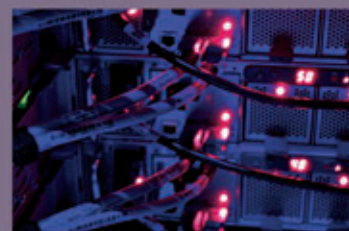
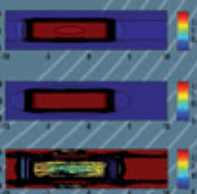
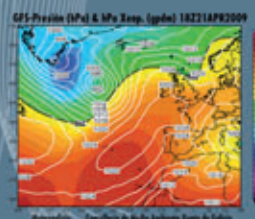
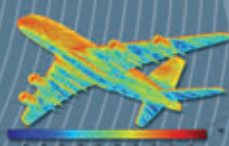
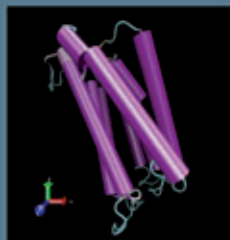
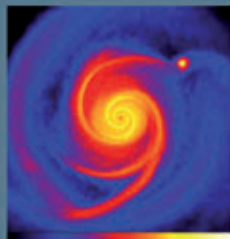
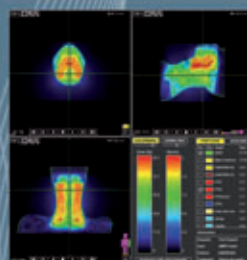
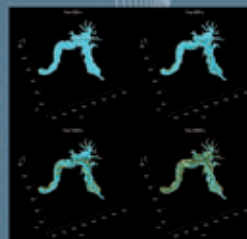
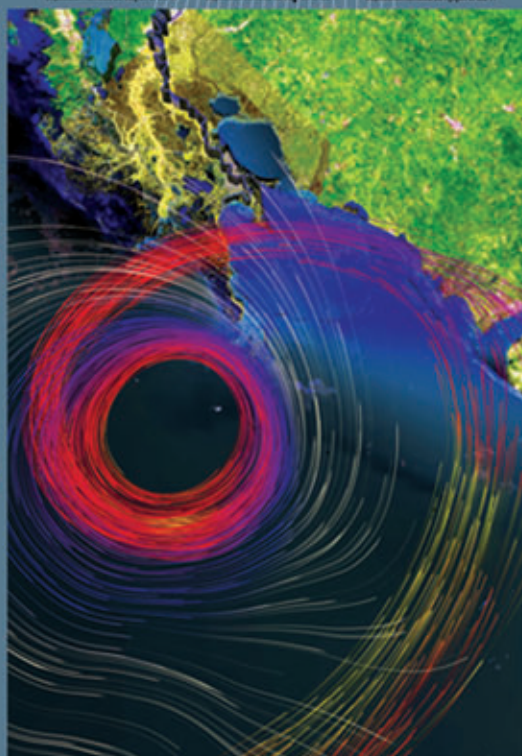
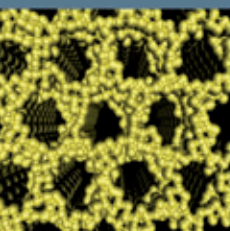
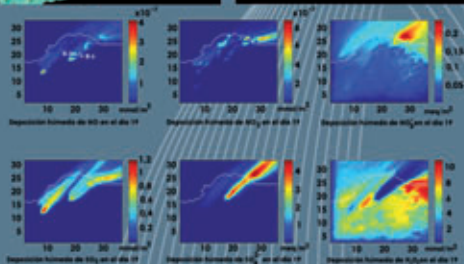
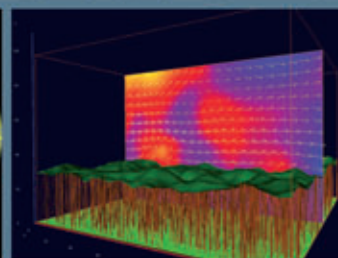
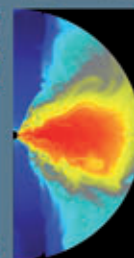
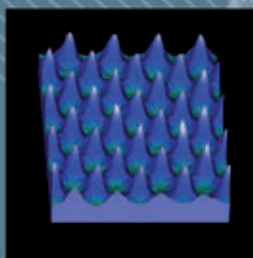
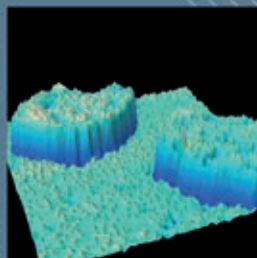
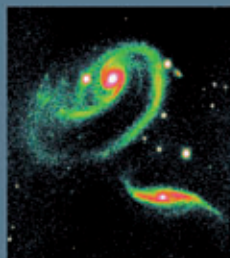


CESGA

ANNUAL ACTIVITY REPORT

2008




XUNTA DE GALICIA
 CONSELLERÍA DE ECONOMÍA
 E INDUSTRIA


**CONSEJO SUPERIOR
 DE INVESTIGACIONES
 CIENTÍFICAS**


FEDER
 FONDO EUROPEO DE
 DESARROLLO REGIONAL


**GOBIERNO
 DE ESPAÑA**

**MINISTERIO
 DE CIENCIA
 E INNOVACIÓN**



CESGA ANNUAL REPORT 2008

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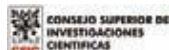
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15705 SANTIAGO DE COMPOSTELA

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Fundación CESGA is a non profit organisation at the service of scientific research since 1993. The Regional Government of Galicia (Xunta de Galicia) and the Spanish National Research Council (CSIC) participate as partners in Fundación CESGA.

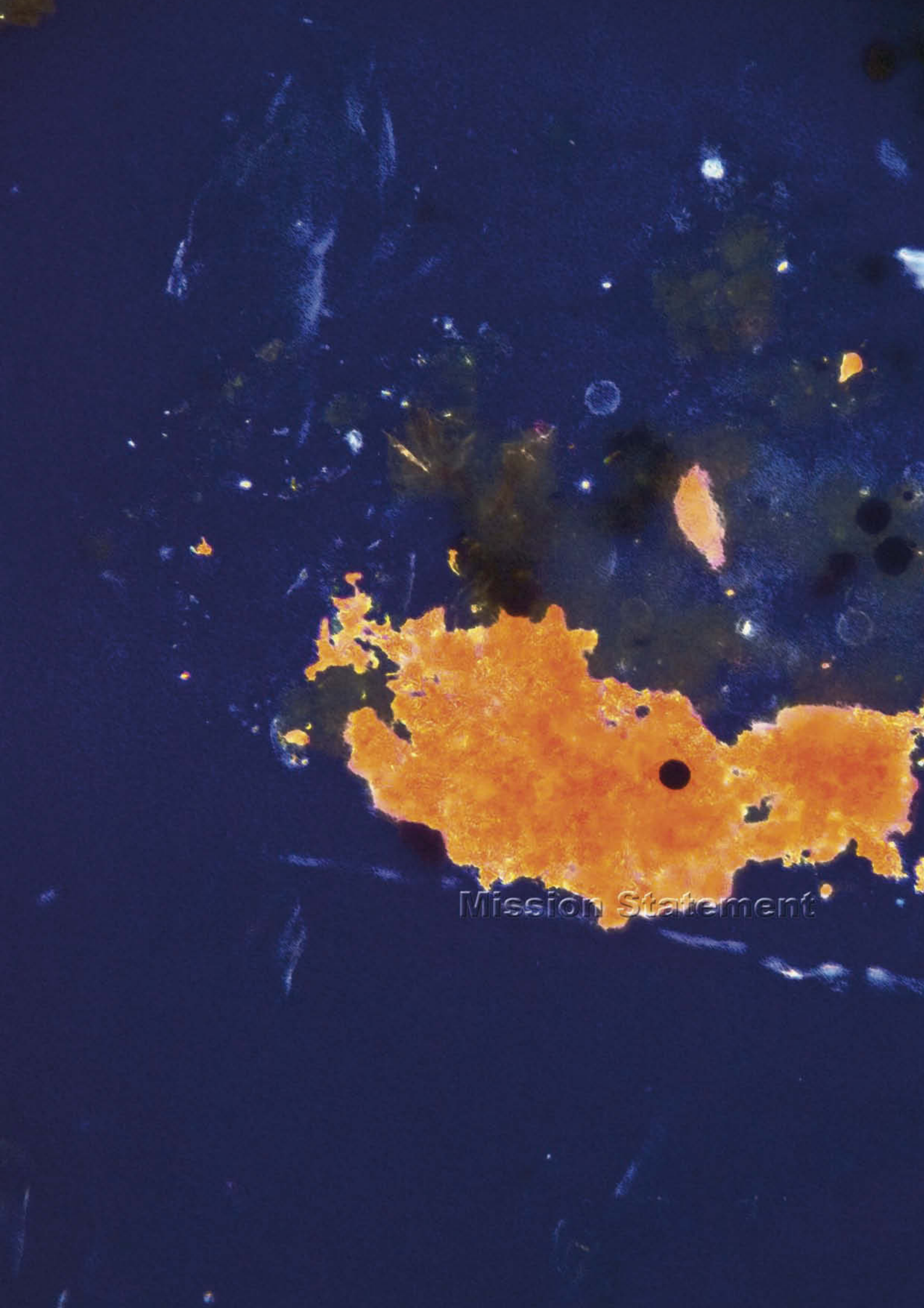


Fundación CESGA's infrastructures have been partially funded by the European Union through the European Regional Development Fund (ERDF) and by the Government of Spain through the Ministry of Science and Innovation (MICYT) as well as by the Xunta de Galicia and CSIC.



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Mission Statement

mission statement

The **mission of CESGA** is:

To provide high performance computing and advanced communications resources and services to the scientific community of Galicia and to the Spanish National Research Council (CSIC) as well as to institutions and enterprises with R&D activity, and

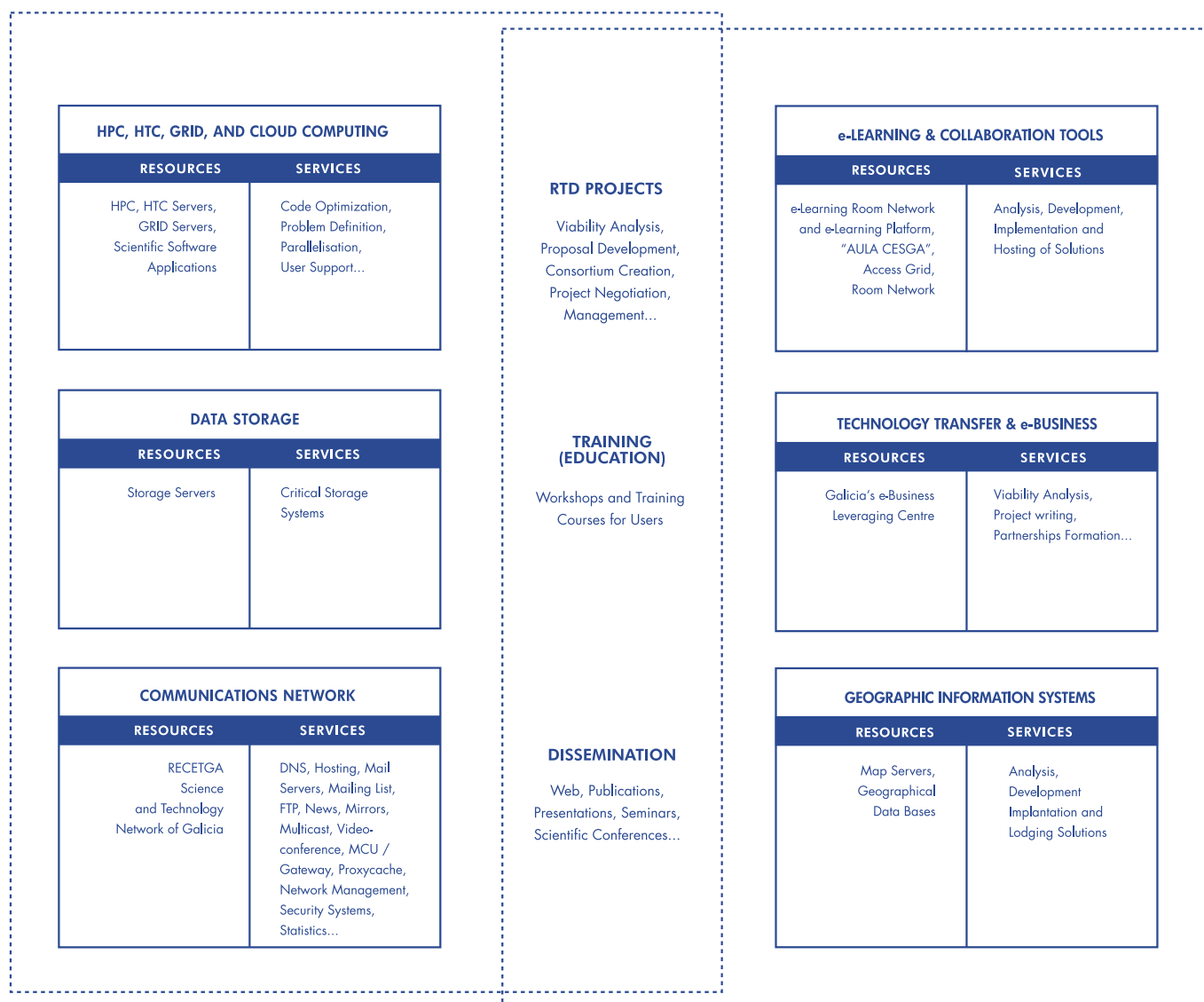
To promote and conduct high quality research in Computational Science in close collaboration with the research community of Galicia as well as other regions or countries around the world thereby contributing to the advancement of science, the transfer of technology to industry

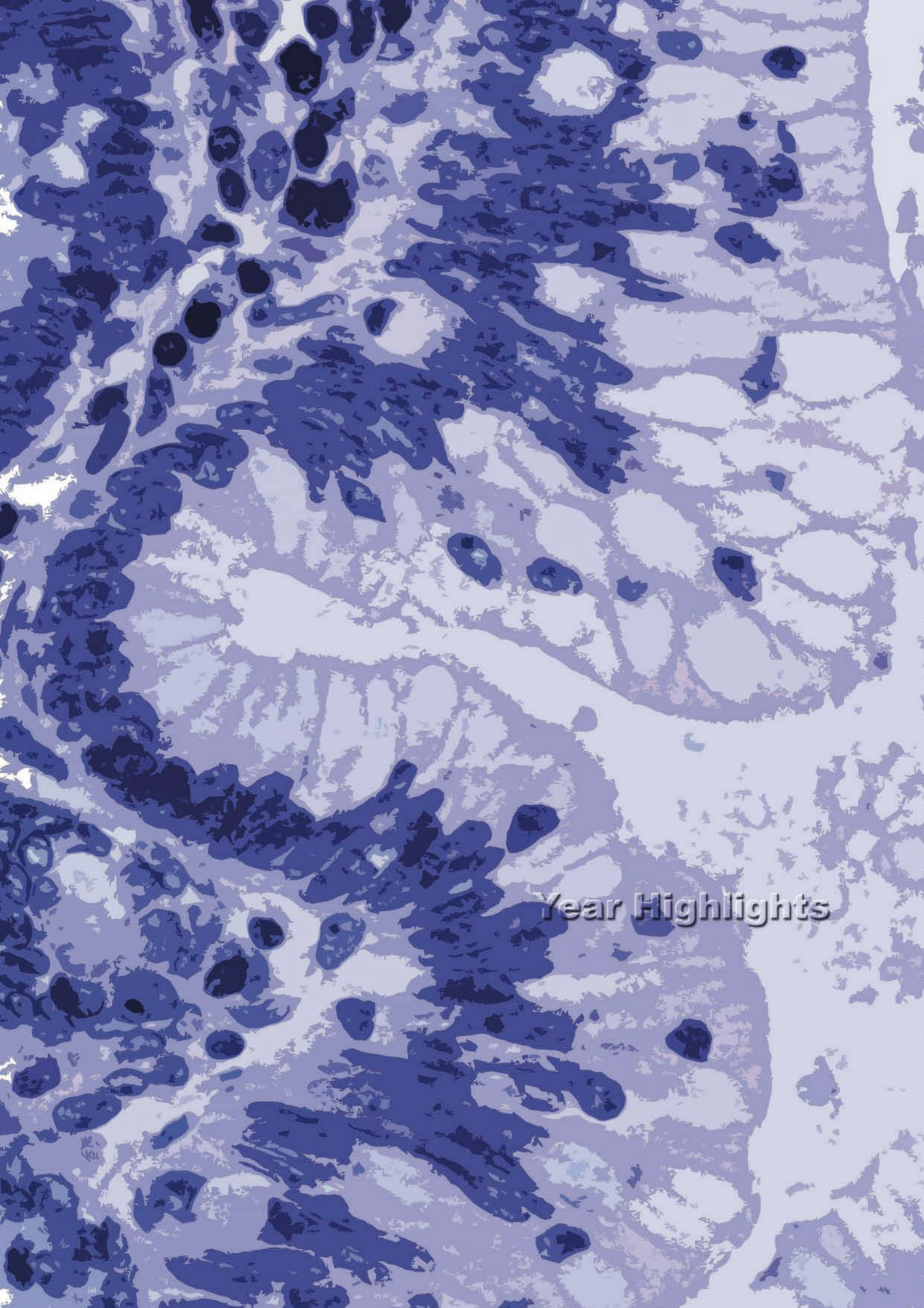
and administrations, and as a consequence, the welfare of society as a whole.

Thus, the Centre's main functions are:

- to supply high performance computing and advanced communications services to users,
- to manage the Science and Technology Communications Network of Galicia,
- to promote and develop cooperation between companies and institutions,
- to promote the use of innovative ICT, and
- to conduct research in Computational Science.

CESGA FUNCTIONAL AREAS



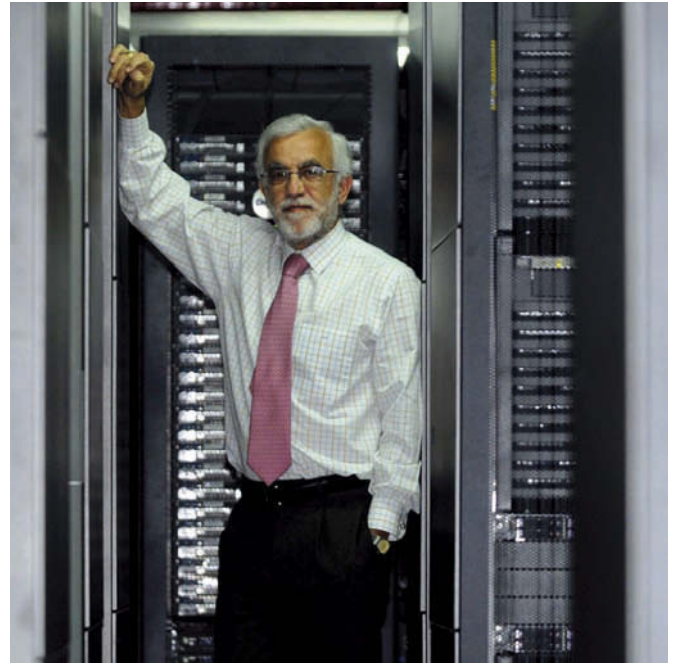


Year Highlights

Introduction

During the year 2008, intense activity was carried out with respect to the organisation, strategies, and infrastructure. The most significant activities accomplished during 2008 are summarised below.

