.

Mandado, M.; González Moa, M.J.; Mosquera, R.A. QTAIM n-center delocalization indices as descriptors of aromaticity in mono and poly heterocycles. Journal of Computational Chemistry. 28, 127-136. 2007.

Estévez, L; González Moa, M.J; Terán, C.; Mosquera, R.A. Conformational study and electron density analysis of 9-[tetrahydropyran-3-yl]purine derivatives. Tetrahedro. 63, 717-726. 2007.

Eskandari, K.; Mandado, M.; Mosquera, R.A. Approximate transferability in conjugated polyenes. Chemical Physics. 437, 1-7.2007.

González Moa, M.J; Mandado, M.; Mosquera, R.A. A computational study on the stacking interactoin in quinhydrone. Journal of Physical Chemistry, A, 111, 1998-2001. 2007.

González Moa, M.J; Mandado, M.; Mosquera, R.A. A computational study on the stacking interactoin in quinhydrone. Journal of Physical Chemistry, A, 111, 1998-2001. 2007.

Vila, A.; Mosquera, R.A. Atoms in molecules interpretation of the anomeric effect in the O-C-O unit. Journal of Computational Chemistry. 28, 1516-1530. 2007.

Mandado, M.; González Moa, M.J; Mosquera, R.A. Chemical Graph Theory and n-center Electron Delocalization Indices: A Study on Polycyclic Aromatic Hydrocarbons. Journal of Computational Chemistry. 28, 1625-1633. 2007.

Otero, N.; Mandado, M.; Mosquera, R.A. Nucleophilicity of indole derivatives: Activating and deactivating effects based on proton affinities. Journal of Physical Chemistry A. 111, 5557-5562. 2007.

Otero, N.; Mandado, M.; Mosquera, R.A. Revisiting the Calculation of Condensed Fukui Functions using QTAIM, Journal of Chemical Physics. 126, 234108. 2007.

Vila, A.; Mosquera, R.A. QTAIM explanation of the anomeric effect in the O-C-O unit II. 2-methoxyoxane and 2,2-dimethoxypropane. Chemical Physics. 443, 22-28. 2007.

De Carvalho, M.F.; Mosquera, R.A.; Rivelino, R. A density functional theory study of the hydrogen bond interactions in glycine dimers. Chemical Physics. 445, 117-124. 2007.

González Moa, M.J.; Mandado, M; Cordeiro, M.N.D.S. Mosquera, R.A. QTAIM electron density study of natural chalcones. Chemical Physics. 446, 1-7. 2007.

Estévez, L.; Mosquera, R.A. A density functional theory study on pelargonidin. Journal of Physical Chemistry. A. 111, 11100-11109, 2007.

Rodríguez, J.L.; García-Tuñón, I.; Taboada, J.M.; Obelleiro, F. Broadband HF Antenna Matching Network Design Using a Real-coded Genetic Algotihm. IEEE Transactions on Antennas & Propagation Special Issue on Synthesis and Optimization Techniques in Electromagnetics and Antenna System Design, vol. 55, no. 3. 611-618. 2007.

Scientific Articles in-press

López Bravo, Cristina; González Castano, Francisco J.; Rodelgo Lacruz, Miguel; Pavón Mariño, Pablo; García Haro, Joan. LBWS: a load-balanced distributed scheduler for WASPNET optical packet switches. European Transactions on Telecommunications. 2007. ISSN: 1124-318X Issues/Year: 6

Mandado, Marcos; Hermida Ramón, José M.; Estévez, Carlos M. Molecular Tweezers as Receptors for Anions. An Energetic and Topological Study. Journal of Molecular Structure, THEOCHEM. Accepted Manuscript, Available online. 2007.

Álvarez, Rosana; Pérez, Martín; Nieto Faza, Olalla; De Lera, Angel R. The Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway.

Rodriguez Molares, Alfonso; Seoane Sobreira, M.A.; Gimenez Pena, A; Guijarro Torres, S. The influence of positional uncertainty in free-field microphone calibration. Provisionaly.

Books/Chapters

Mosquera, R.A.; González Moa, M.J.; Graña, A.M.; Mandado, M.; Vila, A. Exploring basic chemical concepts with the quantum theory of atoms in molecules. Chapter 4 in Chemical Physics

Research Trends (Horizons in World Physics). 252, 165-213, B.V. Arnold (Ed.), NovaPublishers, New York. 2007. ISBN: 1-60021-554-8.

Mandado, M.; González Moa, M.J.; Mosquera, R.A. Exploring basic chemical concepts with the quantum theory of atoms in molecules. II. Aromaticity. Progress in Quantum Chemistry Research, Nova Publishers, New York.

Presentations at Congresses/Conferences

Nieto, R; Gimeno, L; The project VALIMOD. Oral European Geosciences Union, General Assembly 2007 (EGU 2007). Viena, Austria. 2007.

Nieto, R.; Gimeno, L.; Lorenzo, N.; Trigo, R.; de la Torre, L. A trireanalysis climatology of COLs occurrence and an exploratory analysis of their predictability using reforecast. 7th EMS Annual Meeting / 8th ECAM. El Escorial-Madrid, Spain. 2007.

Piñeiro, M.M; Cerdeiriña, C.A; Medeiros, A. Response Functions of fluids: a Microscopic approach based on NpT Monte Carlo. Thermodynamics 2007. Rueil Malmaison, France. 2007.

Nieto, R.; Gimeno, L. The project VALIMOD. WORKSHOP DE LA ACCIÓN COST 733 Harmonisation and Applications of Weather Types Classifications for European Regions. Florence, Italy. 2007.

Nieto, R.; Gimeno, L.; Lorenzo, N.; Trigo, R.; de la Torre, L. A trireanalysis climatology of cut-off low systems occurrence and an exploratory analysis of their predictability using reforecast. 7TH EMS ANNUAL MEETING / 8TH ECAM. EI Escorial- Madrid, Spain, 2007.

Rodríguez Molares, Alfonso; Sobreira Seoane, Manuel A. A Numerical study of the influence of sound lever meter case. 19th International Congress on Acoustics. Madrid, Spain. 2007.