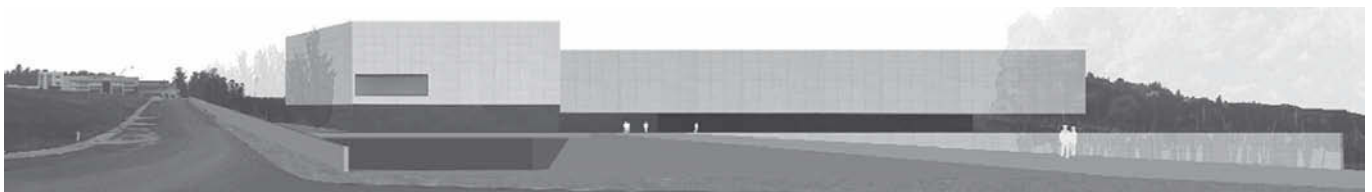
- Finis Terrae Supercomputer was put into operation in the first quarter. Finis Terrae ranked No. 100 on the TOP500 list until June.
- Six (6) supercomputing grand challenges were undertaken: the mathematical problem of the FEKETE points, HEMCUVE ++, that resolved 150 million unknowns which was a world record, wien2k for the solution of what the American Institute of Physics determined to be the 3rd/4th physics problems of today, the genetic algorithm of the IEM-CSIC, and LAMMPS of the IEM.
- The number of computing hours executed was 5 times greater than that of the previous year.
- Signature of a collaboration agreement by the Spanish Ministry for Science and Innovation, the Regional Government of Galicia (Xunta de Galicia), and CESGA to finance the new CESGA Headquarters Building.
- The Tender for Ideas for the new CESGA Headquarters building was published and judged.
- Signature of a collaboration agreement by the DGT (the Spanish department in charge of traffic) and CESGA for the sharing of communications networks and supercomputing infrastructures.
- The Spanish Ministry for Science and Innovation, the Regional Ministry of Innovation and Industry, CESGA and RED.es signed a collaboration agreement for the interconnection



Javier García Tobío. Managing Director

of the Spanish (RedIRIS), the Portuguese (FCCN), and the Galician (RECETGA) academic and research communications networks.

- The Fundación CESGA modified its organisational chart and takes up, the production areas of SAX CESGA.
- The scientific-technological plan of CESGA Computational Science Research Centre (C2SRC) was designed and presented.
- The Strategic Plan for CESGA 2010-2013 was elaborated.
- CESGA received the award, APPLUS+, for quality of management.

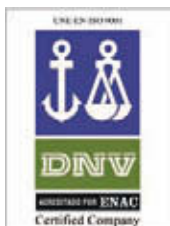
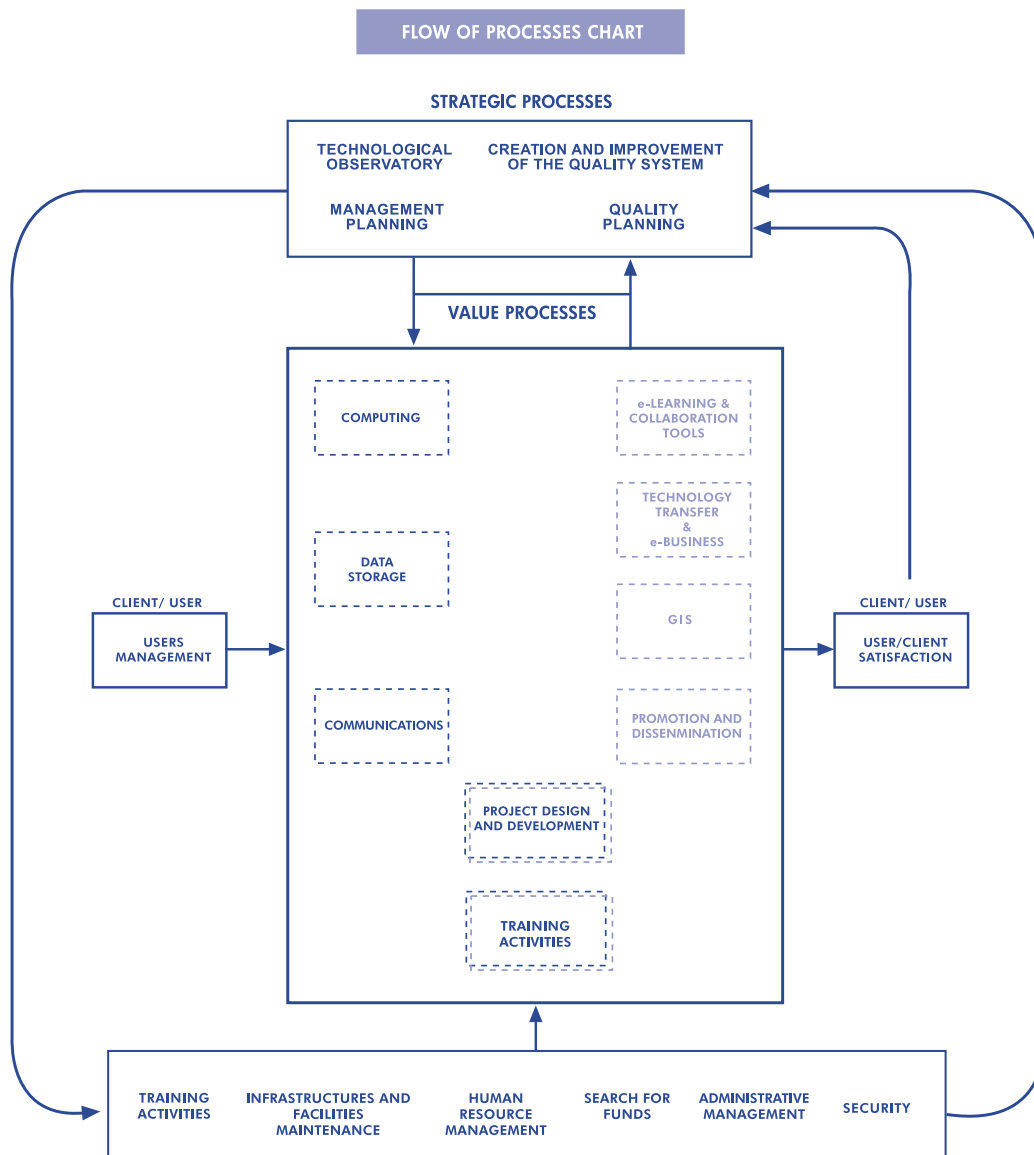


New CESGA Headquarters Building Project



Quality of
Services

quality of services



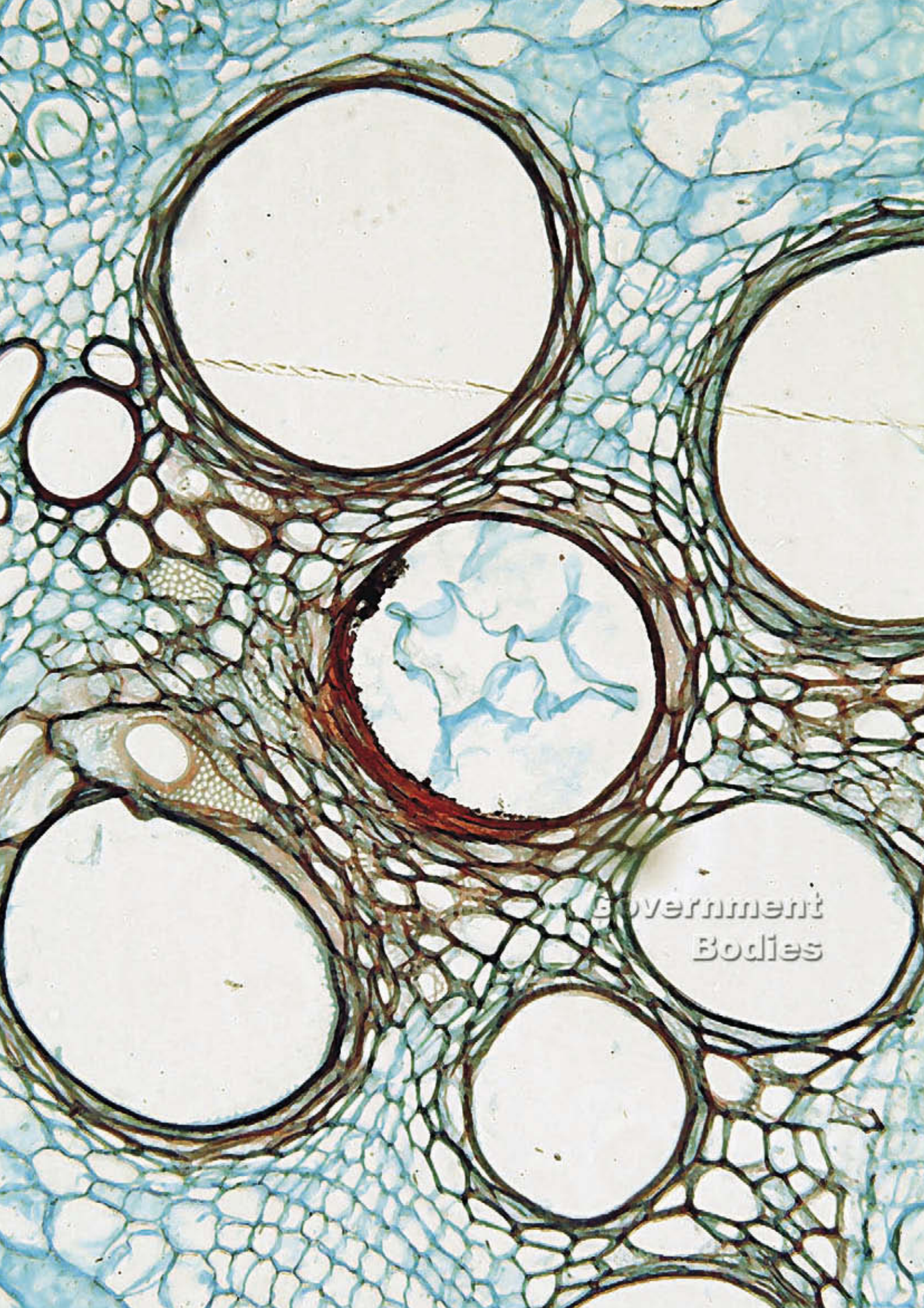
During 2008, CESGA Foundation as well as S.A.X. CESGA renewed the certification of quality, **ISO 9001:2000** that was originally obtained in December 2005. At that time, CESGA became the first supercomputing centre in Spain to hold such certification.

This 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 provided to users.

Quality, a map of processes

Only during this third year in which the certification was in force, 4 processes, 5 procedures, and 4 instructions have been improved. CESGA was audited twice, both with successful results. One audit was internal but performed by external auditors and the other was external.

Additionally, in 2008, continued advances were made in the automating of all processes associated with quality control, with improvements in the monitoring systems of the centre (users, systems, applications, etc.) in accordance with the norm **ISO 9001: 2000**.



Government
Bodies



government bodies of the legal entities that constitute CESGA

BOARD OF DIRECTORS S.A.X CESGA

<p>REGIONAL GOVERNMENT OF GALICIA</p>  <p>XUNTA DE GALICIA</p>	PRESIDENT	Salustiano Mato de la Iglesia Director General for RTD Regional Ministry for Innovation and Industry
	SECRETARY	Patricia Iglesias Rey Legal Adviser Regional Ministry for Innovation and Industry
	MEMBER	Gonzalo Gómez Montaña Director General of the Computing Centre for Tax Management, Finances and Accounting Regional Ministry for Economic Affairs
	MEMBER	M ^a Elena Veiguela Martínez Director General for the Promotion of Industry and Information Society Regional Ministry for Innovation and Industry
	MEMBER	Rogelio Conde Pumpido Director General for the Promotion of Science and Technology in the Galician University System Regional Ministry of Education
	MEMBER	Manuel J. Fernández Iglesias Director General for Audiovisual Communication Secretary General for Communication
	MEMBER	Emilio Nogueira Moure Secretary General Regional Ministry for Innovation and Industry
	MEMBER	Juan J. Gómez Romero Director General for Public Policy Quality Assessment Regional Ministry for the Presidency
<p>SPANISH NATIONAL RESEARCH COUNCIL</p> 	VICE-PRESIDENT	Rosa M. Menéndez López Vice-president for Scientific and Technological Research Spanish National Research Council (CSIC)
	MEMBER	Carlos Manuel Abad Ruíz Deputy Secretary-general of Economic Performance Spanish National Research Council (CSIC)
	MEMBER	Uxío Labarta Fernández Institutional Coordinator Spanish National Research Council Galician Division
	MEMBER	Antonio Álvarez Alonso Researcher Marine Research Institute (CSIC)
	MEMBER	M ^a Concepción Herrero López Vice-President for Research University of A Coruña
	MEMBER	M ^a José Alonso Fernández Vice-President for R&D University of Santiago de Compostela
	MEMBER	Manuel Joaquín Reigosa Roger Vice-President for Research University of Vigo

Data as of 31/12/2008

BOARD OF TRUSTEES OF CESGA FOUNDATION

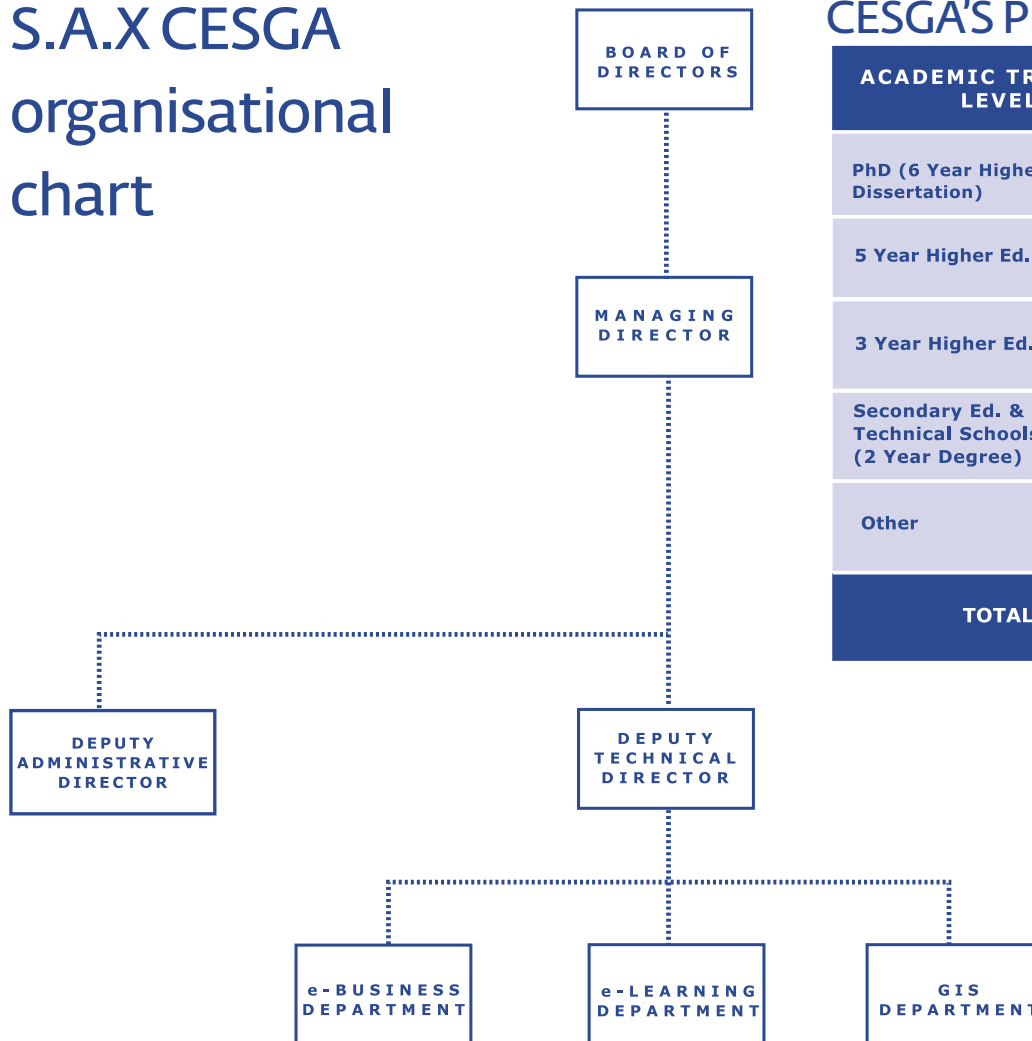
<p>REGIONAL GOVERNMENT OF GALICIA</p>  <p>XUNTA DE GALICIA</p>	<p>PRESIDENT</p>	<p>Salustiano Mato de la Iglesia Regional Ministry for Innovation and Industry</p> <p>Director General for RTD Regional Ministry for Innovation and Industry</p>
	<p>SECRETARY</p>	<p>Patricia Iglesias Rey Regional Ministry for Innovation and Industry</p> <p>Legal Adviser Regional Ministry for Innovation and Industry</p>
	<p>MEMBER</p>	<p>Gonzalo Gómez Montaña Regional Ministry for Economic Affairs</p> <p>Director General of the Computing Centre for Tax Management, Finances and Accounting Regional Ministry for Economic Affairs</p>
	<p>MEMBER</p>	<p>M^a Elena Veiguela Martínez Regional Ministry for Innovation and Industry</p> <p>Director General for the Promotion of Industry and Information Society Regional Ministry for Innovation and Industry</p>
<p>SPANISH NATIONAL RESEARCH COUNCIL</p>  <p>CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS CSIC</p>	<p>MEMBER</p>	<p>Rogelio Conde Pumpido Regional Ministry of Education</p> <p>Director General for the Promotion of Science and Technology in the Galician University System Regional Ministry of Education</p> <p>Rosa M. Menéndez López Spanish National Research Council (CSIC)</p> <p>Vice-president for Scientific and Technological Research Spanish National Research Council (CSIC)</p> <p>Uxío Labarta Fernández Spanish National Research Council Galician Division</p> <p>Institutional Coordinator Spanish National Research Council Galician Division</p>

Data as of 31/12/2008



Organisational
Chart

S.A.X CESGA organisational chart



CESGA'S PERSONNEL IN 2008

ACADEMIC TRAINING LEVEL	NUMBER	MALE
PhD (6 Year Higher Ed.+ Dissertation)	10	10
5 Year Higher Ed.Degree	24	14
3 Year Higher Ed.Degree	4	3
Secondary Ed. & Technical Schools (2 Year Degree)	18	15
Other	1	1
TOTAL	57	43

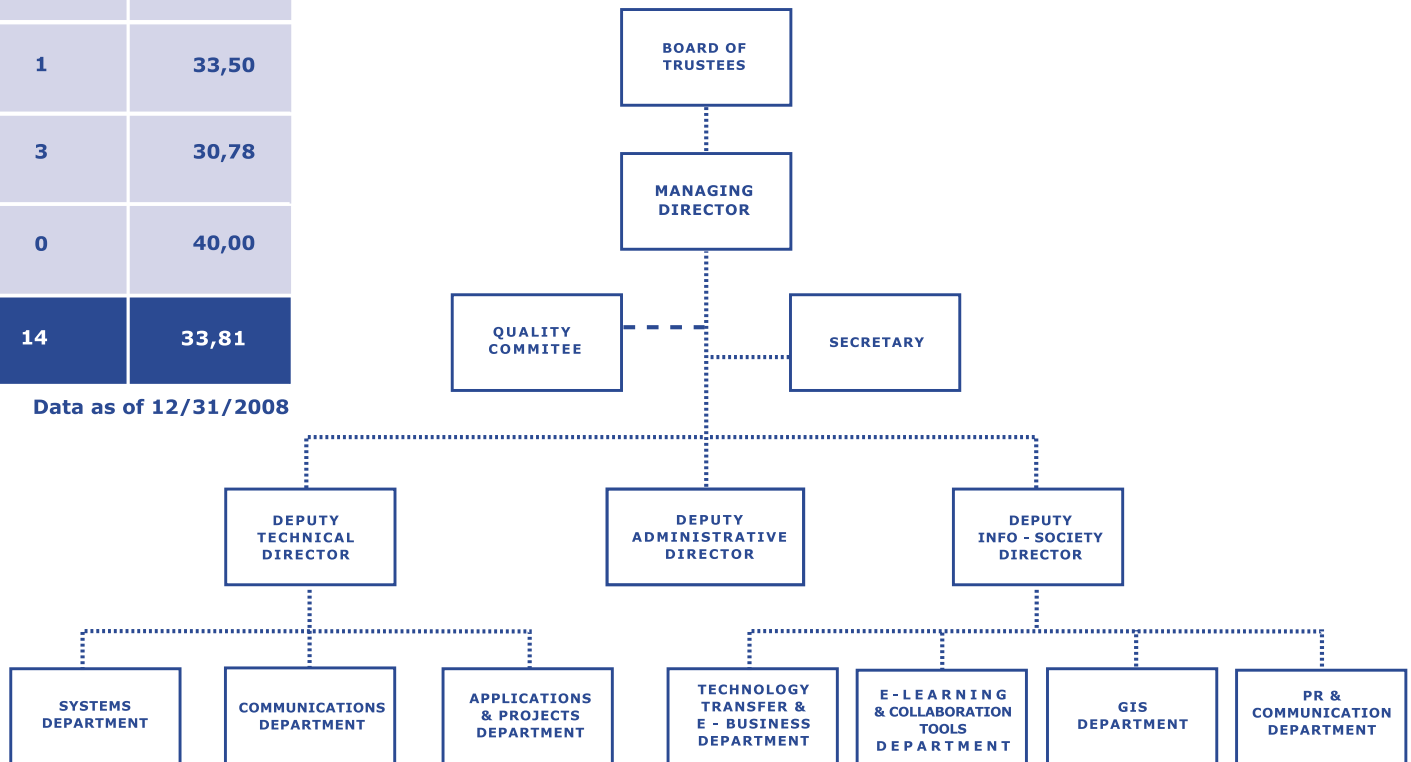
CESGA'S work force, its most valuable asset

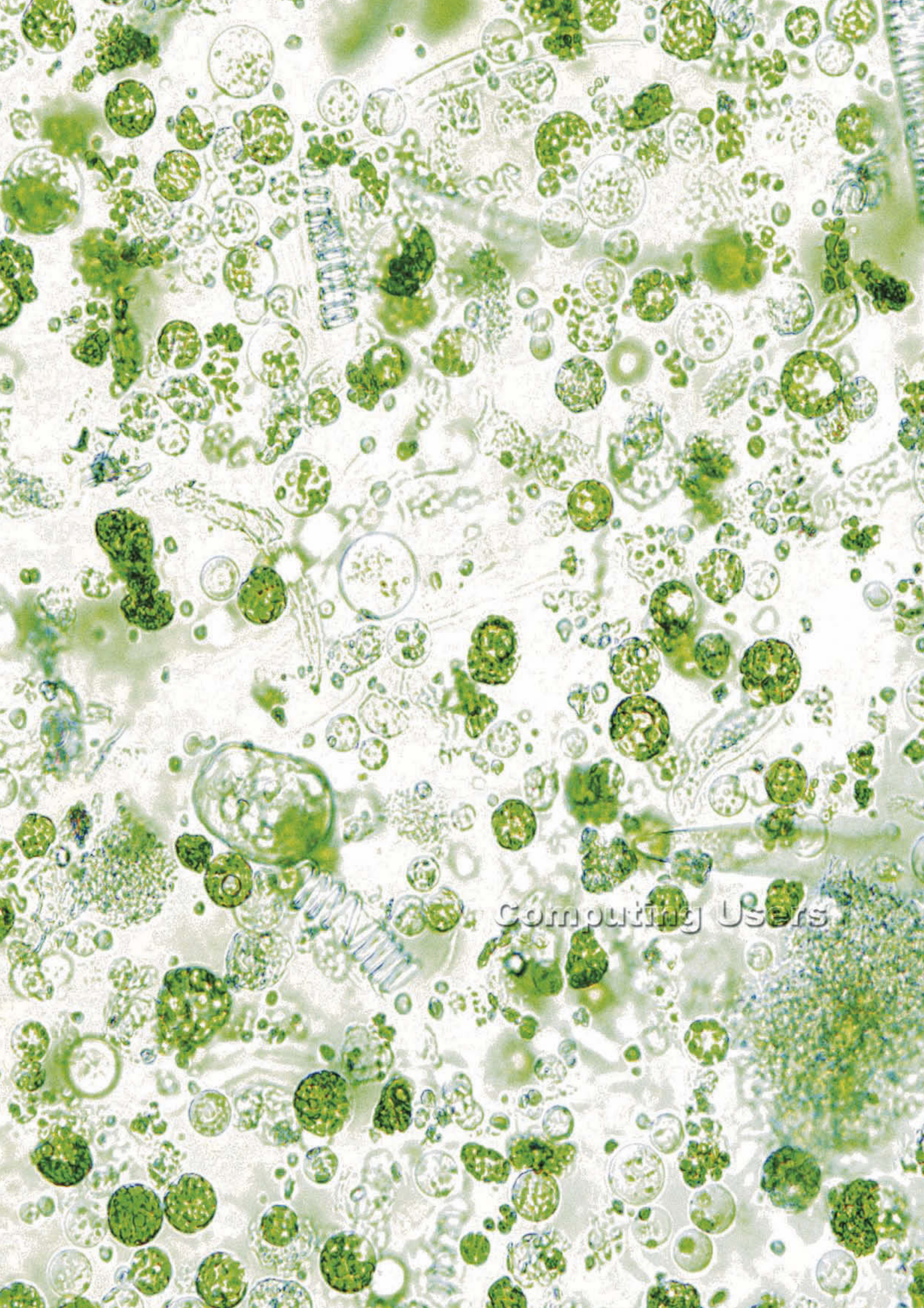


CESGA Foundation organisational chart

FEMALE	AGE AVERAGE
0	35,90
10	35,00
1	33,50
3	30,78
0	40,00
14	33,81

Data as of 12/31/2008





Computing Users

Most active users in 2008 by institution

USER	DEPT./CENTRE	HOURS USED
SANTIAGO DE COMPOSTELA UNIVERSITY (USC)		
Manuel María González Alemany	Applied Physics	574,649.4
Luis Tortajada Iaviu	Condensed Matter Physics	409,140.1
Lucas Vázquez Besteiro	Condensed Matter Physics	329,355.0
Ángel Piñeiro Guillen	Applied Physics	291,328.7
Paola Mendoza Espinosa	Applied Physics	232,715.5
María Pilar Brocos Fernández	Applied Physics	169,876.0
■ ■ ■ ■ ■	■ ■ ■ ■ ■	■ ■ ■ ■ ■
A CORUÑA UNIVERSITY (UDC)		
Daniel Rivero Cebrián	Communications & Information Technologies	152,969.9
Oscar Ibáñez Panizo	Communications & Information Technologies	145,231.7
Daniel Rodríguez Ramos	Chemistry, Physics and Chemical Engineering I	85,894.1
María Isabel Fernández Pérez	Chemistry, Physics and Chemical Engineering I	65,092.3
Sonia Vilarinho Patiño	Fundamental Chemistry	62,876.1
María Fernández González	Fundamental Chemistry	54,704.7
■ ■ ■ ■ ■	■ ■ ■ ■ ■	■ ■ ■ ■ ■
VIGO UNIVERSITY (UVIGO)		
Fernando Obelleiro Basteiro	Signal Theory and Communications	155,254.4
Olalla Nieto Faza	Organic Chemistry	121,971.8
Rosana Álvarez Rodríguez	Organic Chemistry	56,304.0
Laura Estévez Guiance	Analytical Chemistry and Nutrition	34,376.8
Adán Borja González Pérez	Organic Chemistry	32,359.0
José Antonio Souto Salgado	Organic Chemistry	23,786.0
■ ■ ■ ■ ■	■ ■ ■ ■ ■	■ ■ ■ ■ ■
SPANISH NATIONAL RESEARCH COUNCIL (CSIC)		
José Carlos Conesa Cegarra	Group of Fundamental and Applied Catalysis	541,568.4
Víctor Cruz Cañas	Molecular Physics Dept.	540,875.7
Manuel Cobian González	Atomic & Molecular Physics Theoretical Dept.	434,634.2
Octavio Roncero Villa	Atomic & Molecular Physics Theoretical Dept.	265,822.2
Jorge Sánchez Dolado	Nanostructured Materials Unit	253,737.6
Delia Fernández Torre	Molecular Physics Dept.	200,353.8

Both the number of users from CSIC Centres (+54%), and the CPU hours used (+1,032%) by these dramatically increased in 2008

CSIC CENTRES		Department-Group	# of active user accounts		Hours used	
			2007	2008	2007	2008
	Instituto de Tecnología Química (ITQ)	Grupo de carbohidratos	0	1	0	2,453.4
	Centro de Investigaciones Biológicas (CIB)	Estructura y función de proteínas	3	1	13,888	41,976.7
		Microscopía electrónica de Macromoléculas	1	1	1,067.7	1,223.1
		Grupo de Resonancia Magnética Nuclear	3	3	4,648.6	1,098.7
	Centro de Investigación y Desarrollo (CID)	Centro de Investigación y Desarrollo	1	0	5,071.5	0
	Estación Biológica de Doñana (EBD)	Ecología de Humedales, Genética de la Conservación en Peces Litorales	0	1	0	75.2
		Biología Evolutiva; Integrative Ecology Group	1	4	446.8	26,420.3
		Genética de la conservación	2	4	12,181.8	19,832.9
		Evolución de relaciones planta animal	0	2	0	17,356
	Centro Nacional de Biotecnología (CNB)	Estructura de Adenovirus	0	1	0	86,395.2
		Departamento de Estructura Macromolecular	0	4	0	8,483.8
	Instituto de Ciencia de Materiales de Barcelona (ICMAB)	Estructura Electrónica de Materiales	0	9	0	635,169.9
		Departamento Teoría y simulación de materiales	0	2	0	12,783.4
	Estación experimental del Zaidín (EEZ)	Ciencias de la Tierra y Química Ambiental/ Química Teórica y Modelización Molecular	7	3	60,928.5	6,940.7
	Institut Mediterrani d'Estudis Avançats (IMEDEA)	PANCODING	0	1	0	66.5
	Instituto Cajal (IC)	Neurobiología del Desarrollo	1	1	16,680.9	550.2
	Instituto de Análisis Económico (IAE)	Instituto de Análisis Económico	0	1	0	1,923.8
	Instituto de Catálisis y Petrolequímica (ICP)	Grupo de Catálisis Fundamental y Aplicada	2	1	11,129.5	541,568.4
	Instituto de Ciencia de Materiales de Aragón (ICMA)	Química Orgánica	1	1	48	5,804.3
		Química de los Compuestos Organometálicos	1	0	283.3	0
		Química/Grupo Síntesis Orgánica Estereoselectiva	1	1	19,087.6	48,015.5
	Instituto de Ciencias de Materiales de Sevilla (ICMS)	FQM282	0	1	0	20,849.8
		Superficies, intercapas y capas finas	0	1	0	48,511.6
	Instituto de Estructura de la materia (IEM)	Departamento de Física Molecular	3	3	4,282.4	743,093
		Instituto de Estructura de la Materia	4	2	3,979.3	159,259.8
		Departamento de Astrofísica Molecular e Infrarroja	5	5	7,403.3	102,698.7
	Instituto de Física de Cantabria (IFCA)	Departamento de Estructura de la Materia; Grupo de Física Estadística y no Lineal	1	1	41	19,375.7
		Departamento de Astrofísica; Grupo CMB	1	0	89.5	0
	Instituto de Investigaciones Químicas (IIQ)	Grupo de síntesis Orgánica y Reconocimiento Molecular	0	1	0	17.4
	Instituto de Matemáticas y Física Fundamental (IMAFF)	Matemáticas	3	3	4,486.4	76,545
		Departamento de Física Atómica y Molecular Teórica	7	9	18,262.7	534,929.3
	Instituto de Investigaciones Químicas y Ambientales de Barcelona (IIQAB)	Química Teórica y Computacional	0	5	0	122,446.4
	Instituto de Química Médica (IQM)	Quimioterapia	2	2	14,911.3	1,506
	Instituto de Química Orgánica General (IQOG)	Química Orgánica Biológica	4	2	18,017.6	3,906.1
		Laboratorio de Radicales Libres y Química Computacional	0	2	0	2,488.5
		Productos Naturales	1	1	11,458.2	70
	Instituto Nacional del carbón (INCAR)	Texture of Materials for energetic applications	0	2	0	4,161
	Centre d'Estudis Avançats de Blanes	Unidad de Investigación de Ciencias Marinas Operacionales y Sostenibilidad	0	1	0	1,391.7
	Unidad asociada CSIC-LABEIN	Unidad de Materiales Nanoestructurados	1	1	13,193.2	253,737.6
	Centro de Biología Molecular Severo Ochoa (CBM)	Diseño Racional de Encimas-BioWeb	0	1	0	20,042.5
	Instituto de Ciencia y Tecnología de Polímeros (ICTP)	Química Macromolecular	1	1	8,241.9	22,362
TOTAL ACTIVE CSIC ACCOUNTS AND HOURS USED			57	86	316,429	3,605,455.6

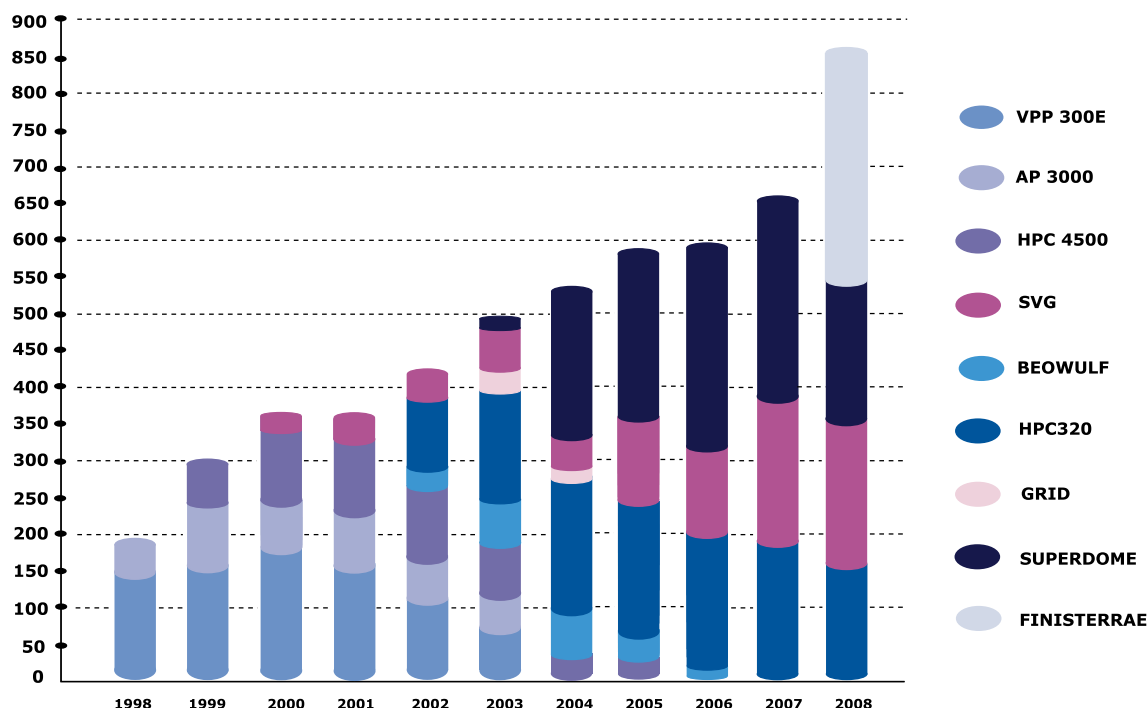
computing users

Number of Active User Accounts

Finis Terrae is the system with the greatest number of active accounts (that is, users with significant CPU time consumption throughout the year) with 313 users during its first year of operation. The SVG system had 213 active user accounts, increasing by 26 that of the previous year, in addition to Grid project users that are included within CESGA's projects and that pertain to national and international institutions present in the different

Grid initiatives in which CESGA participates (The Spanish e-Science Network, European projects such as EGEE, EELA and int.eu.grid, Spanish projects such as RETELAB and CYTEDGRID, and regional projects such as FORMIGA and G-FLUXO). In total, the number of active accounts increased by 53%, from 645 in 2007 to 986 in 2008. This growth was fundamentally motivated by the increase in the number of users of the Finis Terrae system and the incorporation of of Grid computing users.

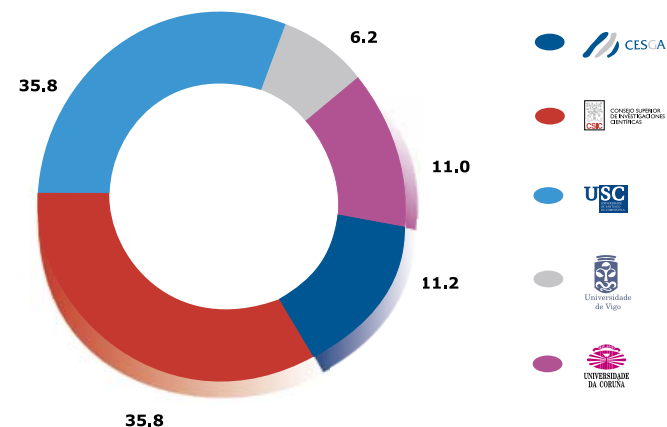
USER ACCOUNT EVOLUTION PER SYSTEM PER YEAR



Distribution by Institutions of the CPU hours Consumed in all Systems

With respect to institutions, the University of Santiago de Compostela and CSIC registered the greatest number of computing hours. The University of Santiago de Compostela consumed 35.8% of the total hours (which is 6.2% less than in 2007) which is the same consumption as CSIC that grew from 17% in 2007 to 35.8% in 2008. As a whole, the three Galician universities represent 53% of the total consumption (decreasing 24.1% with respect to the previous year). The projects in which CESGA participated were responsible for 11.2% of the hours consumed which include some of the computational challenges performed using Finis Terrae.