Araújo, M.G.; García-Tuñón, I.; Taboada, J.M.; Rodríguez, J.L.; Obelleiro, F.; Landesa, L. Modelo de fase progresiva para la

densidad de corriente en el Fast Multipole Method. V Encuentro Ibérico de Electromagnetismo Computacional 2007, Aiguablava-Costa Brava, Spain. 2007.

Taboada, J.M.; Landesa, L.; Araujo, M.G.; Obelleiro, F.; Rodríguez, J.L.; García-Tuñón, I. Compression of the Fast Multipole Method using the Singular Value Decomposition. European Conference on Antennasand Propagation (EUCAP 2007). 11th International Electronic Conference on Synthetic Organic Chemistry. 2007

Araujo, M.G.; Obelleiro, F.; Rodríguez, J.L.; García-Tuñón, I.; Taboada, J.M. Evaluation of Singular Potencial Integrals in the Method of Moments using Linearly Paced RWG Basis Functions. European Conference on Antennasand Propagation (EUCAP 2007), Edinburgh, UK. 2007

Posters in Congresses/Conferences

Dopazo Paz, Ana; González-Salgado, Diego; Romaní, Luís. Molecular simulation of the Thermodynamic Behaviour of the {METHANOL + WATER} system. Thermodynamics. Paris, France. 2007

Dopazo Paz, Ana María. Simulación molecular del comportamiento termodinámico del sistema metanol + agua. XXXI Reunión Bienal de la RSEF. Granada, Spain. 2007.

Nieto, R.; Gimeno, L.; Lorenzo,M.; Trigo, R.; Taboada, I. Predecibilidad de los sistemas de depresiones aislados en niveles altos (DANAs) utilizando datos de repredicción. XXXI Reunión Bienal de la Real Sociedad Española de Física (RSEF). Granada, Spain. 2007.

A. Bermúdez, A; Fernández J.L; Lopez, C; Salgado, P. Análisis of probe response in nondestructive testing of tubes using a volumen integral formulation based on the currente density. COMPUMAG2007 - 16th Internacional Conference on the Computation of Electromagnetic Fields. Achen, Germany. 2007.

Nieto, R; Gimeno, L; Trigo, R; Lorenzo, N. Predictability of cut-off low systems occurrence using reforecasts. Final Workshop de la Acción Cost 723 Data exploitation and modelling for the upper troposphere and lower stratosphere. Sofía, Bulgaria. 2006.

Nieto, R.; Gimeno, L.; Lorenzo, N.; Trigo, R. Predictability of cut-off low systems occurrence using reforecasts. European Geosciences Union, General Assembly 2007 (EGU 2007). 2007.

Nieto, R; Gimeno, L; Lorenzo, M; Trigo, R; Taboada, I. Predecibilidad de los sistemas de depresiones aislados en niveles altos (DANAs) utilizando datos de repredicción. Real Sociedad Española de Física (RSEF). Granada, Spain. 2007.

Rodríguez Barrios, Fátima. Structural and functional modulation of RXR by a series of 3-2 ALKOXYTetrahydronaphthyl-Cinnamic acids. Chemistry in Cancer Research: A vital Partnership. San Diego, USA. 2007.

Rodriguez Perez, Martín. Computational Organic Chemistry. I Xornadas dos Investigadores Parga Pondal e Ramón y Cajal de Galicia, Santiago de Compostela. 2007.

Rodriguez Perez, Martín. Química Orgánica Computacional. ECiMUVI (Encontro Científico Multidisciplinar da Universidade de Vigo). 2007.

PhD Thesis (Defended)

Pérez- Ojeda y Pérez, José Francisco. Contribución a la predicción y medida de la superficie equivalente radar de buques. Universidade de Vigo. 2007.

Pérez Santín, Efrén. Diseño, síntesis y evaluación biológica de buevos retinoides. Universidade de Vigo. 2007.

Alvarez, Susana. Moduladores de receptores de retinoides: diseño, síntesis y caracterización. Universidade de Vigo. 2007.

Master's Thesis/Final Projects

Fontán Filgueira, Noelia. Síntesis de Ureas Simétricas con Potencial Actividad como Inhibidores de las Histonas Metiltransferasas de Aeginina. Directores: De Lera, Angel R; Álvarez Rodríguez, Rosana. Facultad de Química. Universidade de Vigo. 2007.

Garcia Domínguez, Patricia. Aproximación a la Síntesis de los Peyssoneninos A y B. Directores: Angel R. De Lera, Angel; Álvarez Rodríguez, Rosana. Facultad de Química. Universidade de Vigo. 2007.

Otero Martinez, Nicolás. Estudio QTAIM de las protonaciones del indol y derivados. Facultad de Quimica. Universidad de Vigo. 2007.

Lenain, Pieterjan. QTAIM based multicenter delocalization analysis of resonance assisted hydrogen bonds. Universiteit Gent, Belgium. 2007.

OTHER USERS/INSTITUTIONS

Scientific Articles Published

Leo González; Vassilis Theofilis and Rafael Gómez Blanco. Finite Element Methods for Viscous Incompressible BiGlobal Instability Analysis on Unstructured Meshes. American Institute of Aeronautics and Astronautics, AIAA Journal. 0001-1452 vol.45 no.4.840-854.2007

Cesga's Staff Scientific Production

scientific production – CESGA 2007

CESGA Foundation

Conferences: Oral Presentations

A. Gómez, C. Fernández, J.C. Mouriño, J. López, F.G. G. Castaño, D. Rodríguez, L. Domínguez, D. González, J. Pena, F. Gómez, D. G. Castaño, M. Pombar.

Monte Carlo Verification of IMRT treatment plans on the Grid. Oral presentation, HealthGrid, Geneva, Switzerland, 2007.01/04/2007 al 01/04/2007

J.C. Mouriño, A.Gómez, C. Fernández, F. J. González, D.A. Rodríguez, J. Pena, F. Gómez, D. González, M. Pombar.