CPU USE DISTRIBUTION BY INSTITUTION

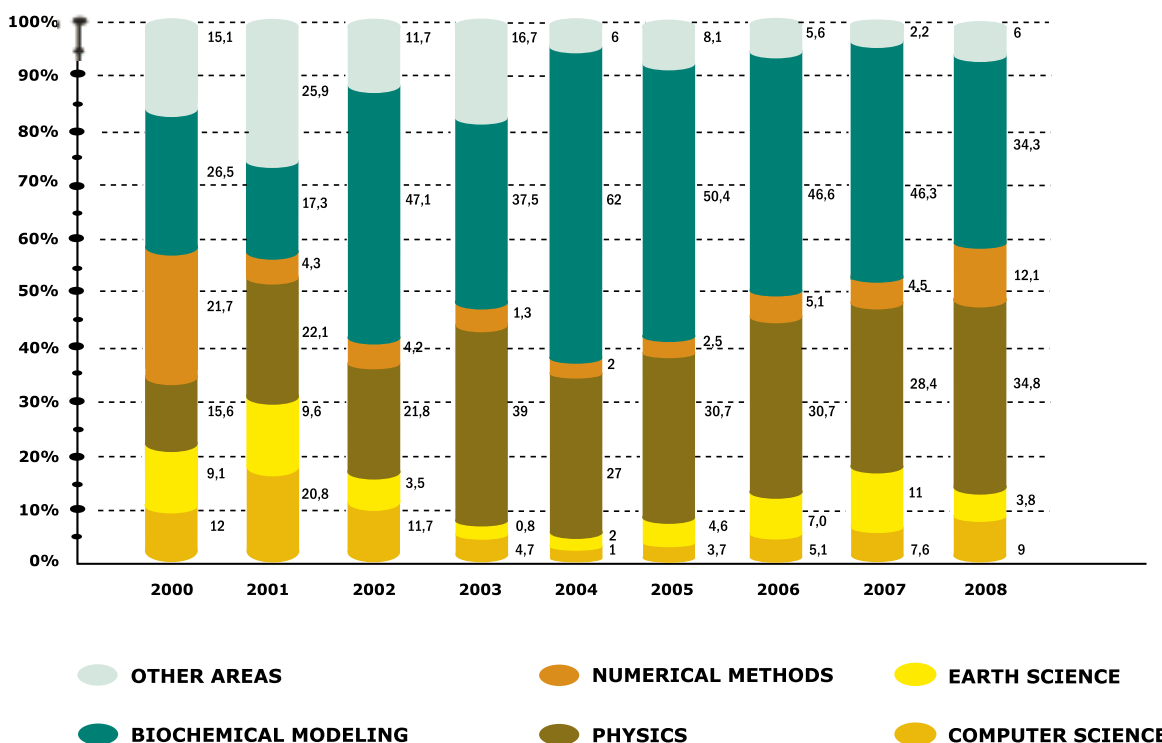


CPU Distribution by Research Area

With respect to research areas, the computing time related to physics represents 34.8% of the consumption, surpassing for the first time biochemical modeling that represents 34.3%

(14.8% less than in 2007). These two areas account for 69.2% of the total hours consumed. It is also important to highlight the increase in the area of Computing Science since 2004.

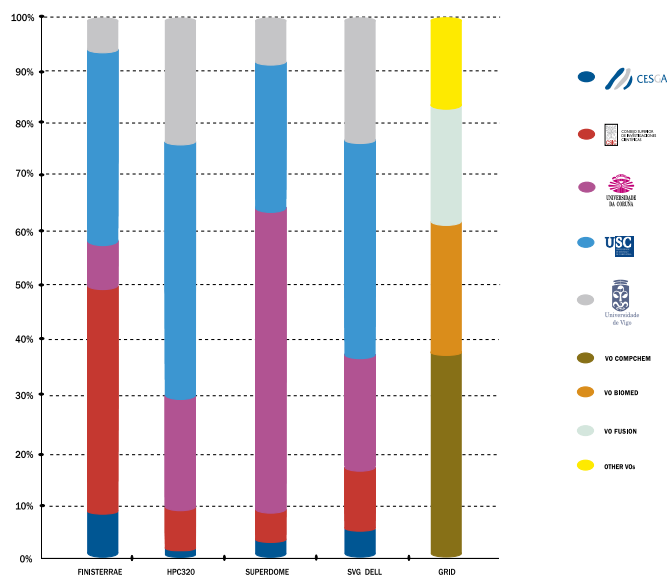
CPU USE DISTRIBUTION BY RESEARCH AREA

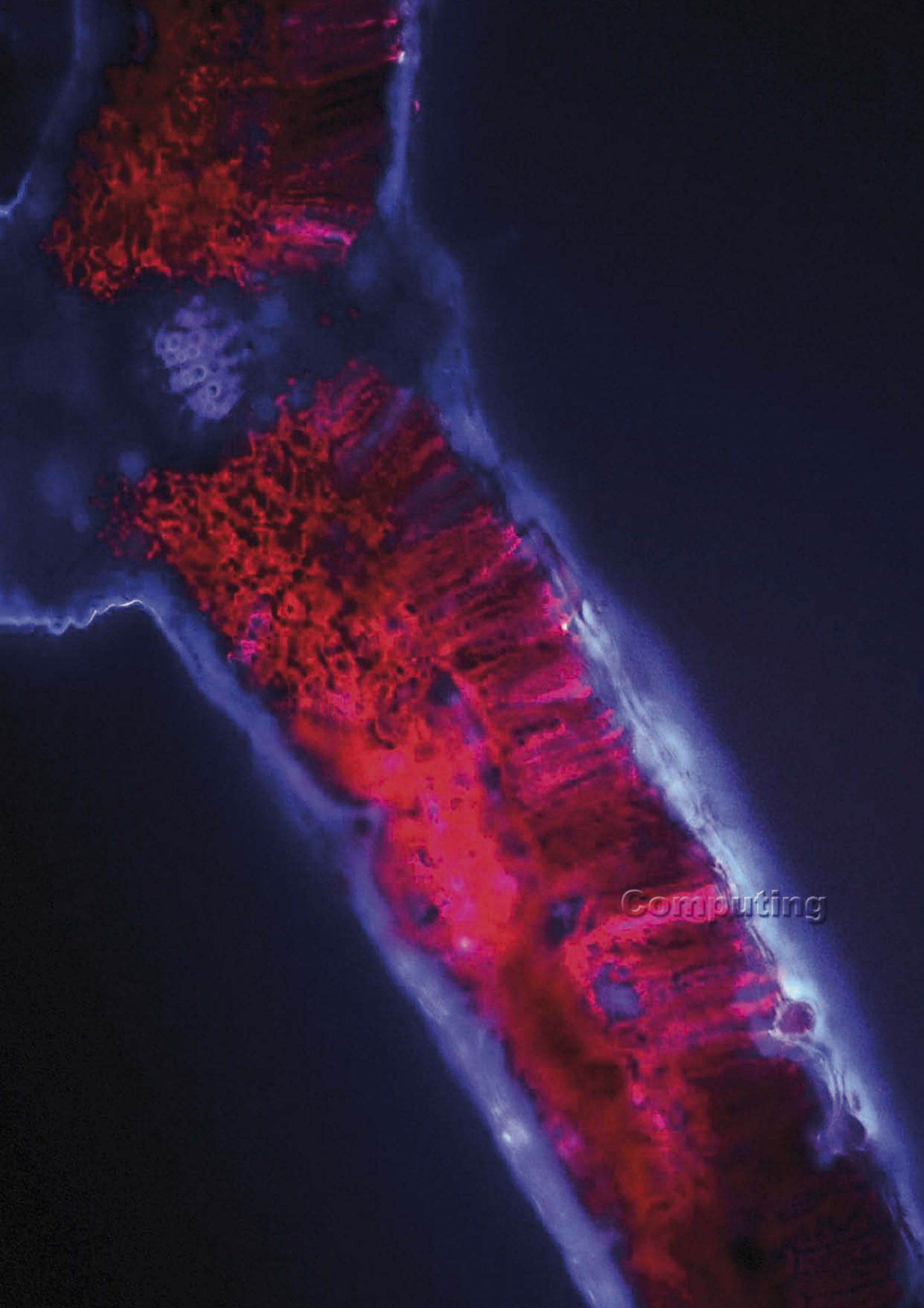


CPU Usage Distribution by Institution and Machine

In this graphic, we can see which of the systems are the most demanded by each one of the institutions that use the computing servers of CESGA. As can be appreciated, CSIC researchers principally utilise the FinisTerra server registering more than 40% utilisation of the system, while the SVG is shared by the researchers of the Universities of Santiago de Compostela and A Coruña. Grid systems are fundamentally used for the projects in which CESGA participates.

CPU DISTRIBUTION BY MACHINE AND INSTITUTION 2008





Computing

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 for their needs.

The highlights of 2008 regarding computing servers were:

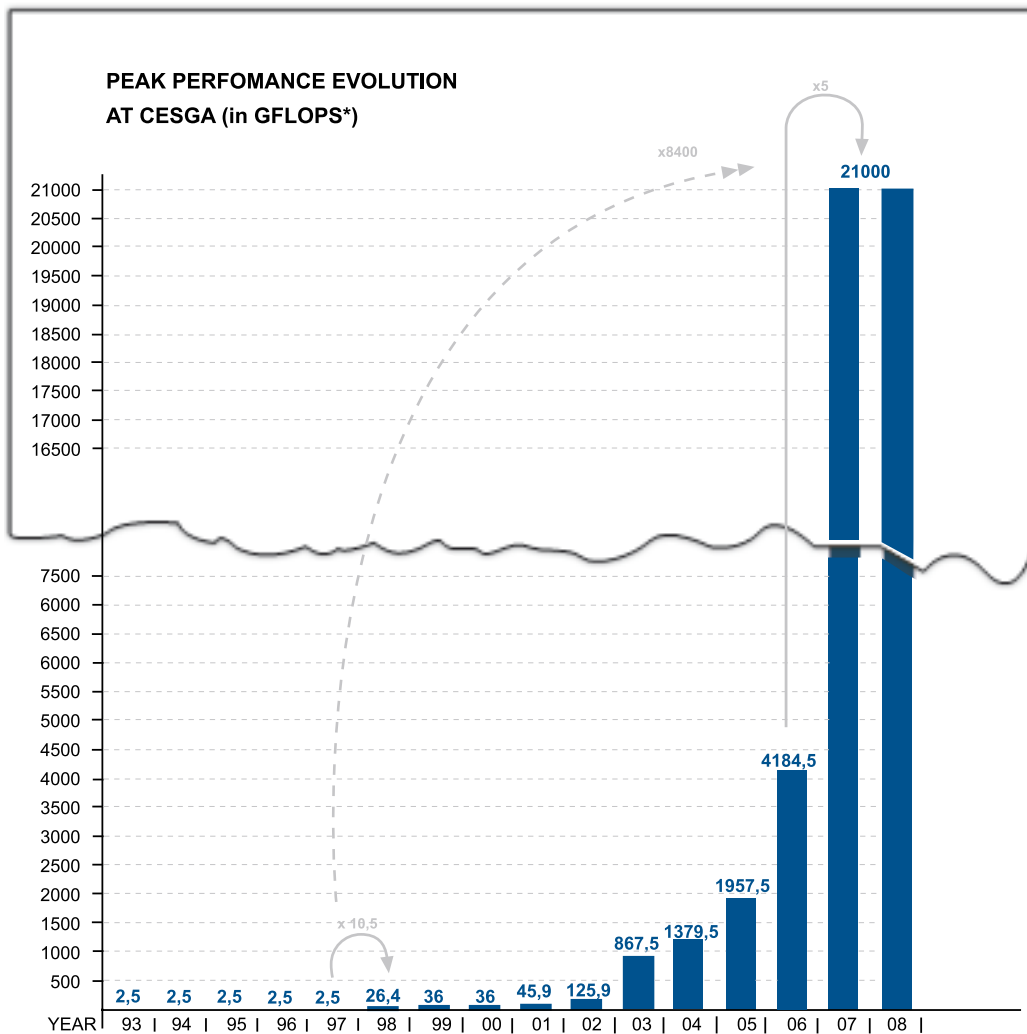
- The installation and the initiation of operation of Finis Terrae,
- The integration of the HP-Superdome servers into the Finis Terrae cluster,
- The HPC-320 server was removed from service, and
- The users employed more than 10 million CPU hours.

In 2008, CESGA centered its efforts on putting Finis Terrae into operation and supporting it. This system ranked number 100 on the TOP500 list of November 2007 and began operation in February 2008 in order to begin to work on relevant computational challenges.

Finis Terrae was made available to all users on April 1, 2008. In 2008, the following computing servers were available to users:



COMPUTING SERVERS IN 2008			
HIGH PERFORMANCE COMPUTING SERVERS			
SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
COMPAQ HPC320	2002	SMP CLUSTER	32 CPU's, 80 GB MEMORY, 64 GFLOPS
FINIS TERRAE	2008	SMP (NUMA) CLUSTER	2,580 CORES, 20 TB, 16 TFLOPS
HIGH THROUGHPUT COMPUTING SERVERS INTEGRATED IN THE GALICIAN VIRTUAL SUPERCOMPUTER (SVG)			
SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
SVG	2001-2006	DISTRIBUTED PC CLUSTER	50 CPU's, 0,5 -1 GB MEMORY CPU, 9,9 GFLOPS , 110 CPU, 300 GFLOPS (2004)
COMPAQ BEOWULF	2002	BEOWULF CLUSTER	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
SERVERS HOUSED AT CESGA			
SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
METEOGALICIA	2004	2 SMP NODES	20 CPU, 40 GB MEMORY, 48 GFLOPS
LHCb-USC	2002-2008	PC CLUSTER	339 CORES, 312 GB MEMORY, 1600 GFLOPS

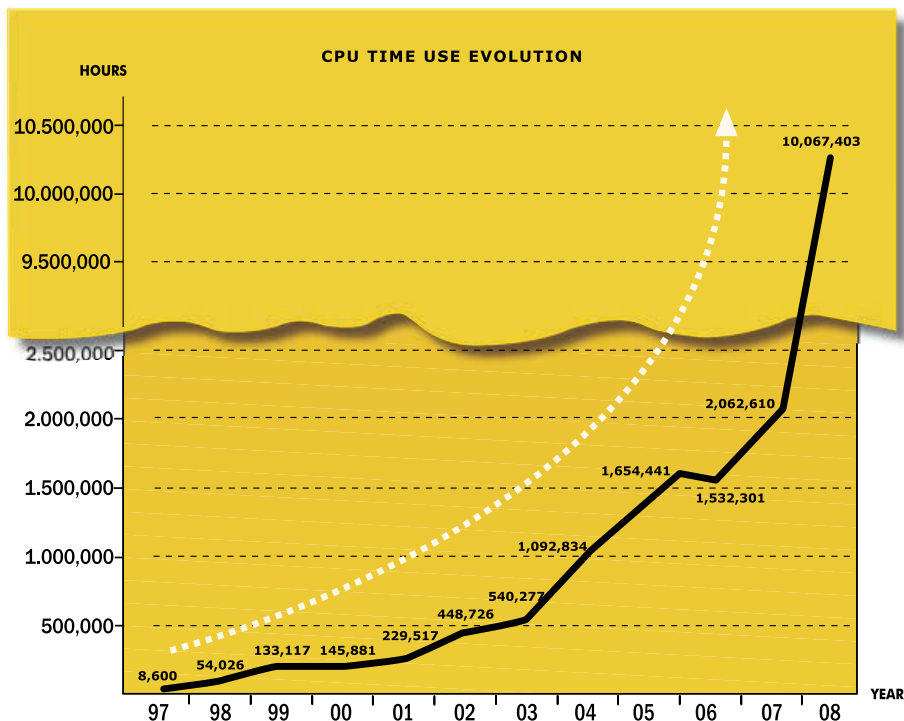


* 1GFLOPS= 1.073.741.824 (floating point operations per second)



Evolution of CPU Consumption

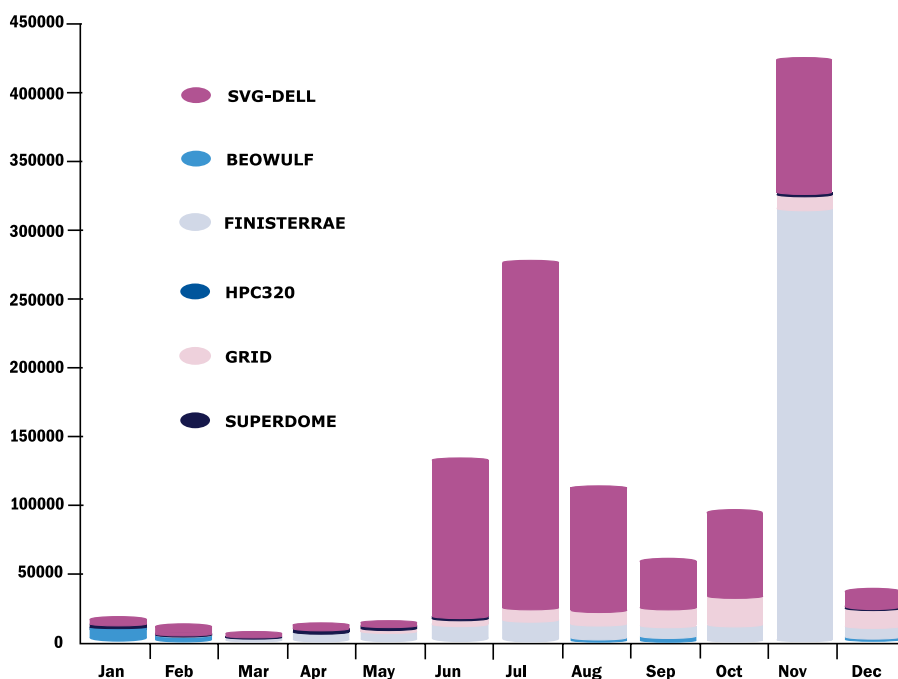
During 2008, the new Finis Terrae system and the SVG cluster were the most utilised servers. In order to facilitate the transition to Finis Terrae for the users, one of the HP Superdome systems was maintained in operation for the duration of the year. The number of hours consumed increased significantly, multiplying the total by 5, going from 2 million hours (2,062,610 actual hours) for 2007 to a total of 10,067,403 hours for 2008.



Number of Jobs Executed

The number of jobs executed represents the quantity of simulations that the users performed on each one of the computing servers. This value does not only depend on the available computing capacity but also on the resources necessary for the execution of the simulations. The SVG cluster and Finis Terrae were the most utilised systems. The SVG was especially important given that it is a server that is oriented to productivity, that is, the performance of a great number of independent projects with relatively low computing needs. In summary, the 2008 total number of jobs of 1,214,079 was much higher than that of 2007 (215,883).