The elMRT project: Planning and Verfication of IMRT treatments on the GRID. Oral presentation, IBERGRID, Santiago de Compostela. 14/05/2007 al 16/05/2007

F.J. González-Castaño, P.S. Rodríguez-Hernández, R.P. Martínez-Álvarez, A. Gómez-Tato

Support vector machine detection of peer-to-peer traffic in high-performance routers with packet sampling: a nonlinear kernel approach.

Oral presentation, ICCS 2007 7th International Conference of Computational Science, Beijing, China. 27/05/2007 to 30/05/2007

M.David, G. Barreira, G. Boreges, N. Dias, J. Gomez, J.P. Martins, E. Acción, C. Borrego, M. Delfino, G. Merino, K. Neuffer, A. Pacheco, M.C. Porto, A. Sainz, J. López, P. Rey, C. Fernández, A. Simón, A. Lumbreras, F. Pérez, G. Amoros, J. SALT, A. Fernández, A. Lamas, South-West Regional Operations Centre

Operation and management as part of the EGEE Grid infrastructure. Oral presentation, IBERGRID, Santiago de Compostela. 14/05/2007 al 16/05/2007

P. Rey, C.Fernández, J.López, D.Kant, y J.Gordon The accounting infrastructure in EGEE. Oral presentation, IBERGRID, Santiago de Compostela.14/05/2007 al 16/05/2007

G.Borges, M.David, J.Gomes, J.López, P.Rey, A.Simón, C.Fernández, D.Kant, y K.M.Sephton

Sun Grid Engine, a New Scheduler for EGEE Middleware. Oral presentation, IBERGRID, Santiago de Compostela. 14/05/2007 al 16/05/2007

C.Fernández, L.García, C. Veiga, J.López, I.Campos, S.Stork, and M.Plociennik

The Study and Implementation of Virtual Servers for a Parallel Grid. Oral presentation, IBERGRID, Santiago de Compostela. 14/05/2007 al 16/05/2007

Conferences: Posters

Sagarminaga, Yolanda; Pérez, Javier; López, Ignacio; Cotos, José RETELAB: The development of a laboratory. Virtual Poster, XII Congress of the Spanish Association of Teledetection, Mar de Plata, Argentina, September 2007.

J.C. Mouriño, A. Gómez, C. Fernández, J. López, F.J. González Castaño, D.A. Rodríguez, J. Pena, F. Gómez, D. González-Castaño, M. Pombar

The elMRT project: The planning and verification of IMRT treatments on the GRID. Poster, XVI National Congress of Medical Physics, Granada, May 22 - 25, 2007.

Publications (journals, magazines, book chapters, etc.)

García Tobío, Javier; Doallo Biempica, Ramón; López Cabido, Ignacio; Martín Santamaría, Mª José; Gómez Tato, Andrés; Touriño Domínguez, Juan (Editors) - 1st Iberian Grid Infrastructure Conference Proceedings, book ISBN 978-84-611-6634-3.

J.Carlos Mouriño, Aurelio Rodríguez Benchmarks for the analysis of new architectures: Xeon Single, Dual and Quadcore. Technical report. CESGA-2007-001.

Jesús Otero, Andrés Gómez The integration of biomedical slides in tele-assistance systems. Technical report, CESGA-2007-002.

S. A. X. CESGA

Conferences: Oral Presentations

Gromaz Campos, Manuel; Rodríguez Malmierca, María José "E-Hospital: e-learning experiences with hospitalized adults". Presentation, Online Educa, Madrid, May 2007.

Rodríguez Malmierca, María José "Aula Cesga, a virtual campus for innovation based on Software Libre". Presentation, Xornadas de Inforensino, Lugo, September 2007.

Rodríguez Malmierca, María José "Aula Cesga, a virtual campus for innovation based on Software Libre". Presentation, I Xornadas de Software Libre no Ensino. OUSLI. Ourense, October 2007.

Gromaz Campos, Manuel; Rodríguez Malmierca, María José; Manoel Baña Castro; Beatriz López González A virtual environment for the improvement of the quality of life of families with functional diversity. Presentation, IX Congreso Internacional Galego-Portugues de Psicopedagoxía. A Coruña, September 2007.

Rubio Gayo, Bruno; Rodríguez Malmierca, María José; Gromaz Campos, Manuel (et al.) eHospital project: Aportación de la Tecnología Educativa a la Educación Hospitalaria. Presentation, Encontro Galego sobre Actividades Físicas e Saúde nos Lesionados Medulares. XXIV Jornadas Nacionales SEP. XIII Simposio de ASELME. II ,A Coruña, June 2007.

Rodríguez Malmierca, María José "Ethical concerns related to the use of ICT for the integration of marginalised young people". Presentation, "Ethical Aspects of Inclusion in the Information Society Workshop", European Commission: Information Society & Media, Brussels, November 2007.

Ramón Basanta BizPoint presentation: Conferencia Internacional sobre Xanelas Únicas Empresariais, A2B e apoio a empresas. Santiago de Compostela, Spain, Feb. 2, 2007.

Ramón Basanta Presentation, III Forum Vale do Minho: Proxectos de cooperación interrexional. Monçao, Portugal, March 30, 2007.

Ramón Basanta Presentation, The new European programmes and opportunities for Local Authorities and SMEs. Brussels, Belgium, Dec. 04, 2007.

Ramón Basanta Presentation, EISCO 2007: Government in Local Authorities. Hameenlinna – Finland, April 17-18, 2007.

Ramón Basanta Presentation, SINDUR, Santiago de Compostela, November 2007.

Conferences: Posters

Ramón Basanta Organización e ponencias BizPoint: Conferencia Internacional sobre Xanelas Únicas Empresariais, A2B e apoio a empresas. Santiago de Compostela, Feb. 15, 2007.

Publications (journals, magazines, book chapters, etc.)

Rodríguez Malmierca, María José (coord), Gromaz Campos, Manuel, García Tobío, Javier (et al) The state of e-learning in Galicia: analysis in the university and in business-2006. Book, 978-84-690-4560-2.

Manuel Gromaz Campos; Beatriz Cebreiro López; Carmen Fernández Morante; María José Rodríguez Malmierca; Javier García Tobío "Generating work proposals among professors in order to improve the utilization of TIC: The EFELCREN Project". Journal article, Quaderns Digitals Nº 45. [on line]. [consultation, Jan. 20, 2008] http://www.quadernsdigitals.net/index.php?accionMenu=hemeroteca.VisualizaArticuloIU. visualiza&articulo_id=9676. ISSN 1575-9393.

Manuel Gromaz Campos; Javier García Tobío; María José Rodríguez Malmierca; Bermejo Paradela, Miguel (et al) "The Galician Observatory of e-learning: methodology, techniques, and instruments". The Iberoamerican Journal of Distance Education. Volume 10. N°1. ISSN: 1390-3306. http://www.utpl.edu.ec/ried/index.php?option=com_content&task=view&id=443&Itemid=152 Arti-

cle, The Iberoamerican Journal of Distance Education - RIED. Vol 10, no 1. June 2007. ISSN 1138-2783.

ICHNOS Partners Project WhiteBook, Book.

ICHNOS Partners Green Paper, Book.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al Xanelas Únicas Empresariais en Europa, Article, ISBN: 84-690-3457-X.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Administrative Simplification for the creation of businesses. Article, ISBN: 84-690-3459-6.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Interoperability in Public Administrations. Article, ISBN: 84690-3460-X.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. A Administración Electrónica de cara ás empresas. Article, ISBN: 978-84-690-3709-6.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Support to businesses in Galicia. Article, ISBN: 978-84-690-3710-2.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Portelo ou Punto de Contacto Único para empresas: O caso galego. Article, ISBN: 978-84-690-3708-9.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al Xanelas Únicas Empresariais en Europa. Monograph, ISBN: 84-690-2166-4.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. The creation of businesses: the role of administrative simplification. Monograph, ISBN: 84-690-3461-8.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Interoperabilidade nas Administracións Públicas. Monograph, ISBN: 84-690-3462-6.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Apoio a empresas en Galicia. Monograph, ISBN: 84-690-3463-4.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Electronic administration and business. Monograph, ISBN: 84-690-3464-2.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. O Punto de Contacto Único para Empresas: Caso Galego. Monograph, ISBN: 84-690-3465-0.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Bizpoint - From global to local. Monograph, ISBN: 84-691-3268-0.

Javier García Tobío, Ramón Basanta Cheda, Diego Nieto, Iria Veiga et. al. Puntos de Contacto Únicos para Empresas. Book, ISBN: 978-84-690-7351-3.

Ramón Basanta (Coord.) Rafael M.ª García Rodríguez, M.ª Teresa García Álvarez, José López Rodríguez, Rosa M.ª Mariz Pérez, Elías Rebuge Estudo do Impacto das TIC nas PEMEs Galegas. Book.

DEA projects/Final projects

D. Nieto. The design and implementation of ROLAP data storage for the study of patients with cardiopulmonary sleep disorders. Advanced Studies Diploma (DEA).

Intelligent Systems Group | Department of Electronics and Computation | USC.



geographic information systems area (GIS)

The objectives of the Area of Geographic Information Systems include conducting analysis and calculus projects in the area of Geographic Information Systems (GIS), working with and processing raster and vectorial geo-referenced information, such as alphanumerical data bases, conducting studies in the field that include analysis, programming, visualization and diverse outputs (print, applications, intranet, Internet). In addition, it is responsible for the promotion and support of the use of GIS technology in the research community.

Noteworthy Activity in 2007

Sueloempresarial.com.- Operative maintenance of the Web of industrial parks developed for the Consortium Zona Franca de Vigo.

Risks M.A.- Having developed the part of risks for the agriculture and livestock sectors as well as its tool, the department is developing the part concerning atmospheric contamination, to be concluded in the next year.

SIFI Galicia.- Having collected the cartography of reference (Administrative, Infrastructures, Hydrographic and Natural Spaces), businesses data in the Galician sector of forestry were implemented and geo-referenced, forestry information was obtained and incorporated into the application, and the programming of an application for the management of the data base was initiated.

Patrimony 2007 Government-The development of a system of automatic cartography and the implementation of sub-aquatic Patrimony, such as models of spatial data.

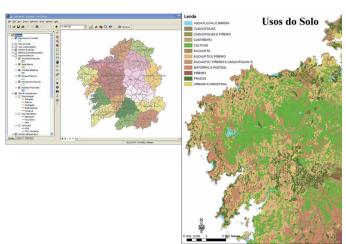
Map of Surnames of Galicia-The operative maintenance of the Map of Surnames developed for ILGA in Internet.

REDIX.-The presentation of a proposal for a European network, "Network on Distributed Collaborative Geographic Information

Systems", in the European Science Foundation of the UE formed by 11 countries and 2 global networks. The organization of training sessions for "GIS Day" in Lugo with a presentation of the projects integrated in the Network. Moreover, a manager has been contracted to be responsible for the research Network

The Area of Graphic Information Systems collaborated in the offering of technological training days for the diffusion of GIS technology, including the National Congress of Infrastructures of Spatial Data (IDEE) celebrated in Santiago de Compostela in October 2007.







e-learning

Objectives

- » Research in the area of e-learning in different contexts.
- » Promotion and dissemination of the Information and Communication Technologies (ICT) applied to teaching and learning processes.
- » Promotion of the integration of educational institutions in the Information Society.

Technological resources of CESGA in e-learning

- » Online Learning and Collaborative Suite (Aula Cesga)
- » Video Streaming for training sessions
- » Video-conference equipment
- » Distribution lists
- » Webminar tool
- » Training room

Outstanding activities in e-learning Area in 2007

- » E-intervention (Study and impact analysis of ICT use for the support of people with disabilities and their families: Quality of life and self-management): a project co-financed by the Directorate General for RTD, Regional Government of Galicia.
- » SUMA (Integration of E-learning Services through Standards): a national project financed by Plan Avanza in collaboration with other leading private and public institutions, part of the E-learning Workgroup in the INES Spanish Software and Services Technological Platform.
- » Five European projects. Three within the Socrates-Grundtvig program: E-hospital (e-learning applied to hospitalised adult patients), Parents (ICT Support for Parents as family
- » vocational advisers for children), and IEPTL (Integrating European Projects in Teaching and Learning). One within the Socrates-Leonardo program: YES (Youth Employment Support, an e-learning system for SMES to support earlyschool leavers). One within the Socrates-Comenius 2.1 program: Efelcren (Educational FLExible and CReative Environments).