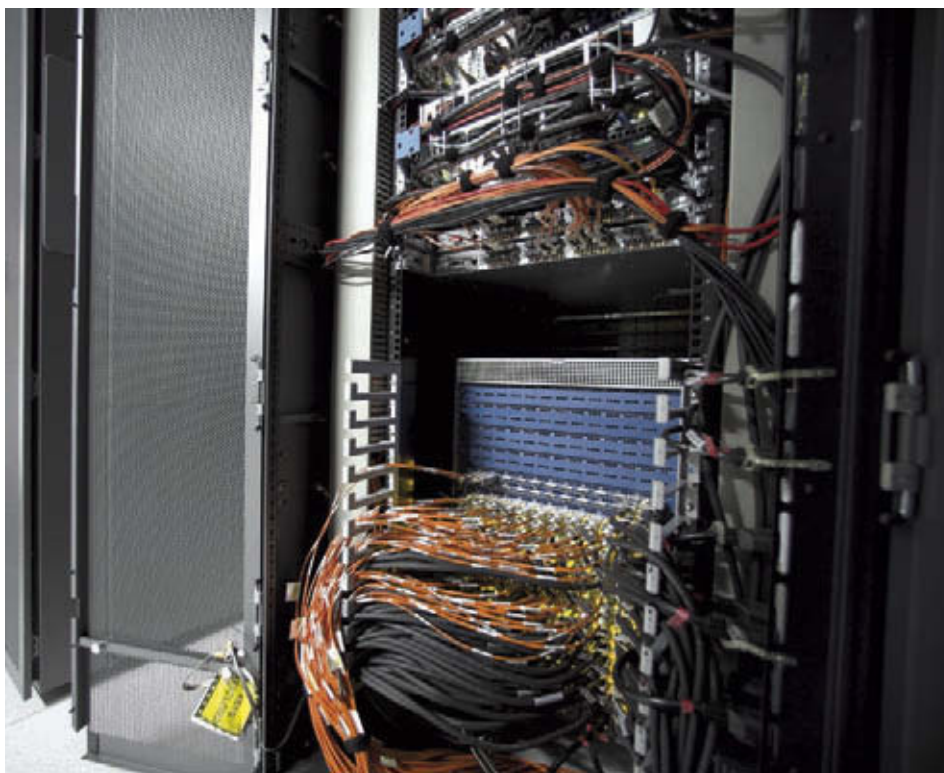
JOBS EXECUTED PER SYSTEM



Average in-queue time

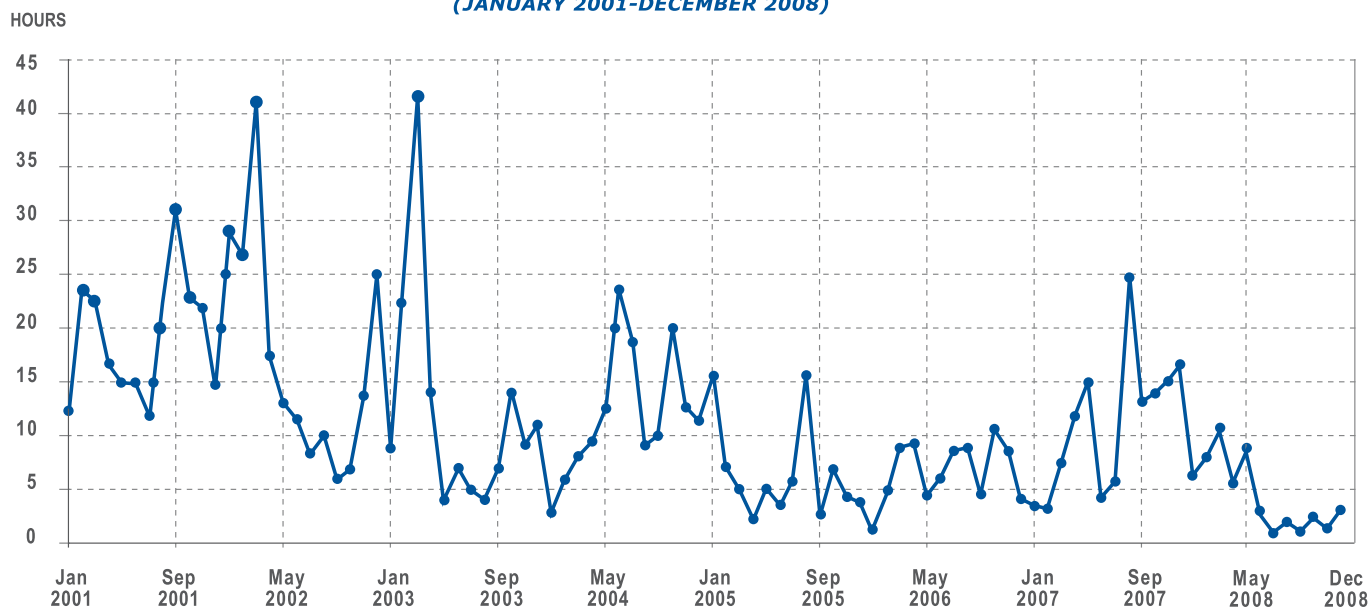
The average in-queue time represent the average amount of time that users must wait from the moment that they request CESGA resources until their simulations begin running on the systems. This time varies as a function of the quantity of simulations that are being performed and desirably it should be the closest possible to zero in order to avoid that users have to wait much time until they receive the results of their simulations.

Logically, the higher the level of occupation of the computing systems, the more time it is necessary to wait until the necessary resources are available. This average is a good indicator of the level of saturation that exists in the computational resources. Normally, the waiting times decrease in summer and during the Christmas holidays, and they increase significantly as new users are incorporated. In summary, the waiting times have decreased in great measure thanks to the incorporation of the Finis Terrae server, reducing the waiting time from an average of more than 7 hours



in 2007 to an average of only 2 hours for all of the computing servers in 2008. Even more important is the decrease in waiting time in the server with the greatest capacity. In 2007, the average for the HP Superdome was 43 hours and it decreased to less than 2 hours for Finis Terrae. This allows researchers to run more simulations and to receive their results in less time, thereby increasing their competitiveness.

**AVERAGE IN QUEUE TIME FOR ALL PROCESSES IN ALL SYSTEMS
(JANUARY 2001-DECEMBER 2008)**



HPC: high performance computing servers

Different server architectures for High Performance Computing (HPC) are available for CESGA users. These involve 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 memory size, utilizing internal networks with a low latency time and a high transfer capacity.

During 2008, the users had access to three different high performance systems.

Finis Terrae

The supercomputer FINIS TERRAE was installed at CESGA in December, 2007. It is an integrated system with shared memory nodes, with SMP NUMA architecture. A list of the components of FINIS TERRAE follows.

A total of 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, and
- 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, and
- 2,200,000 GB on tape (cartridge robot).

An interconnect Infiniband 4x DDR at 20 Gbps.

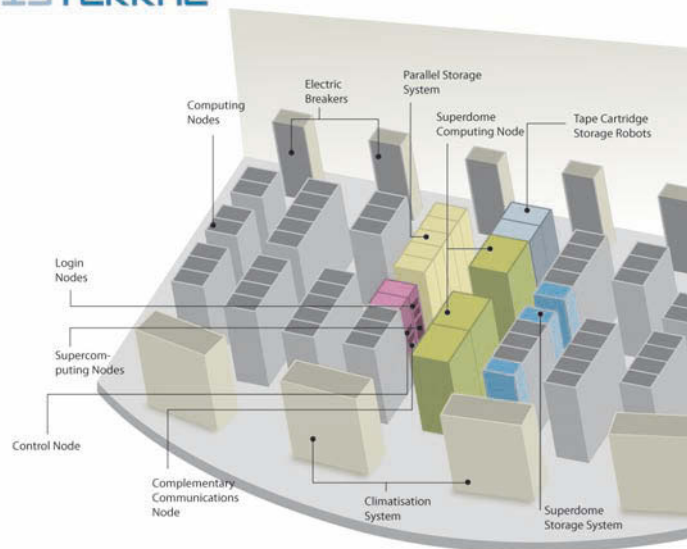
An external network at 10 Gbps.

The system concurrently supports multiple operating systems 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



FINISTERRAE CLUSTER SMP NUMA TECHNICAL SPECIFICATIONS	
COMPUTER	Integrity rx7640/Superdome Itanium 2 Cluster
APPLICATION 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 etc...
COMPILERS, LIBRARIES & DEVELOPMENT TOOLS	Intel C/C++ and Fortran, Intel MKL, Vtune, HP-MPI and HP UPC
NODE INTERCONNECT	Infiniband 4x DDR at 20 Gbps
EXTERNAL NETWORK CONNECTION	10 Gbps
PROCESSOR	Intel IA-64 Itanium 2 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 & 384 GB memory
PROCESSING CORES	2,580
MEMORY	19,670 GB
STORAGE NODES	22 nodes with 96 cores
HIERARCHICAL STORAGE	390,000 GB on disk & 2,200,000 GB on tape



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 disk. An Infiniband network between the two nodes is available. For permanent data, the user had an HP EVA-3000 disk rack for massive storage with FibreChannel technology. During 2008, this server was integrated into Finis Terrae which means that its operating system is Linux SLES10SP1 and can be accessed using the same batch system.

COMPAQ HPC 320

This cluster was 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 were interconnected by means of a Memory Channel Dual Rail network. After 5 years of extraordinary service to CESGA's community of researchers, COMPAQ HPC 320 reached the end of its technological life and was finally retired from service in June, 2008.

HTC: high throughput computing & grid servers

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

This type of architecture is ideal for iterative processes with low dependency between themselves, such as, genetic algorithms, massive processing of experimental data, the rendering of images, parametric computing, etc.



Supercomputer (SVG). In 2007, 32 processors and 32 GB of memory were added.

SVG reflects the wager that the Centre made back in 1999 for low cost cluster systems as an ideal solution to the increase in 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 or to learn new operating systems.

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 into the Galician Virtual

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

SIGNIFICANT COMPUTING INICIATIVES IN WHICH CESGA PARTICIPATES

housing of computing equipment



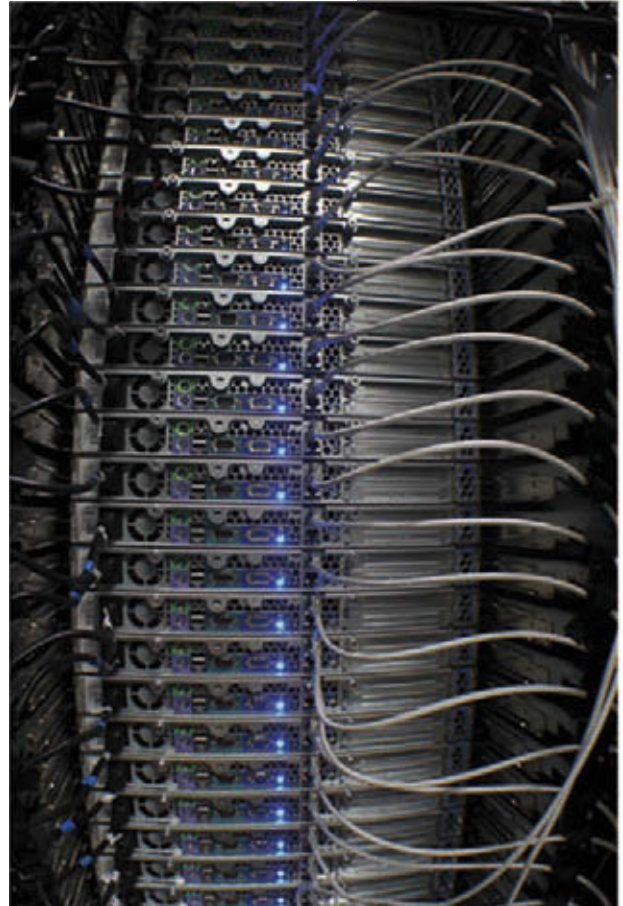
SUN NODES METEOGALICIA

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 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 forecasts. In addition to this SUN machine, Meteogalicia regularly used the following servers in 2008: Finis Terrae, HP Integrity Superdome, HPC 320, and the Galician Virtual Supercomputer (SVG).

LHCb-USC CLUSTER



LHCb-USC

Since 2002, the Experimental Group of High Energy Physics of the University of Santiago de Compostela (GAES) has had 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. Since it was first housed at CESGA, this cluster has steadily grown with the addition of new computing cores.

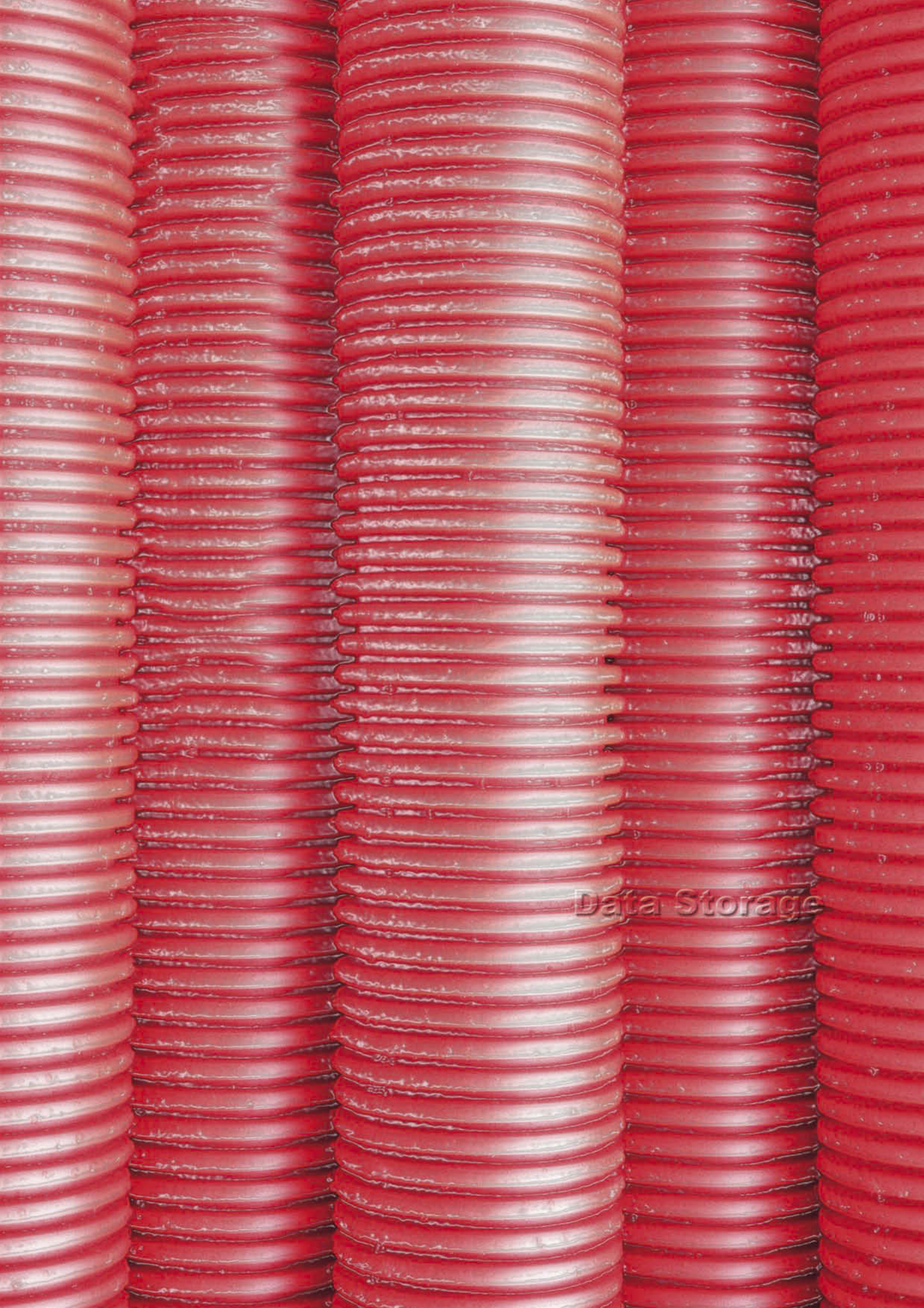


XUNTA DE GALICIA
 CONSELLERÍA DE MEDIO AMBIENTE
 E DESENVOLVEMENTO SOSTIBLE
 Dirección Xeral de
 Desenvolvemento Sostible

METEOGALICIA



Worldwide LHC Computing Grid
 Distributed Production Environment for Physics data Processing



Data Storage

data storage

The total storage capacity available to CESGA users did not increase significantly in 2008 since the incorporations of Finis Terrae had been produced and accounted for in the prior year. The storage capacity on the 465.6TB tape was the only memory increase noted after the acquisition of 291 new LTO-4 tapes for the robotic library, reaching a total of 625.6TB. In total, available storage for users by the end of 2008 reached 1013 Terabytes which represented an increase of 57% with respect to the previous year.

The data storage service now uses a type of hierarchy for the data that is stored in order to assure the best quality of service as a function of the information (criticality of data and velocity of access). There were 77 requests for storage service of which 40 had an increase in their usage quota on the computing servers, 27 concerned massive data storage and 10 concerned security copies to disk (some users subscribe to more than one service).

Storage service

Criteria for the classification of information

In 2008 the Centre maintained the criteria introduced in 2004 regarding the classification of the types of data in the storage service.

This system permitted the accommodation of the different 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 optimisation 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. Regarding 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, as a 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 wide bandwidth to access the servers. Back-ups can be made according to demand.