- » Coordination of the Aula Molina project, financed by the Director General for Foreign Cooperation, Government of Galicia, for the analysis, knowledge transfer and implementation of a virtual campus at the Universidad Nacional Agraria La Molina, in Lima (Perú).
- » Collaboration with the Regional Ministry of Education Director General of Vocational and Special Education) for training activities for teachers such as the production of an e-learning course about a Didactics Mathematics Database, (MathDi, MathEduc), and collaboration on an e-learning course on GIS in secondary education. Consulting activities in the field of new technologies applied to teaching for Teacher Training Centres and training services at Galician universities and secondary schools.
- » Collaboration in, the planning, development, and evaluation of the training activities of CESGA personnel and HPC users.
- » Collaboration with training activities in the Network of Technological Centres of Galicia (Retgalia).
- » Participation in the e-learning work group at the INES platform (Spanish Software and Services Technological Platform).
- » Guest speakers at the Special Workshop on E-inclusion: "Ethical Aspects of Inclusion in the Information Society" in Brussels,organised by the Director General for the Information Society and Media of the European Commission.
- » Members of a Spanish Learning Objects Thematic Network dealing with the design of learning objects and activities

- (REDOAPA), together with 18 other institutions and national universities.
- » Publication of 1 book, 2 articles in scientific journals and presentations at 5 congresses in the sector of education and technology.
- » Analysis and implementation of an online open source based tool that facilitates videoconferences and virtual seminars as a service for researchers.
- » Maintenance and updating of the e-learning section at the CESGA Website.

» A total of 6 R&D projects were submitted and 4 of them obtained financing.



Holger Bienzle, Théo Bondolfi, Marie-Claude Esculier, Elisabeth Frankus, Carmen ernández Morante, Uwe Hoppe, Maria Jose Rodríguez Malmierca, Joanna Szczecin

E-Learning in hospitals at work:

Documentation of seven informal e-learning programme
piloted by the eHospital project







e-business

The Area of e-Business has the objectives of promoting the use of information technologies in Galician businesses as well as promoting the awareness, innovation and diffusion of the same. To these ends, this area is responsible for the design and production of innovative projects in the TIC environment and business, identifying lines of work and research in this field by means of observation and the performance of studies. The e-business area anticipates cooperation with other organizations in order to realise activities and projects that promote regional development by means of the use of TIC in businesses.

Noteworthy Activities in 2007:

During 2007, the area of e-Business continued to develop projects of innovation and technology centred in the business context as well as to support business projects.

The contracted European projects, ICHNOS y CIC-Commerce, were completed and new projects, i.e., CMMI/SPICE and CoopTIC were presented and contracted. In addition, specific meetings of support were organized with Galician organizations and businesses in order to evaluate possible projects of an innovative character. Last but not least, 102 consultations were conducted via Internet.

Various reports and publications were produced in association with contracted projects. They concerned unique business advantages in Galicia, Spain, and Europe, the interoperability of public administrations, and studies of the impact of TIC on Galician SMEs, among others.

BizPoint

Same BizPoi

Activities of the Centre were maintained in relation to TIC, innovation, and business by means of access to information sources, event attendance, etc.

The department organized an international conference in Santiago de Compostela concerning unique business advantages, A2B and support to businesses, Bizpoint, etc. and participated in various international and national technical meetings and panels, as listed below.

EISCO 2007: Government in Local Authorities", Hameenlinna,

Finland

SINDUR: Santiago de Compostela

ICHNOS: Steering and Scientific committees

III Forum Vale do Minho: Interregional cooperation projects

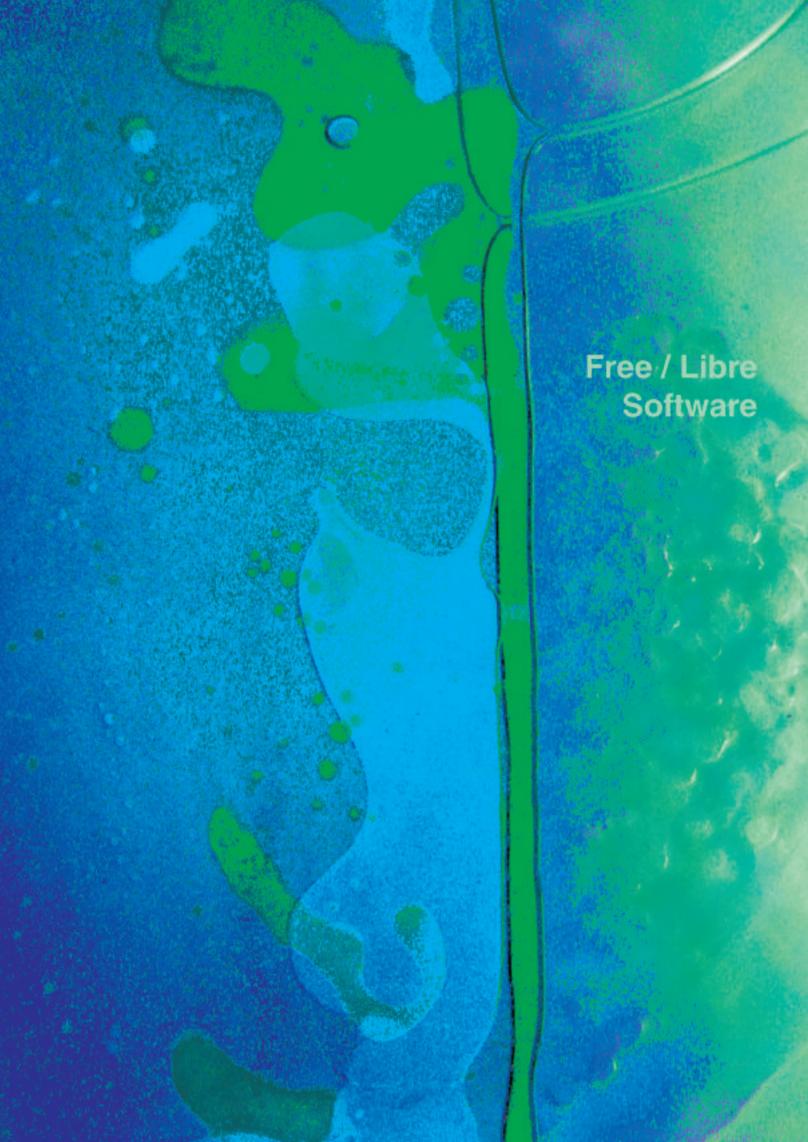
"The new European programmes and opportunities for Local

Authorities and SMEs" Brussels Course: Agents of Innovation, Lugo

Other activities of the e-Business Department of CESGA in 2007 include the development of the website of the BizPoint Conference as well as of the Registry of Private Agents of Innovation in addition to numerous meetings with agents involved in the TIC sector in Galicia and in Europe. By means of this participation, e-Business was able to contribute to the generation of knowledge in work environments.







galician iniciative for free/libre software



Mancomún

Activities relative to Free Software are managed according to the agreement of collaboration with the Director General of Industrial Promotion and the Information Society via Mancomún. The objective is the establishment of Free Software in Galicia, thereby facilitating industrial and innovative development of the SME in the TIC sector in Galicia. In this manner, the Information and Knowledge Society can be delivered to the Galician society with the expectation of potentiating the use of computer applications in the Galician language as well as promoting the utilization of open standards in order to achieve technological independence. Mancomún is to serve as a meeting point for the different initiatives relative to Free Software that are being developed in different environments: institutional, business, educational, volunteer, etc.

The most noteworthy activities undertaken in 2007 are listed below.

The Free Software Observatory

- » Technological observation of politics and initiatives: Notices published daily in mancomun.org and trimester reports by the USC and the UDC, respectively.
- » Distribution of the study, "Report about Free Software in Galician organisations".
- » Elaboration of a second study of observation concerning the situation of Free Software in Galician organisations at the end of the year.
- » Creation of the sections, "Success Cases" and "Interview" of the portal www.mancomun.org. Interviews related to success cases concerning the establishment and use of free

software in diverse environments, educational centres, city governments, and TIC businesses were conducted. These can be consulted in the interviews section of the mancomun. org. website.

Dissemination

- » Production and maintenance of the "Web mancomun.org-Galician Initiative for Free Software" with the goals of making the website more accessible and of standard and of energising the same by means of:
 - The incorporation of automatic translation to Spanish of mancomun.org,
 - The inclusion of social aggregates to the news for greater diffusion.
- » The organization of approximately 30 events of TIC literacy in coordination with the LUG (Groups of users in GNU/Linux de Galicia).
- » Participation as speakers in some 30 diffusion events for Free Software.
- » Participation in international congresses: BrOffice in Brazil and the OpenOffice.org Conference in Barcelona.

Repository of Free Software

- » Collaboration with the UDC in the activation and energising of Forxa: forja.mancomun.org.
- » Establishment of the open tool, "Linguistic corpus search engine" in Forxa.
- » Relocation of Forxa to the Council's Pilar platform in the 1st trimester of the year.

Advice in the SwL for the PYME

- » An agreement of collaboration was established between CESGA and the Galician universities to produce a series of events for the development and introduction of Free Software. These events are grouped in three categories.
- » The completion of a study and the promotion of numerical simulation in industry by way of SL.
 - The completion of a study concerning software solutions for business management in order to determine the state of maturity as well as for its introduction in the SME, and
 - The development of tools based on open technologies that favour computer access to groups of persons with functional diversity.
- » Elaboration of DVD Computer tools for the SME with the compilation of all of the applications translated to Galician regarding business management as well as office automation and collaborative work.
- » Presentation of the DVD to businesses and communication media in a work session; participation was high.
- » Elaboration of a "Guide: Learning to make FLOS" directed toward the SME in the FAQ format.
- » Sponsorship of the diffusion material of AGASOL, the Association of free software business in Galicia.
- » Production of the SME directory that includes 61 businesses.
- » Elaboration of manuals as a result of SME support activities:
 - Elaboration of contents for the TIC business: Tools for Web development
 - A study of SL specifically for businesses that derived from the generation of the CD "Personal Financial Managers".
 - How to set up a web service of automatic translation with Opentrad/Apertium.

Technical Support

- » Technical support to users of mancomun.org, SMEs, city governments, administrative organs, etc.
- » Technical support for energising the Web:
 - Elaboration and production of the visual Y-Sign Web of the leveraging Network, and
 - Installation and maintenance of the Jabber message server for the promoters of the Information Society.

Translation of SwL

- » Maintenance of the translation of writing applications: Firefox, thunderbird, pidgin, sunbird, gimp, Gnome
- » Translation of the different versions of OpenOffice.org and the distribution of approximately 5000 CDs.
- » Collaboration in the technical revision of the grammatical corrector of Galician for Ooo and its presentation.
- » Elaboration of an optimized version of the orthographic corrector of Galician for Ooo.
- » Maintenance and advancement of the on-line translation application, Entrans.
- » Improvements in the application, "Linguistic corpus search engine".

Training Activities

» 1,600 hours of training in SwL directed to the SME and the dissemination in general society, awarded to PcCarrier as a result of a sealed-bid tender, taking responsibility for the management of these hours in the leveraging Network.Collaboration with the Council of Education regarding courses oriented to teachers:

- Course "Entrans: the Galician language and the translation of Free Software for Galicia", co-organized by the Council of Education and the Council of Innovation and Industry
- · Course "Introduction to Free Software", co-organized by the Council of Education and the Council of Innovation and Industry.
- » Elaboration of the contents of the course, "Didactic Applications of OpenOffice.org".

Other Training Activities

- » Training course, in collaboration with CEFORE of Coruña, in the Secondary Centre of Betanzos, "Free software in educational centres".
- » Collaboration with the personnel of the Secondary Centre, IES San Clemente of Santiago of Compostela, for a course in GNU/Linux.
- » Sponsorship of the training sessions organized by OUSLI.
- Creation of manuals of diverse applications in the wiki of mancomun.org.