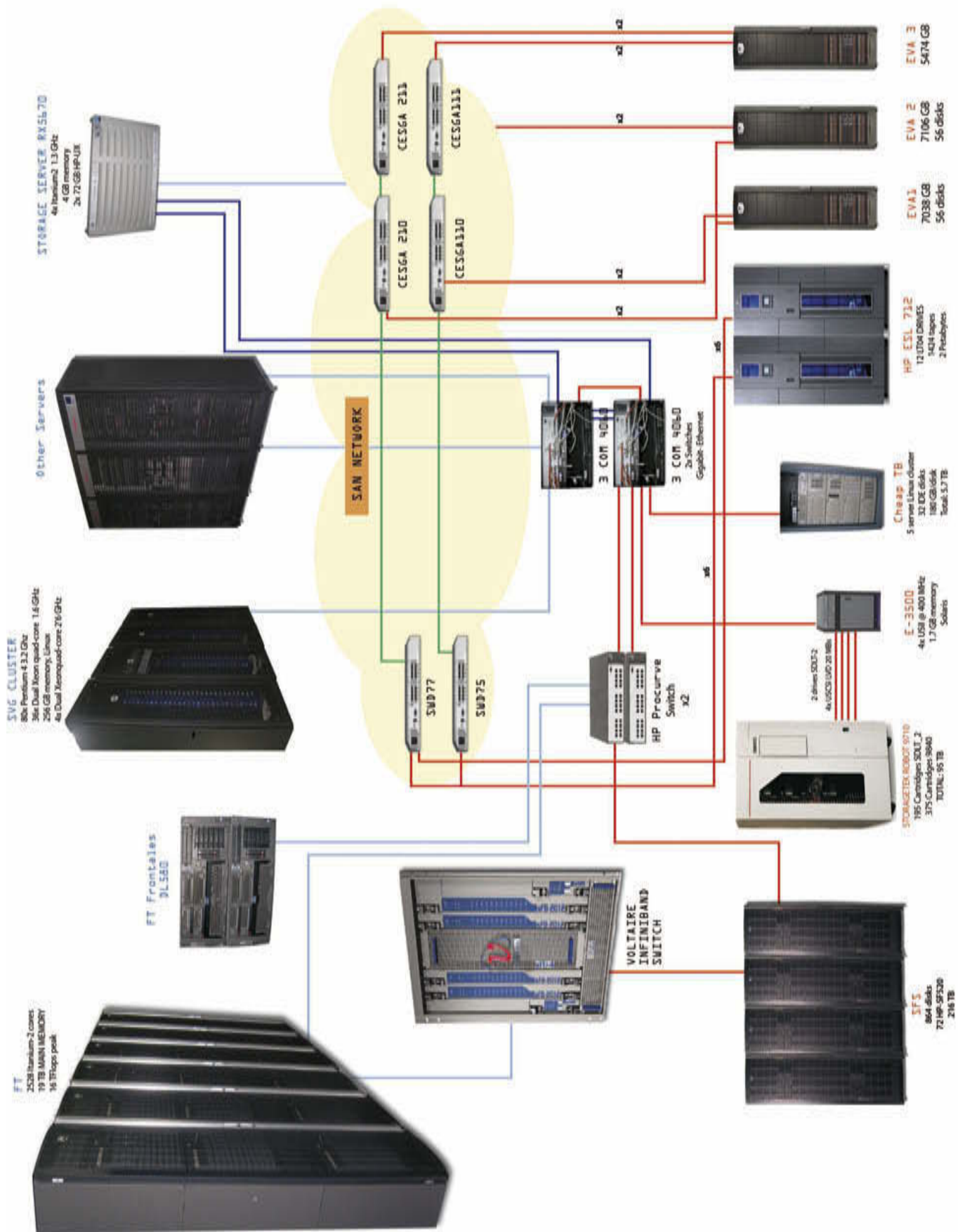
Back-ups to disk are the copies of the data that users make with their own servers or PCs are stored in CESGA's systems in order to have a secure copy of their data. The availability of the service may be low. The service is offered by means of the network for which it is not necessary that the type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

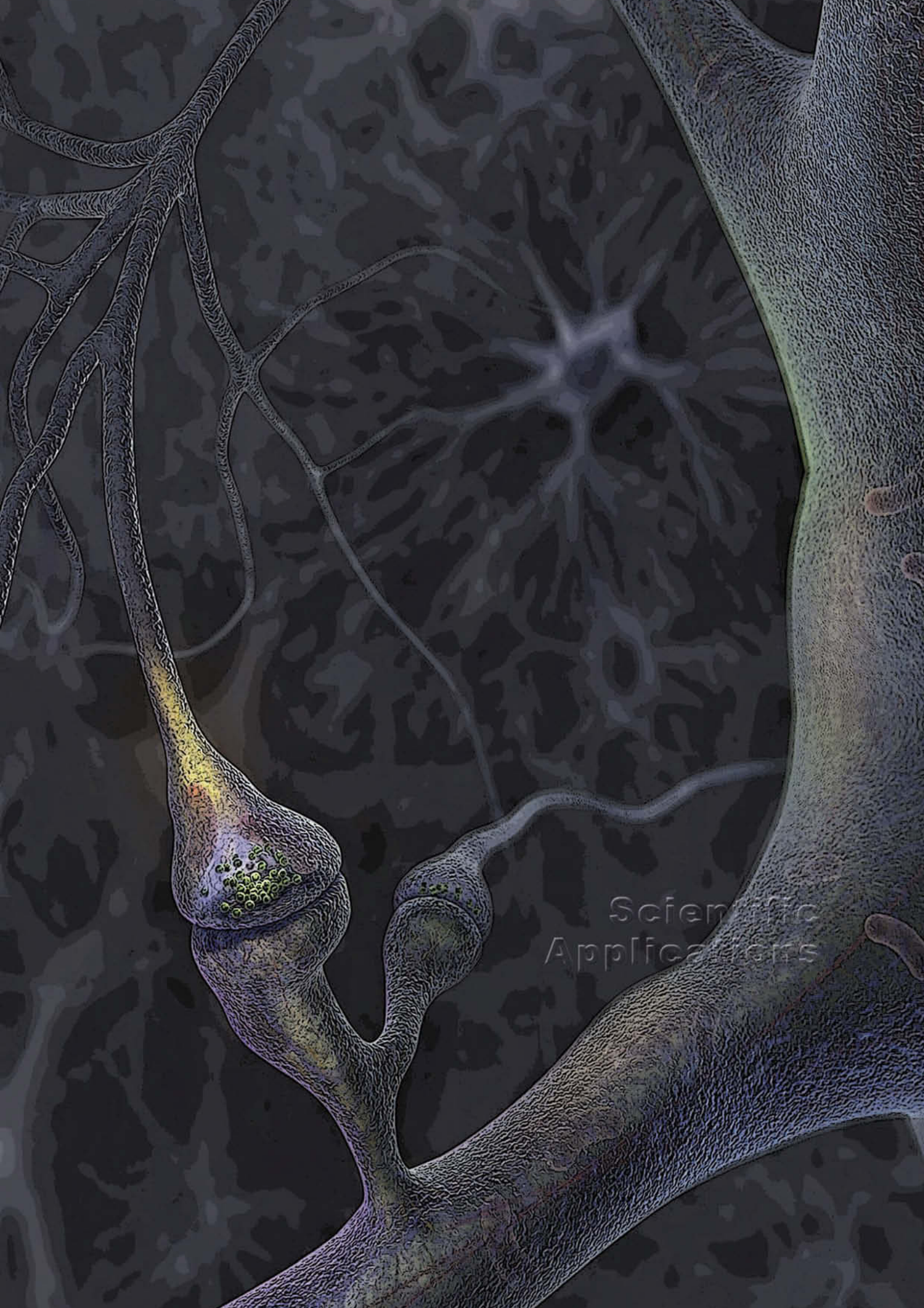
Scratch Parallel is very high performance (very low latency and maximum band width), similar to the first type with the addition that, in this case, the scratch data is shared between all of the nodes of the cluster and distributed among all of them). This permits an increase in both the access bandwidth 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.

DATA STORAGE USED

TYPE OF STORAGE	CAPACITY (Gbytes)
Temporary or Scratch	133,480
Temporary Parallel	228,800
Permanent Disk	25,538
Tape	625,600
TOTAL	1,013,422

DATA STORAGE RESOURCES 2008





Scientific
Applications

scientific computing applications

There was a significant increase in activity in the area of applications during 2008 due to the installation of the new super-computer, Finis Terrae and the demonstration of its capacities in the execution of scientific challenges. Specifically, the following activities were performed in 2008.

- The execution of 6 scientific challenges, 4 in February and 2 during the rest of the year.
- A high number of support activities (241) during the year which represents an interannual increase of 96%.
- The installation of almost all the applications supported by CESGA in the Finis Terrae server, as well as other applications that users demand. This required the porting of several applications to Finis Terrae. A list of the ported elements is presented below.

Applications, such as:

- Amber version 9.0
- CHARMM version c34b2
- CPMD version 3.11.1
- Crystal version 06
- deMon2k version 2.3
- Elmer version 5.4.1
- FLEXPART version 8.0
- FLUENT version 6.3
- Gamess versions 24 MAR 2007 (R1) & 11 APR 2008 (R1)
- Gaussian 03 version E.01
- Grads version 2.0.a1
- Gromacs versions 3.3, 3.3-2, 3.3-3, 4.0 y 4.0.2
- LAMMPS versions 21May2008 & 22Jan2008
- Leadmix version 28-08-2005
- Macaulay 2 version 1.1
- Materials Studio version 4.3
- MOLCAS version 6.4
- Molden version 4.6
- molpro version 2006.1
- MrBayes version 3.1.2
- NAMD version 2.6
- NWChem version 5.1
- R versions 2.7.0 & 2.7.2
- SIESTA version 2.0.1
- Singular version 3.0.4

- Stata/MP version 10.0
- Turbomole version 5.10
- udunits version 1.12.4
- VASP version 4-6-28
- VMD version 1.8.6
- Wien2k version 08.1
- XcrySDen version 1.4

Libraries, such as:

- CGAL version 3.3.1
- FFTW versions 3.1.2 & 3.2alpha3
- HDF versions 4.2r3-ia64 & 5.1.8.1
- HP MPI 2.2.5.1
- Intel MPI Library 3.0 3.1 2 3.2.0.011
- Jrokit R27.5.0-jdk1.5.0_14
- MKL 10.0.011 10.0.2.018 9.1 10.1.0
- NumPy 1.0.4
- pyMPI 2.5bo
- Ncarg 5.0.0
- NetCDF 4.0 3.6.2

Compilers, such as:

- Intel C++ Compiler versions 9.1.052, 10.1.012 & 11.0.069
- Intel Fortran Compiler versions 9.1.052, 10.1.012 & 11.0.069

Software management utilities, such as:

- Modules version 3.1.6
- Subversion version 1.5.3

The installation of the majority of Intel development tools in the SVG server, thereby unifying the development tools supported by CESGA's servers.

The organisation of internal and external training courses on topics related to applications and tools.

Solely organised by CESGA:

- Free/Libre software tools for the debugging and the analysis of applications performance
- Parallel programming by means of OpenMP directives
- Fortran course (1st edition)
- Fortran course (2nd edition)
- Intel development tools

Many new applications or libraries of utilities were incorporated in 2008 at the request of users or for the installation of new versions (see Table below).

APPLICATION	TASK
SCIENTIFIC DATA BASES	
CSD (Migrated to the SVGD server; new version, V5.30 (2009) installed)	Cambridge Structural Database is a data base that collects bibliographic, chemical, and crystallographic information regarding organic and organometallic obtained by the diffraction of X-rays and the diffraction of neutrons. http://www.ccdc.cam.ac.uk/products/csd
MOLECULAR SIMULATION	
Amber (new installation, version 9.0, in Finis Terrae)	AMBER is a set of programs that allows the user to perform molecular dynamics simulations, fundamentally in biomolecules, based on theories of force fields. http://ambermd.org
CPMD (new installation, version 3.11.1, in Finis Terrae)	CPMD is an implementation of the theory of the functionality of density using plane waves/pseudopotentials that are particularly designed in order to carry out ab initio molecular dynamics studies. http://www.cpmc.org
Gamess (New installation, versions 11 APR 2008 (R1) and 24 MAR 2007 (R1), in Finis Terrae)	This is an analogue package for GAUSSIAN that incorporates ab initio methods, although it does offer specific solutions for the description of orbits and other methods of optimisation. http://www.msg.chem.iastate.edu/gamess/gamess.html
Gaussian 03 (new installation version E.01, in Finis Terrae)	Gaussian 03 is one of most used packages in Computational Chemistry that permits the prediction of properties (energies, frequencies of vibration, optimal geometry, etc.) of molecules and intermediates of reaction, fundamentally by means of theoretical ab initio methods. http://www.gaussian.com
Gromacs (New version, 3.3.2, in the SVG. New installation, versions 4.0.2, 4.0, 3.3, 3.3.3 Y 3.3.2, in Finis Terrae)	GROMACS is versatile software for molecular dynamics calculations, i.e., it simulates the equations of Newton regarding movement for systems with hundreds of millions of particles. It is principally designed for the study of biochemical molecules such as proteins and lipids with a large number of complex bonding interactions. http://www.gromacs.org
LAMMPS (new installation, versions 21 May 2008 and 22 Jan 2008, in Finis Terrae)	LAMMPS is a molecular dynamics simulator. It runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionality. http://lammps.sandia.gov
Molden (new installation, version 4.6, in Finis Terrae)	Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK, GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac, it also supports a number of other programs via the Molden Format. Molden reads all the required information from the GAMESS / GAUSSIAN outputfile. Molden is capable of displaying Molecular Orbitals, the electron density and the Molecular minus Atomic density. http://www.cmbi.ru.nl/molden/molden.html

APPLICATION	TASK
NAMD (new installation, version 2.6, in the SVG and in Finis Terrae)	NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. http://www.ks.uiuc.edu/Research/namd/
NWChem (new installation, version 5.1, in Finis Terrae)	NWChem is a computational chemistry package designed for execution on high performance parallel supercomputers as well as for conventional work station clusters. It is intended to be scalable in its capacity to deal with large problems in an efficient manner such as in its use of available parallel computational resources. http://www.emsl.pnl.gov/docs/nwchem/nwchem.html
SIESTA (new installation, version 2.0.1, in Finis Terrae)	SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and its computer program implementation, to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. http://www.icmab.es/siesta
Applications with limited licensing (User or single institution) RESTRICTED TO SPECIFIC USERS	
CHARMM (new installation, version c34b2, in Finis Terrae)	CHARMM (Chemistry at Harvard Macromolecular Mechanics) is a versatile and widely used program for molecular simulation that has many applications to multiparticle systems. http://www.charmm.org
Crystal (new installation, version o6, in Finis Terrae)	Crystal is a computational tool for simulations of solid state physics and chemistry. http://www.crystal.unito.it/
DeMon2k (new installation, version 2.3, in Finis Terrae)	deMon (density of Montréal) is a software package for density functional theory (DFT) calculations. It uses the linear combination of Gaussian-type orbital (LCGTO) approach for the self-consistent solution of the Kohn-Sham (KS) DFT equations. The calculation of the four-centre electron repulsion integrals is avoided by introducing an auxiliary function basis for the variational fitting of the Coulomb potential. http://www.demon-software.com/public_html/program.html
Materials Studio (new installation, version 4.3, in Finis Terrae)	Materials Studio is a modelling and simulation package that is easy to use for the study of chemical substances and materials. It provides tools for modelling crystal structure and crystallization processes, for the study of polymer properties, catalysis, and the study of structure-activity relationships. http://accelrys.com/products/materials-studio
MOLCAS (new installation, version 6.4, in Finis Terrae)	MOLCAS is a quantum chemistry software developed by scientists to be used by scientists. MOLCAS emphasizes the multiconfigurational approach for quantum chemical calculations, which allows studies of systems where a single configuration does not give a good representation of the electronic structure. Examples are excited states, transition states for chemical reactions, heavy element systems (transition metals, lanthanides, actinides), and much more. http://www.teokem.lu.se/molcas
MOLPRO (new installation, version 2006.1, in Finis Terrae)	Molpro is a complete system of ab initio programs for molecular electronic structure calculations. As distinct from other commonly used quantum chemistry packages, the emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem through the multiconfiguration-reference CI, coupled cluster and associated methods. http://www.molpro.net

APPLICATION	TASK
Turbomole (new installation, version 5.10, in Finis Terrae)	TURBOMOLE is one of the fastest and most stable codes available for standard quantum chemical applications. Unlike many other programs, the main focus in the development of TURBOMOLE has not been to implement all new methods and functionals, but to provide a fast and stable code which is able to treat molecules of industrial relevance at reasonable time and memory requirements. http://www.cosmologic.de/index.php?cosName=main_turbomole
VASP (new installation, version 4-6-28, in Finis Terrae)	VAMP/VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. http://cms.mpi.univie.ac.at/vasp
WIEN2K (new installation, version 08.1, in Finis Terrae)	The program package WIEN2k allows users to perform electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. http://www.wienzk.at
BIOINFORMATICS	
IM (new version 3/2/2008 in the SVG)	IM is a program for the fitting of an isolation model with migration to haplotype data drawn from two closely related species or populations. IM is based on a method originally developed by Rasmus Nielsen and John Wakeley (Nielsen and Wakeley 2001 Genetics 158:885). Large numbers of loci can be studied simultaneously, and different mutation models can be used. http://lifesci.rutgers.edu/~heylab/HeylabSoftware.htm#IM
Lamarc (new installation, versions 2.1.2b and 2.1.3, in the SVG)	Lamarc is a program for doing Likelihood Analysis with Metropolis Algorithm using Random Coalescence. Lamarc estimates effective population sizes, population exponential growth rates, a recombination rate, and past migration rates for one to n populations assuming a migration matrix model with asymmetric migration rates and different subpopulation sizes. http://evolution.genetics.washington.edu/lamarc/lamarc_prog.html
Leadmix (new installation, version 28-08-2005, in the SVG and Finis Terrae)	LEADMIX is a Fortran program to estimate the admixture proportions and genetic drift using data on genetic markers, based on the likelihood method http://www.zoo.cam.ac.uk/ioz/software.htm#LEADMIX
MrBayes (new installation, version 3.1.2, in Finis Terrae)	Mrbayes is a program for the Bayesian phylogenesis estimation based on a simulation technique known as Markov chain Monte Carlo (or MCMC). http://mrbayes.csit.fsu.edu/index.php
Structure (new installation, version 2.2.3, in the SVG)	The program structure is a free software package for using multi-locus genotype data to investigate population structure. Its uses include inferring the presence of distinct populations, assigning individuals to populations, studying hybrid zones, identifying migrants and admixed individuals, and estimating population allele frequencies in situations where many individuals are migrants or admixed. http://pritch.bsd.uchicago.edu/structure.html
Unphased (new installation, version 3.0.13, in the SVG)	UNPHASED is a versatile application for performing genetic association analysis. http://www.mrc-bsu.cam.ac.uk/personal/frank/software/unphased

APPLICATION	TASK
METEOROLOGICAL SIMULATION	
ECBILT/CLIO (new installation, version 3, in the SVG)	The ECBilt-Clio model is an 'intermediate-complexity', three-dimensional coupled atmosphere-ocean-sea ice General Circulation Model. http://www.knmi.nl/onderzk/CKO/ecbilt.html
Field (new installation, version 1.2 in the SVG)	The Field library provides high-level access to gridded data fields in a data format independent manner. This library is required for models such as ECBILT. http://www.knmi.nl/onderzk/CKO/tools.html
STRUCTURAL MODELLING, FLUIDS, AND MAGNETISM	
Elmer (new installation, version 5.4.1, in Finis Terrae)	Elmer is an open source multiphysical simulation software developed by CSC. Elmer includes physical models of fluid dynamics, structural mechanics, electromagnetism, heat transfer and acoustics, for example. These are described by partial differential equations which Elmer solves by the Finite Element Method (FEM). http://www.csc.fi/english/pages/elmer
OpenFOAM (new version, 1.4.1, in the SVG)	The OpenFOAM® (Open Field Operation and Manipulation) CFD Toolbox can simulate anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics, electromagnetism and the pricing of financial options. OpenFOAM is produced by OpenCFD Ltd and is freely available and open source, licensed under the GNU General Public Licence. http://www.opencfd.co.uk/openfoam
Applications with limited licensing (User or sole institution) RESTRICTED TO SPECIFIC USERS	
FLUENT (new installation, version 6.3, in Finis Terrae)	FLUENT software is a powerful and flexible general-purpose computational fluid dynamics (CFD) package used for engineering simulations of all levels of complexity. It offers a comprehensive range of physical models that can be applied to a broad range of industries and applications. http://www.fluent.com
SIMULATION	
FLEXPART (new installation, version 8.0, in Finis Terrae)	FLEXPART is a model of particle dispersion that is used more and more every day. http://transport.nilu.no/flexpart
Macaulay 2 (new installation, version 1.1, in Finis Terrae)	Macaulay 2 is a software system devoted to supporting research in algebraic geometry and commutative algebra. http://www.math.uiuc.edu/Macaulay2
MATLAB (new versions, R2007b and R2008b, in the SVG)	MATLAB® is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran. It is possible to use MATLAB in a wide range of applications, including signal and image processing, communications, control design, test and measurement, financial modeling and analysis, and computational biology. http://www.mathworks.com/products/matlab
SCIENTIFIC VISUALISATION AND ANIMATION	

APPLICATION	TASK
Grads (new installation, version 2.0.a1, in Finis Terrae)	The Grid Analysis and Display System (GrADS) is an interactive desktop tool that is used for easy access, manipulation, and visualization of earth science data. The format of the data may be either binary, GRIB, NetCDF, or HDF-SDS (Scientific Data Sets). http://www.iges.org/grads
HDF (new installation, version 4.2r3-ia64, in FinisTerrae)	At its lowest level, HDF is a physical file format for storing scientific data. At its highest level, HDF is a collection of utilities and applications for manipulating, viewing, and analyzing data in HDF files. Between these levels, HDF is a software library that provides high-level APIs and a low-level data interface. http://www.hdfgroup.org/products/hdf4
HDF5 (new installation, version 1.8.1, in Finis Terrae)	HDF5 is a unique technology suite that makes possible the management of extremely large and complex data collections. http://www.hdfgroup.org/HDF5
JASPER (new installation, version 1.900.1, in Finis Terrae)	The JasPer Project is an open-source initiative to provide a free software-based reference implementation of the codec specified in the JPEG-2000 Part-1 standard (i.e., ISO/IEC 15444-1). http://www.ece.uvic.ca/~mdadams/jasper
Ncarg (new installation, version 5.0.0, in Finis Terrae)	NCAR Graphics is a Fortran and C based software package for scientific visualization. http://ngwww.ucar.edu/
NCO (new installation, version 3.9.3, in the SVG)	The netCDF Operators, or NCO, are a suite of programs known as operators. Each operator is a standalone, command line program which is executed at the UNIX shell-level. The operators take netCDF files as input, then perform a set of operations (e.g., deriving new data, averaging, hyperslabbing, or metadata manipulation) and produce a netCDF file as output. http://nco.sourceforge.net
NetCDF (new installation, versions 3.6.2 and 4.0, in Finis Terrae. New version, 3.6.2, in the SVG)	NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. http://www.unidata.ucar.edu/software/netcdf
Udunits (New installation, version 1.12.4, in Finis Terrae)	The UDUNITS package supports units of physical quantities (e.g., meters, seconds). Specifically, it supports conversion between string and binary representations of units, arithmetic manipulation of units, and conversion of numeric values between compatible units. http://www.unidata.ucar.edu/software/udunits
VMD (new installation, version 1.8.6, in Finis Terrae)	VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. http://www.ks.uiuc.edu/Research/vmd
XcrySDen (new installation, version 1.4.1, in Finis Terrae)	XCrySDen is a crystalline and molecular structure visualisation program, which aims at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. http://www.xcrysdem.org

APPLICATION	TASK
MATHEMATICAL LIBRARIES	
CGAL (new installation, version 3.3.1, in Finis Terrae)	The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C++ library. CGAL is used in various areas needing geometric computation, such as: computer graphics, scientific visualization, computer aided design and modeling, geographic information systems, molecular biology, medical imaging, robotics and motion planning, mesh generation, numerical methods... http://www.cgal.org
FFTW (new installation, versions 3.1.2 and 3.2.alpha3, in Finis Terrae)	FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data (as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST). FFTW, which is free software, should become the FFT library of choice for most applications. The benchmarks, performed on a variety of platforms show that FFTW's performance is typically superior to that of other publicly available FFT software, and is even competitive with vendor-tuned codes. In contrast to vendor-tuned codes, FFTW's performance is portable: the same program will perform well on most architectures without modification. http://www.fftw.org
Libmcrypt (new installation, version 2.5.8, in the SVG)	Libmcrypt is the library which implements all the algorithms and modes found in mcrypt and facilitates a standard mechanism of access to them. http://mcrypt.hellug.gr/lib/index.html
Mcrypt (new installation, version 2.6.7, in the SVG)	Mcrypt allows developers to use a wide range of encryption functions, without making drastic changes to their code. It allows users to encrypt files or data streams without the necessity of advanced knowledge of cryptography. http://mcrypt.sourceforge.net
MKL (new installation, versions 9.1, 10.0.011, 10.0.2.018 and 10.1.0, in Finis Terrae. New versions, 9.1.023 and 10.0.3.020, in the SVG)	Intel® Math Kernel Library (Intel® MKL) is a library of highly optimized, extensively threaded math routines for science, engineering, and financial applications that require maximum performance. Core math functions include BLAS, LAPACK, ScaLAPACK, Sparse Solvers, Fast Fourier Transforms, Vector Math, and more. Offering performance optimizations for Intel next-generation microarchitecture, it includes improved integration with Microsoft Visual Studio*, Eclipse*, and XCode*. Intel MKL allows for full integration of the Intel Compatability OpenMP* run-time library for greater Windows*/Linux* cross-platform compatibility. http://software.intel.com/en-us/intel-mkl
NumPy (new installation, version 1.0.4, in Finis Terrae)	NumPy is the fundamental package needed for scientific computing with Python. It contains a powerful N-dimensional array object, sophisticated broadcasting functions, basic linear algebra functions, basic Fourier transforms, sophisticated random number capabilities and tools for integrating Fortran and C/C++ code. http://numpy.scipy.org
SCIENTIFIC ANALYSIS	
R (new installation, versions 2.6.1, 2.7.0 and 2.7.2, in Finis Terrae)	R is a language and environment for statistical computing and graphics. It is a GNU project that provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering, ...) and graphical techniques, and is highly extensible. http://www.r-project.org

APPLICATION	TASK
Singular (new installation, version 3.0.4, in Finis Terrae)	SINGULAR is a Computer Algebra System for polynomial computations with special emphasis on the needs of commutative algebra, algebraic geometry, and singularity theory. http://www.singular.uni-kl.de
Applications with limited licensing (User or sole institution) RESTRICTED TO SPECIFIC USERS	
Stata/MP (new installation, version 10.0, in Finis Terrae)	Stata is a complete, integrated statistical package that provides everything you need for data analysis, data management, and graphics. Stata/MP is a version of Stata/SE that runs on multiprocessor and multicore computers. http://www.stata.com/statamp/index.html
JAVA	
JROCKIT (new installation, version R27.5.0-jdk1.5.0_14, in Finis Terrae)	The Oracle JRockit JDK provides tools, utilities, and a complete runtime environment for developing and running applications using the Java programming language. The JRockit JDK includes the Oracle JRockit Java Virtual Machine (JVM). The Oracle JRockit JVM is developed and optimized for Intel architectures to ensure reliability, scalability, and manageability for Java applications. http://www.oracle.com/technology/products/jrockit/index.html
PARALLEL LIBRARIES	
HP MPI (New installation, version 2.2.5.1, in Finis Terrae)	HP-MPI for Linux is a high performance and production quality implementation of the Message-Passing Interface (MPI) standard for HP servers and workstations. HP-MPI uses enhancements whenever appropriate to provide low latency and high bandwidth point-to-point and collective communication routines. It supports multi-protocol execution of MPI applications on clusters of shared-memory servers so that applications can take advantage of the shared memory for intra-node communications. http://www.hp.com/go/mpi
Intel MPI Library (New Installation, versions 3.0, 3.1 3.2.0.011, in Finis Terrae)	Intel® MPI Library focuses on making applications perform better on IA-based clusters—implementing the high performance MPI-2 specification on multiple fabrics. It enables you to quickly deliver maximum end user performance even if you change or upgrade to new interconnects, without requiring major changes to the software or operating environment. Use this high-performance message-passing interface library to develop applications that can run on multiple cluster fabric interconnects chosen by the user at runtime. http://software.intel.com/en-us/intel-mpi-library
PyMPI (new installation, version 2.5b0, in Finis Terrae)	pyMPI is a fully functional Python interpreter that just happens to include a large subset of MPI functions. pyMPI has extensive support for running parallel Python scripts and has been tested on a number of clusters and other scientific machines. http://pympi.sourceforge.net
COMPILERS	
Intel C++ Compiler (new installation, versions 9.1.052, 10.1.012 y 11.0.069, in Finis Terrae. New installation, version 10.1.017, in the SVG)	Intel® C++ Compiler offers the best support for creating multi-threaded applications. It offers the breadth of advanced optimization, multi-threading, and processor support that includes automatic processor dispatch, vectorization, auto-parallelization, OpenMP*, data prefetching, and loop unrolling, along with highly optimized C++ templates for parallelism, math processing, and multimedia libraries. http://software.intel.com/en-us/intel-compilers

APPLICATION	TASK
<p>Intel Fortran Compiler (new installation, versions 9.1.052, 10.1.012 and 11.0.069, in Finis Terrae. New installation, version 10.1.017, in the SVG)</p>	<p>The Intel Fortran Compiler for Linux delivers rapid development and winning performance for the full range of Intel® processor-based platforms. It is a full-language Fortran 95 compiler with many features from the Fortran 2003 standard, plus a wide range of popular extensions. It automatically optimizes and parallelizes software to take best advantage of multi-core Intel processors, including dual-core mobile, desktop, and enterprise platforms. http://software.intel.com/en-us/intel-compilers</p>
<p>PGI Fortran Workstation (New version, 8.0.1, in the SVG)</p>	<p>The PGI Fortran Workstation Fortran compilers deliver outstanding performance on 64-bit x64 and 32-bit x86 processor-based workstations and servers, and enable simple portable parallel programming for both shared-memory and clustered computing systems. http://www.pgroup.com/products/workpghpf.htm</p>
SOFTWARE MANAGEMENT	
<p>Modules (new installation, version 3.1.6, in Finis Terrae. New installation, version 3.2.6, in the SVG)</p>	<p>The Environment Modules package provides for the dynamic modification of a user's environment via modulefiles. Modules abstracts the details about a software package's installation, environment, and software dependencies so that from a user's perspective, all software is accessed in the same way. http://modules.sourceforge.net</p>
<p>Subversion (new installation, version 1.5.3, in Finis Terrae)</p>	<p>Subversion is an open source version control system. It is used to maintain current and historical versions of files such as source code, web pages, and documentation. Its goal is to be a mostly-compatible successor to the widely used Concurrent Versions System (CVS). http://subversion.tigris.org</p>



computing challenges on FINISTERRAE

During its first year of operation, Finis Terrae executed 6 computing challenges, that is, large computational problems that either had not been proposed until that moment or that could now be executed thanks to the excellent computing potential that this equipment offers.

Three problems were first approached during Finis Terrae's test period with a dual intent. First, to take advantage of the fact that the machine was not occupied, and second, to measure the capacity of the machine itself and to detect possible bottlenecks, hardware errors, or misconfigurations. Following the success obtained with the first 3 computing challenges, 3 additional challenges were selected from those proposed by CSIC researchers. The six challenges executed are described below.

Fekete

The VARIDIS group of the Department of Applied Mathematics III in the Universitat Politècnica de Catalunya has tested a new robust, effective and versatile algorithm, the Forces Method, for the solution of the Fekete problem. This problem consists in minimising under general constraints a potential functional energy depending on the relative distances between N particle points. The Fekete points are the optimal configurations obtained in these types of problems. Finding an efficient algorithm for the search of good estimations of such optimal points for the logarithmic energy in the 2-sphere is the centre of S. Smale's "7th Mathematical problem for the 21st century". More precisely, Smale asks for a real number algorithm which computes these optimal points in polynomial time in N .

The Forces Method has been used to perform a massive computation program with the objective of producing significant statistical information in order to extract conclusions about Smale's 7th problem. In total, we consumed approximately 350,000 hours of computation in FinisTerraee in about two



weeks of real time and using 50% of its capacity (which is equivalent to 40 years using only one CPU).

The obtained results confirmed all the predictions about the behaviour of the Forces Method, overcoming the uncertainty related to convergence conditions or cpu-time estimations which emerge in other optimisation algorithms.

As a result of this challenge, more than 50 million local minima for the logarithmic energy in the 2-sphere are obtained. This is the greatest sample ever obtained for the Fekete problem and for Smale's 7th problem. From the statistical analysis of this sample information, a positive answer to the probabilistic Smale's 7th problem could be concluded. Furthermore, this analysis allows the identification of the master lines of a possible proof.

The results of this challenge are reported in the following scientific publications:

- E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto, A. Gómez, C. Mouriño, M.T. Sánchez, Computational cost of the Fekete problem I: the Forces Method on the 2-sphere, *Journal of Computational Physics* 228 (2009), 3288 – 3306.
- J.M. Gesto, Estimation of Fekete points, Dissertation, Departament de Matemàtica Aplicada III, Universitat Politècnica de Catalunya, 2008.

Hemcuve:

A mixed group of researchers in computational electromagnetism from the Universities of Vigo and Extremadura, along with CESGA staff, have implemented a code in order to perform electromagnetic calculations. That code is in constant development and it is based on an algorithm that is now out of date for these kinds of problems, considerably surpassed by more recent multilevel algorithms, but it has the particularity that it is more scalable. Multilevel algorithms are very efficient with only a few processors but they present scalability problems. The developed monolevel approximation which in principal is much more computationally intensive, scales almost linearly above 100 CPUs, and allows dealing with larger problems.

The first challenge attempted a problem of 35 million unknowns, close to the world record of 42 million. This challenge was finally achieved after multiple adaptations of the application to the platform, using 512 CPUs and 8 TB of RAM memory (64 full nodes of FT). After this execution, some unbalancing and bottlenecks were detected, limiting the scalability.

A new improved version of the code was developed and a challenge of 150 million unknowns was executed during the summer using 1024 CPUs and 5.4 Tb of memory, the biggest run at that moment in the world.

Note that the new problem, 5 times larger, consumes less memory than the previous one, due to the optimisations performed in the code. A new improved version of the code is under development and we plan to execute a problem with more than 500 million unknowns during January 2009.

For the execution of these challenges, a hybrid parallelization was implemented and half of FT was fully occupied, using MPI for inter-node communications and OpenMP within the nodes. This demonstrates that FT is perfect for these kinds of problems due to its great amount of memory per CPU.

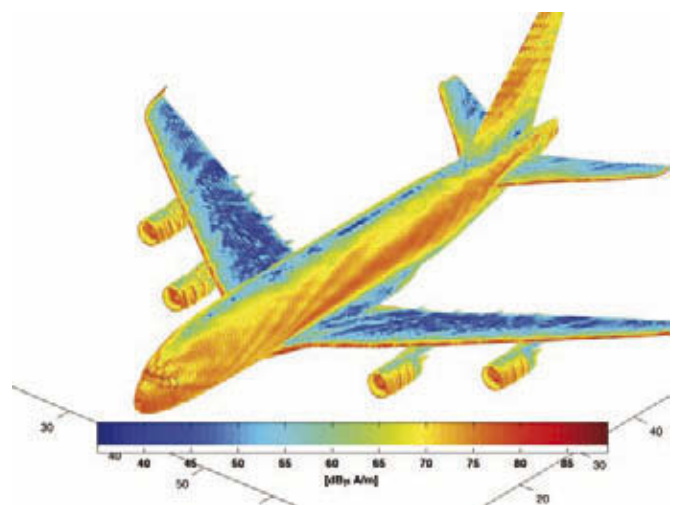
This project is applicable for the solution of electromagnetic problems in large structures equipped with radio systems, such as ships, planes, or satellites. In that manner, the elec-

tromagnetic behaviour of the structures in their stage of design can be simulated, in order to verify and guarantee the electromagnetic requirements and to minimise later problems during the manufacturing process.

The following scientific publications were produced as a result of this challenge.

- L. Landesa, J.M. Taboada, F. Obelleiro, J.L. Rodríguez, J.C. Mouriño, A. Gómez, "FMM in electromagnetic problems with tens of millions of unknowns", XXIII National Symposium of the International Scientific Radio Union (URSI 2008), Madrid, September 22-24, 2008.
- L. Landesa, J.M. Taboada, F. Obelleiro, J.L. Rodríguez, J.C. Mouriño, A. Gómez, "Fast Multipole Method in Supercomputers", VI Iberian Meeting of Computational Electromagnetism, Chiclana de la Frontera, Cádiz, October 21, 2008.
- J.C. Mouriño, A. Gómez, L. Landesa, J. M. Taboada, F. Obelleiro, J. L. Rodríguez, "High Performance Computing Electromagnetics Challenge: solving tens of millions of unknowns." Proceedings of IBERGRID 2008, Oporto (Portugal), May 12-14, 2008.

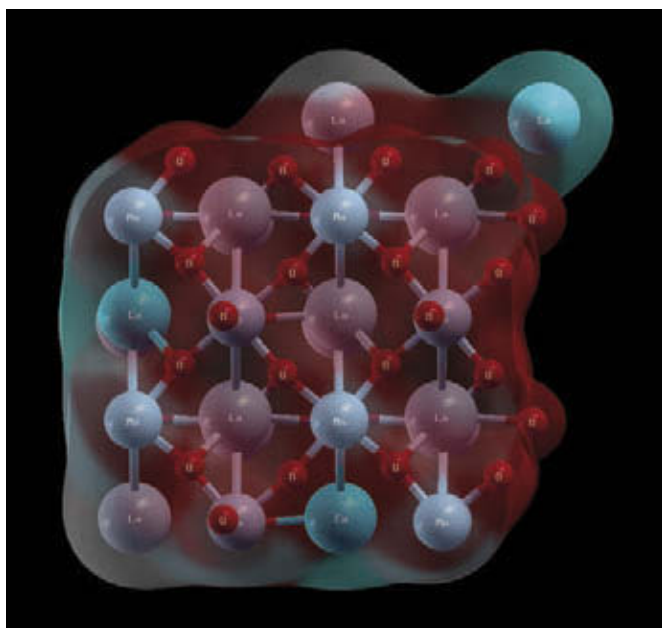
Other scientific articles have been presented for review but, at this moment, none have been published nor completely accepted.



Phase Transitions

A group of researchers from the Department of Applied Physics of the University of Santiago de Compostela, coordinated by Professor Daniel Baldomir along with CESGA staff, intend to solve the 3rd/4th most important physics problems of the decade according to the American Institute of Physics. The problem consists of discovering how exactly the phenomenon called "phase transition" is produced. This deals with the critical point in which a material acquires effective magnetic properties as a result of human intervention, concretely, adding other compounds or varying the temperature. Until now, the manipulation of the magnetic characteristics of a compound have been common, although we could only understand the dynamics in an approximate way. Due to the exhaustive understanding yielded by this discovery, it will be able to be controlled and, as a consequence, its applications can be refined.

To carry out the problem, 24 of all 142 computation nodes of Finis Terrae (which adds up to a total of 384 cores) were used, during an accumulated time of almost 68,000 hours, using 100 GB of memory and approximately 300 GB of disk space. These challenge results can open up many research lines. Some of those are the optimisation of battery technology for mobile telephones, a qualitative improvement in the memories of portable computers, or the optimisation of the sensors used to detect very small magnetic fields, and other multiple applications. At this moment, none of the obtained results have been published but work is in progress.



Genetic Algorithm for the Astrophysics of Massive Stars

This challenge was proposed by Francisco Najarro, a researcher in the Department of Infrared Molecular Astrophysics (DAMIR) of the Institute of the Structure of Material (IEM) at CSIC.

They have proposed genetic algorithms as an alternative method to obtain the stellar parameters that are generated by observations of astrophysical models of the atmosphere of massive stars.