The Forge

DEVELOPMENT

- · Golfiño
- · Entrans · Corpus
- SME DVD

DISSEMINATION

Associative Movement

Events Schedule

Content Creation

Presentations

TRAINING

Content Creation, Training Aids, Courses...

Collaboration with the Regional Ministry of Education

Training software catalog

TECHNICAL SUPPORT

Manuals, Documentation

Mailing Lists

Help Desk

Mancomun.org:

OBSERVATORY

Technological Observation Project Following

Collaboration with the Galician Observatory for Information Society

SOFTWARE LOCALISATION

Translation Methodology

Support

Translation Tools

- Entrans
- Corpus

Linguistic Edition

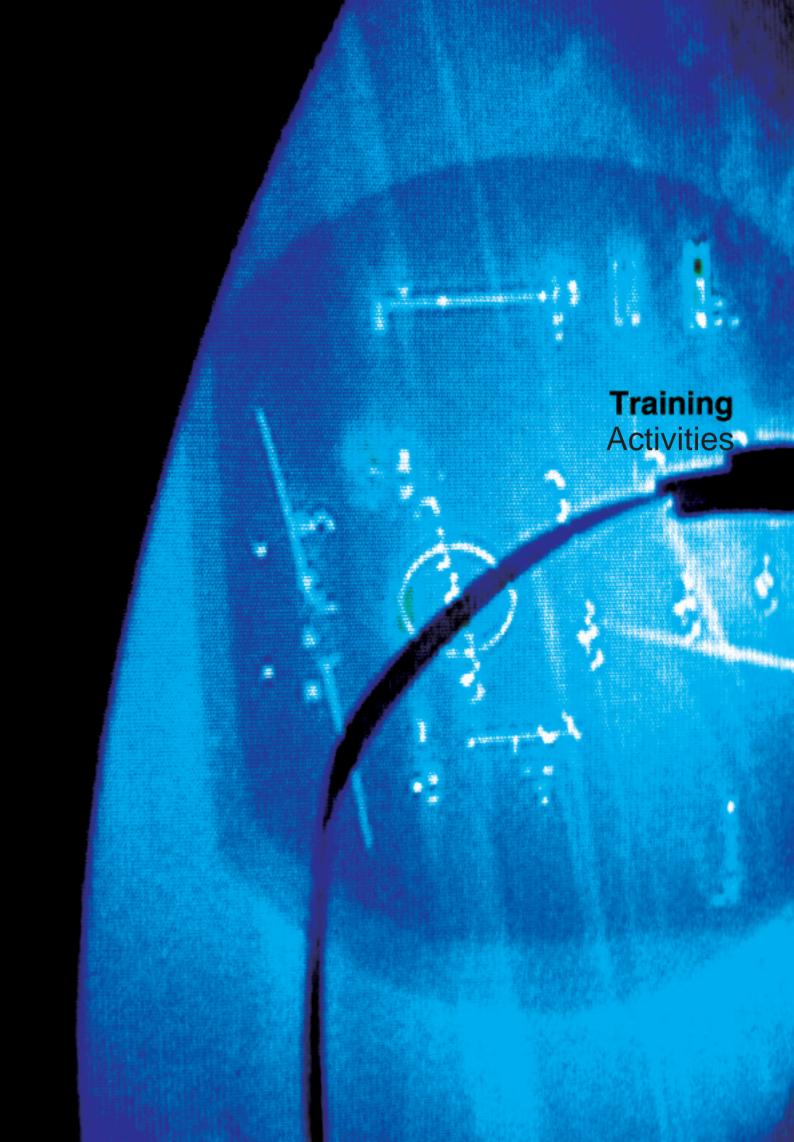
IMPLEMENTATION

DEMO System

Business Directory

Best Cases

Consulting



training activities

The Training of CESGA's Users and Personnel

During 2007, the Centre participated in the organization of a total of 28 training activities, distributed as indicated in the Table below.

Training Activities organized by or participated in by CESGA between 2004 and 2007

Concretely, it is the users of the Centre, the RTD personnel of businesses, and the public administration, teachers, researchers, and students of secondary and higher education who benefit from these activities. The same is true for the personnel of CESGA itself as stipulated by the Annual Training Plan.

The majority of these activities were related to the establishment and the optimal use of advanced technologies. The average length of the courses was 11.35 hours and promoted aspects such as compilation, programming languages, or content management.

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DETAIL OF THE TRAINING ACTIVITIES ORGANIZED BY OR PARTICIPATED IN: CESGA-2007

Training Activity Title	Type	In Collaboration with	Date of Activity	Duration (h)
Programming with UPC	Course	HP	4th Trimester	15
Advanced SUSE	Course	Intel	4th Trimester	10
Globus 4	Course	UDC	4th Trimester	40
Parallel Programming using OpenMP directives	Course	UDC	4th Trimester	15
HP MPI and IB	Course	HP	4th Trimester	25
DataProtector	Course	Intel	4th Trimester	24
Insight Manager	Course	HP	4th Trimester	18
Expert in the Administration and 250	Course	Globa	ll Estrategias	2nd Trimester
Management of e-Learning Projects				
Optical Networks	Course	UVIGO	2nd Trimester	4
Personal Data Protection (LOPD) Seminar	Course	EOSA	2nd Trimester	5
MPI	Course	USC	1st Trimester	15
Computational Mathematics	Course	UDC	1st Trimester	15
"AJAX: a practical approach"	Course	UVIGO	1st Trimester	8
OpenOffice	Course	Compostela Wireless	1st Trimester	8

DETAIL OF THE SEMINARS AND CONFERENCES ORGANIZED BY, OR PARTICIPATED IN: CESGA-2007

Title of the Activity	Туре	In collaboration with	Date
"Applications of Inductive Logic Programming	Seminar	Rui Camacho	
		Nuno Fonseca	
(ILP) in Molecular Biology problems"		(IBMC Universidade do Porto)	9/28/2007
1st Iberian GRID Infrastructure	Scientific Conference	CESGA	5/14–16/2007
Conference IBERGRID			
ISOC-ES Conference Cycle:	Seminar	CESGA	10/18/2007
"Social Networks as an Economic Asset".			
ISOC-ES Conference Cycle: "The 10 Internet	Seminar	CESGA	12/20/2007
Changes of Greatest Impact in 2007".			
ISOC-ES Conference Cycle: "An Internet	Seminar	CESGA	11/15/2007
Radio. A Basque Country Experience".			
ISOC-ES Conference Cycle: "Internet, a	Seminar	CESGA	04/18/2007
Common Good: the Governance of Internet".			

CESGA NODE ACTIVITIES IN THE I-MATH PROJECT

Mathematica.nodo.cesga.es	Туре	Responsible organisation	Date
Computational Math: Compiling,	Course	CESGA	03/26-28/2007
execution and program optimization			
Parallel Programming using OpenMP Directives	Course	CESGA	11/12-14/2007
Quantitative Finances FC-2007	Seminar	USC, Caixa Galicia	07/06/2007
Interaction: Applied Math and Industry	Seminar	USC	04/24/2007
Mathematics in the Biomedical Industry MIB-2007	Seminar	UDC	04/12/2007
Mathematical Modeling and Numerical	Seminar	UVIGO	11/29-30/2007
Simulation of Forest Fire Propagation			
AUTO Industry - i-MATH - CTAG	Seminar	Galician Auto Industry	09/18/2007
		Technological Centre, USC , CESGA	



dissemination

Noteworthy Activities in 2007

The objectives of the area of Promotion and Communication at CESGA include the planning, coordination, and execution of the PR & Communication activities of S.A.X. and the Foundation. The goal is to inform the users and the different social agents of the resources and services that are available to researchers through the Centre, as well as the improvement of the relations with the users and with the technical and general communication media. The most relevant activities of the area in 2007 are presented below.

- » One of the most important activities during the year was the organization of the 1st Iberian Grid Infrastructure Conference, IBERGRID, and the subsequent publication of the Proceedings.
- » The drafting and the implementation of the CESGA Communication Plan, 2007-2008.
- » The planning of the CESGA corporate video, the CESGA technical newsletter, and other activities described in the Communication Plan.
- » The writing and distribution of press releases and press calls to the technical and general communication media concerning projects and initiatives of the Centre.
- » Cooperation with requests made by radio, television, and print media throughout the year and collaboration with media representatives and invited authors in publications regarding the preparation and writing of reports about Centre projects.
- » Support services to the Press Departments of the Regional Ministry for Innovation and Industry.
- » Support for the organisation of the exhibition, "Dos ábacos aos computadores" ("From abacus to computers"), organized by the Vice-President for Culture of the University of Santiago de Compostela and sponsored by Caixanova.

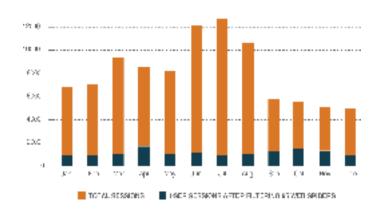
The Area of Promotion and Communication is also responsible for the development and maintenance of the dissemination tools: "Díxitos" magazine, Web, conferences, events, etc.

- » The quarterly publication of "Díxitos" of which 1,350 copies were distributed.
- » The publication of the ANNUAL 2007 that reports the activities of the Centre, maintaining a stable number of copies (1,500).
- » The establishment of the video-on-demand repository of training and dissemination activities, tv.cesga.es

In addition, the area is also in charge of supporting the elaboration of the CESGA publications, including the studies conducted as a result of projects developed in the Centre, communications, and posters created for presentation in scientific conferences, project websites, etc.

» The preparation of presentations, dossiers, and reports for management and personnel of the Centre, including the presentation of FINIS TERRAE, the proposal for the creation of the CESGA Computational Science Research Centre (C2SRC), and the proposal for the creation of a node of the Spanish Institute of Mathematics in Galicia (IEMath), among others.

DAYLY AVERAGE OF USER SESSIONS IN WWW.CESGA.ES 2007



- » Support to the following projects: ENSIGNA, e-HOSPITAL, T-MAESTRO, MANCOMUN, CAPITA, ISOC, "Programa ConCiencia", elMRT, RECETGA, I-MATH and FINIS TERRAE.
- » The planning of the Bibliographic study of the Scientific Production of the users of the Centre in collaboration with BUGALICIA. The collection of data relative to the scientific production of the 2006 users and the preparation of the campaign to collect data from the 2007 users.
- » The planning of satisfaction surveys for the users of CESGA computing, storage, and communications services, promoting the adoption of measures in accordance with the survey results.
- » The planning of the survey regarding satisfaction and knowledge of CESGA services and resources on the part of the users; in collaboration with CIDADANIA.
- » Support to the Spanish Royal Society of Mathematics (RSME), the Society of Statistics and Operative Investigation (SEIO) and the European Courses in Advanced Statistics (ECAS) for the hosting of their websites in the CESGA servers.
- » Support for the publication of the strategic research agenda of VINDEIRA (Galician ICT Technological Platform.)
- » Participation in the review process of dissemination projects within the frame of the call launched under the Program of Social Awareness associated with the PGIDT and driven by the Director General for RTD.
- » Participation in the Scientific Commission of the Forum of Communication and Science, organized by the Director General for RTD and the Professional Association of Galician Journalists.
- » Support for thematic networks: the organisation of RedeGRID training events. Maintenance of the website and the distribution list of RedeBioinfo, the Galician Network of Bio-informatics, as well as the Galician Network of High Performance Computing (GHPC Network).

- Communication support to the Technological Centres Network, RETGALIA, and to the ICT Technological Platform in Galicia, VINDEIRA.
- » Creation of the contents concerning CESGA for the Annual Report of the CSIC delegation in Galicia.

Finally, in the area of Promotion and Communication, the logistical organisation of the Annual Training Project for CESGA's users and personnel

- » Collaboration in the organisation of the training events of the Centre
- » Maintenance of the content management application for www.cesga.es. The implication of the personnel of all of the departments of the Centre in the maintenance of the contents of the website.







www.turgalicia.es

TODOS OS RECURSOS E ALOXAMENTOS TURÍSTICOS DE GALICIA