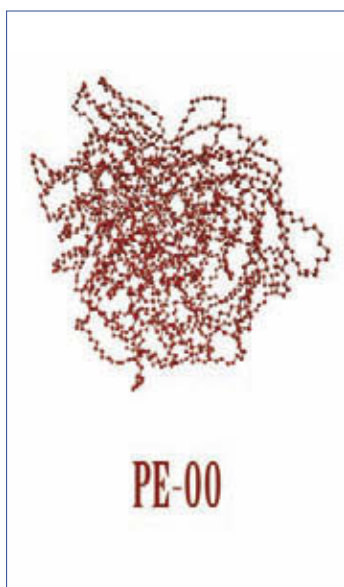
The precision and efficiency of the genetic algorithms depend in great part on the fine tuning of the genetic parameters to the problem of optimisation. This work has consisted of the adequation of the necessary diagnostics, the spectral lines, the genetic parameters, the codification, and the number of parameters in order to approach the astrophysical problem in a realistic manner.



In this challenge, the quantitative study of massive stars was initially based on infrared observations. Until now, these methods were only used in the stellar optical spectrum. Infrared is important because it permits the study of regions, such as the centre of our galaxy, that are optically dark and cannot be observed.

The studies, still in course, are revealing the enormous potential of this method. Actually, we are adapting our observation for later automatic analysis using the genetic algorithm implanted in Finis Terrae.

The typical resources used in the method correspond to the computation of about 20,000 to 40,000 models with an average time of 15 minutes per model. The method is highly parallel and scales linearly with the number of processors available. The tests are performed with a maximum of 80 cores. Work is underway to publish results of these computations.



Mathematical Sciences

The researcher Ana María Mancho from the Institute of Mathematical Science in CSIC used Finis Terrae to carry out her research.

The objective was to justify a new definition of Distinguished Trajectory (DT) which generalises the concepts of fixed point and periodic orbit to aperiodic flows. Finis Terrae made possible the exploration of this definition in an incredibly short period of time while, before the FT era, the work was progressing slowly, dragging through months. The required computational resources were between approximately 10000 and 15000 hours.

The obtained results are collected in the following publications:

- J. A. Jiménez Madrid, Ana M. Mancho. Distinguished trajectories in time-dependent vector fields. Accepted in Chaos.
- A. M. Mancho. Numerical studies on the self-similar collapse of the α -patches problem. In preparation.

Crystallization process of macromolecular systems

CSIC Researchers from the Macromolecular Physics Department of the Institute of Material Structure have proposed a problem concerning the crystallization process of macromolecular systems to be solved by means of molecular dynamics techniques using the public domain, massively parallel program, LAMMPS.

At this time, 16 computation nodes of Finis Terrae (256 cores) have been used during an accumulated time of more than half a million CPU hours. Preliminary results derived from molecular dynamics simulations of polyethylene models containing short chain branches concerning the molecular mechanisms involved in the formation of ordered structures during the early stages of crystallization have been obtained.



**Recetga
Communications**

science and technology network of Galicia:

The Science and Technology Network of Galicia (RECETGA) is a high-capacity communications infrastructure that provides connectivity and Internet services of the highest quality standards to the research community in Galicia. It was established in 1993 and, after successive technological changes in accordance with the new technologies of transmission and transport, today it interconnects 43 technological centres, research units in hospitals, research institutes, and the totality of Galician university campuses. RECETGA's main mission is to provide advanced network services as well as a technological environment that makes possible research, development, and innovation in the field of communications and that favours the development of the Galician Information and Knowledge Society.

RECETGA is managed by CESGA who is licensed as a Class C

Internet Service Provider by the Spanish Telecommunications Authority (CMT).

The network is based on Gigabit Ethernet lines and ATM circuits. RECETGA permits access to services supplied by CESGA, interconnects research centres, allows access to other academic networks, and to the Internet.

RECETGA is connected with European scientific and academic networks by way of RedIRIS10. This Spanish academic network has one of its most important nodes located at CESGA. It is through RedIRIS10 that CESGA's users have access to the European Science and Technology Network, GEANT.

Network users include:

- Research Centres and Laboratories of the Regional

RECETGA TECHNICAL SPECIFICATIONS

BACKBONE NETWORK

- Based on Dark Fibre and SDH Radio Links
- Gigabit and ATM Links
- JUNIPER M20, M10 & M10i Gigarouters
- FORE ATM Switches

ACCESS NETWORK

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

NETWORK MANAGEMENT

- Own developments based on open source software

CONNECTION TO RedIRIS

- Five links at 2.5 Gbps

CESGA INTERNAL NETWORK

- Gigabit Ethernet-Fast Ethernet
- 3COM, JUNIPER & ENTERASYS Switches
- DELL, HP & 3COM Switches
- JUNIPER & ENTERASYS Switchrouters

SERVICES AVAILABLE TO CONNECTED CENTRES

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

Government, Xunta de Galicia.

- University System of Galicia.
- Spanish National Research Council (CSIC) Centres in Galicia.
- Other Public and Private R&D institutions.

The Communications department staff at CESGA provides support to RECETGA, RedIRIS, CESGA's internal communications, and other internal services. They also manage network security and technical coordination with connected centres.

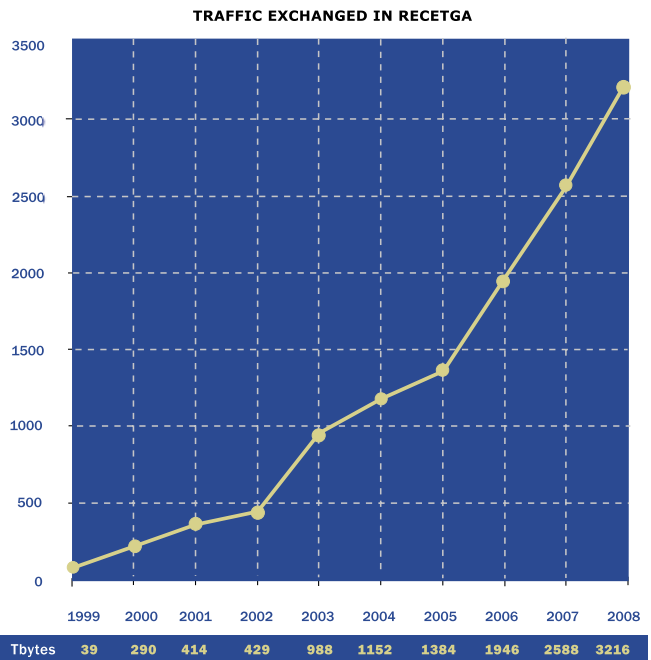
RECETGA's most relevant activities during 2008 are summarised below.

Network management and monitoring:

The Galician Science and Technology Network offered its services with 99.743% availability. This percentage of availability was affected in some centres because they do not have personnel working on the weekends and, for that reason, such events such as cuts in electrical supply are not attended to until the next work day.

Activities were undertaken in 2008 to guarantee the evolution and improvement of the network. They are listed below.

- A comparative study of the costs of different network maintenance alternatives.
- The migration of FEUGA and DXIDI to gigabit technology.
- A study of the migration of SERGAS and the CHUS to gigabit technology.
- The set up of a backup link for the Institute of Marine Research in Vigo (CSIC).
- The migration of the CEIDA connection to Fast Ethernet.
- The signing of a Collaboration Agreement with the DGT (Spanish Motorway Traffic Authority) to share computing and telecommunications infrastructures of interest including highway service galleries.
- The signing of an Agreement of Collaboration with RED.es to connect the Portuguese Science & Technology Network with RECETGA and RedIRIS.

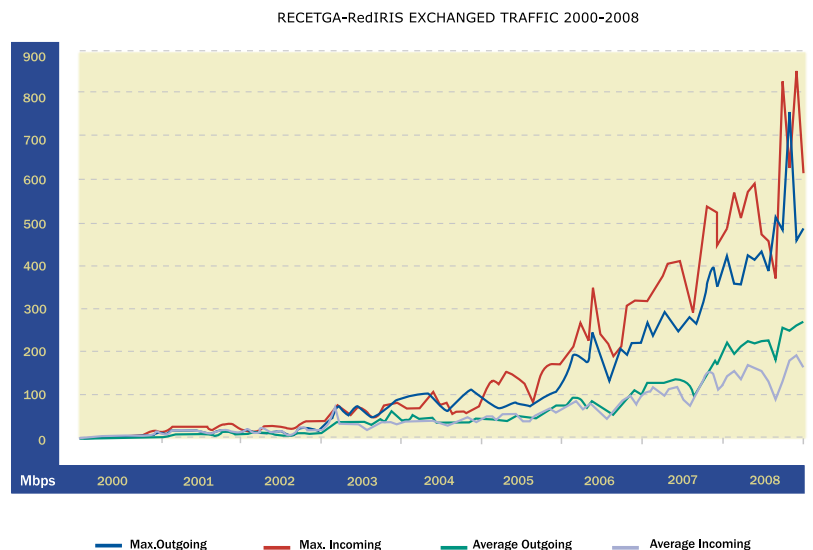


Diffusion and conference activity during 2008:

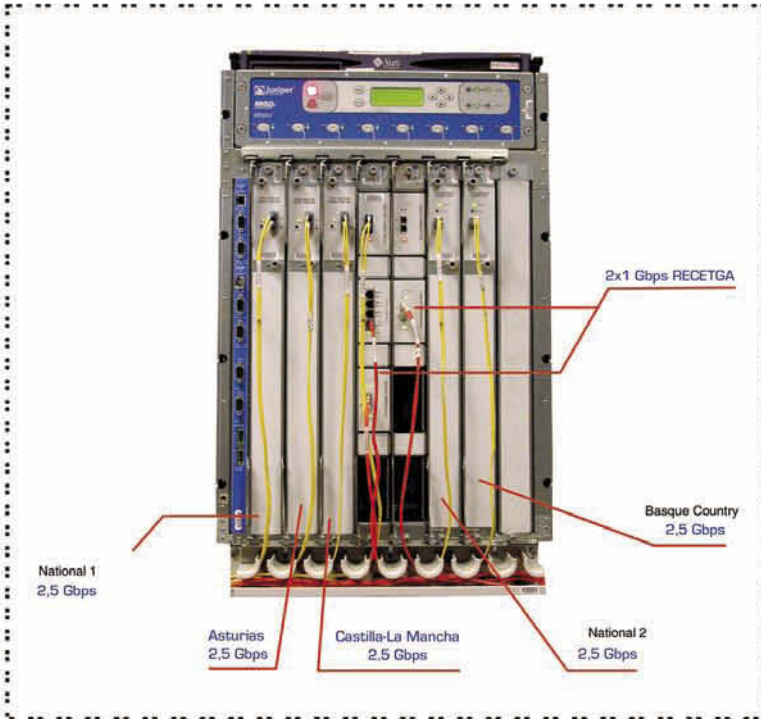
- Contribution to the diffusion of multimedia technologies via a presentation in the IIR Tele-Presence in Spain Conference.

Adaptation of internal network infrastructures to accommodate the Finis Terrae Supercomputer:

Due to the arrival of Finis Terrae, CESGA had to adopt various measures in order to adequately adjust the infrastructure to the requirements of this new system. These operations affected the area of communications. The work initiated in 2007 continued during the first months of 2008.



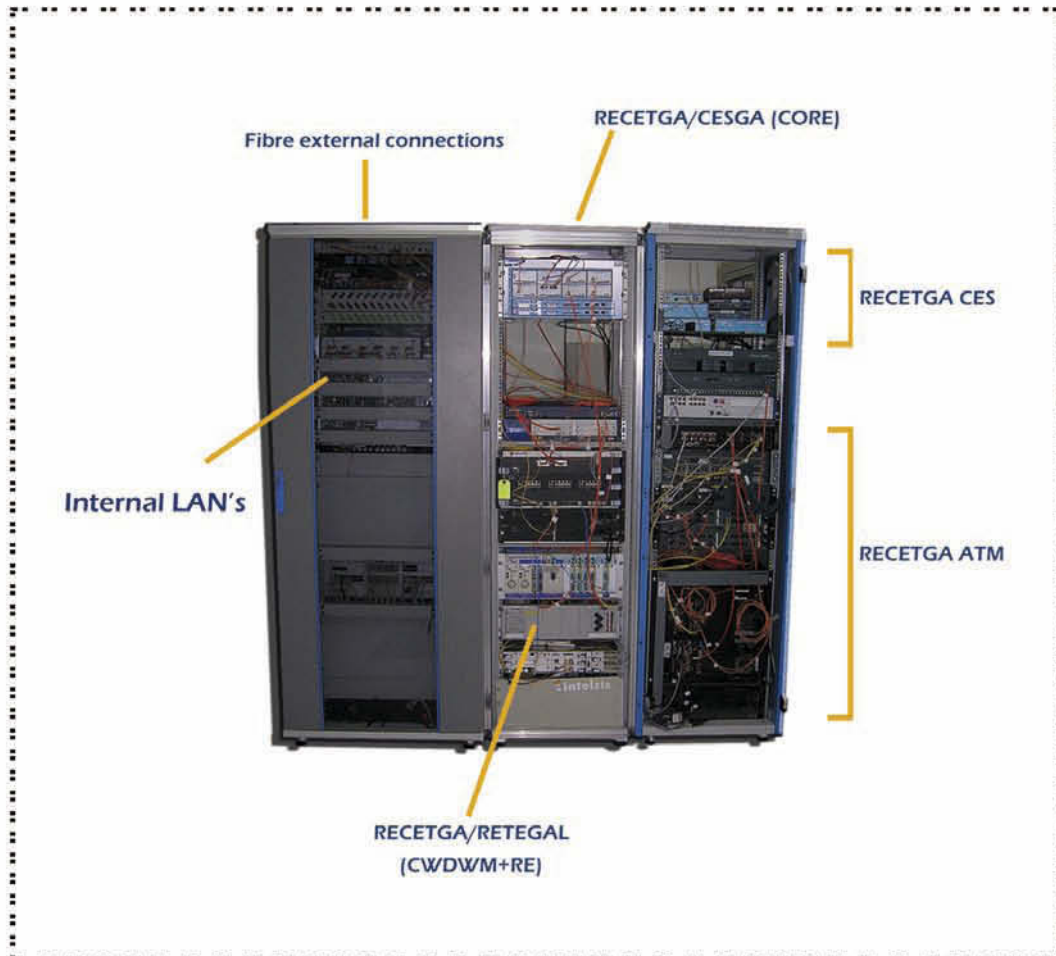
RedIRIS PoP IN GALICIA (JUNIPER M40E)



EXTERNAL CONNECTIONS THROUGH



RECETGA CENTRAL NODE INSTALLED AT CESGA



Centres Connected to RECETGA

CENTRE	LINK	AVAILABILITY
Universidade da Coruña		
Coruña Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155Mbps	99,999%
Ferrol Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155Mbps	99,972%
Universidade de Santiago de Compostela		
Santiago Campus	2 Fibre Optics (1Gbps)	99,999%
Lugo Campus	Fibre Optics (1Gbps)	99,943%
Universidade de Vigo		
Vigo Campus	2 Fibre Optics (1Gbps)	99,925%
Pontevedra Campus	Fibre Optics (1Gbps)	99,940%
Ourense Campus	Fibre Optics (1Gbps)	99,946%
Universidade de Minho		
BUGALICIA		
Consorcio de Bibliotecas Universitarias de Galicia	Fibre Optics (155Mbps)	98,805%
RTD Centres		
ANFACO - CECOPECA (Vigo)	FastEthernet (100Mbps)	99,859%
Aula de Produtos Lácteos (USC - Lugo)	Radio Link 4x2 Mbps	99,810%
Centro de Investigacións Forestais (Lourizán)	ATM Radio Link at 155 Mbps	98,833%
Centro Superior Bibliográfico de Galicia	Fibre Optics (155Mbps)	98,985%
Centro de Investigacións Lingüísticas "Ramón Piñeiro"	ATM Radio Link at 155 Mbps	99,999%
Centro Tecnolóxico Armando Priegue AJMEN	Radio Link 4x2 Mbps	99,400%
Estación de Viticultura e Enoloxía (Leiro)	ISDN (64 Kbps)	NA
Centro de Cultivos Mariños (Ribadeo)	ISDN (64 Kbps)	NA *
Centro de Investigacións Agrarias de Mabegondo	Radio Link 4x2 Mbps	99,973%
Centro de Control de Calidade do Medio Mariño (Vilaxoán)	ATM Radio Link at 155 Mbps	99,977%
Centro de Investigacións Mariñas (Corón)	Radio Link 4x2 Mbps	99,985%
Centro de Supercomputación de Galicia	2 Fibre Optics (1Gbps)	99,997%
Centro Tecnolóxico del Mar (CETMAR)	Wireless (11/22 Mbps)	99,394%
Centro de Innovación e Servicios (Ferrol)	ATM Radio Link at 155 Mbps + Wireless (11/22 Mbps)	97,430%
Fundación Empresa - Universidade de Galicia (Vigo)	FastEthernet (100Mbps)	99,859%
Fundación Empresa - Universidade de Galicia (Santiago)	Fibre Optics (16 Gbps)	99,628%
CEIDA (Santa Cruz)	Wireless (11/22 Mbps)	99,725%
Dirección Xeral de I+D+i	Fibre Optics (1 Gbps)	99,999%
Centro Tecnolóxico del Automóvil (CTAG)	Radio Link 4x2 Mbps	99,984%
Centro Multimedia de Galicia		99,996%
Hospitals		
Hospital Clínico Universitario de Santiago de Compostela	Fibre Optics (155Mbps)	99,996%
Complexo Hospitalario "Xeral - Cies"	Radio Link ATM at 155 Mbps	99,605%
Complexo Hospitalario Universitario "Juan Canalejo"	ATM Radio Link at 155 Mbps	99,999%
Unidade de Investigación do Hospital do Meixoeiro	ATM Radio Link at 155 Mbps	99,841%
Centro Oncolóxico de Galicia	Wireless (11/22 Mbps)	99,734%
IEO		
Instituto Español de Oceanografía - A Coruña	Wireless (11/22 Mbps)	99,889%
Instituto Español de Oceanografía - Vigo	ATM Radio Link at 155 Mbps	99,844%
I.E.O Delegación de Vigo sede Bouzas		99,868%
CSIC		
Misión Biolóxica de Galicia	Radio Link 4x2 Mbps	98,392%
Instituto de Investigacións Agrobiolóxicas de Galicia	Fibre Optics (1Gbps)	99,999%
Instituto de Investigacións Marinas	Fibre Optics (155 Mbps)	99,413%
Instituto de Estudos Galegos "Padre Sarmiento"	Radio Link 4x2 Mbps	99,982%
Delegación Institucional del CSIC en Galicia	FastEthernet (100 Mbps)	99,999%
Other Centres		
Palacio de Exposicións e Congresos de Galicia	Fibre Optics (155 Mbps)	NA **
Parque Tecnolóxico de Galicia	Fibre Optics (155 Mbps)	99,723%
Meteogalicia	Fibre Optics (155 Mbps)	99,805%
Exchange with other Networks		
ONO	2x100 Mbps	99,985%
RedIRIS	5x2,5 Gbps	99,998%
RETEGAL	155 Mbps	99,984%
SERGAS	155 Mbps	99,993%

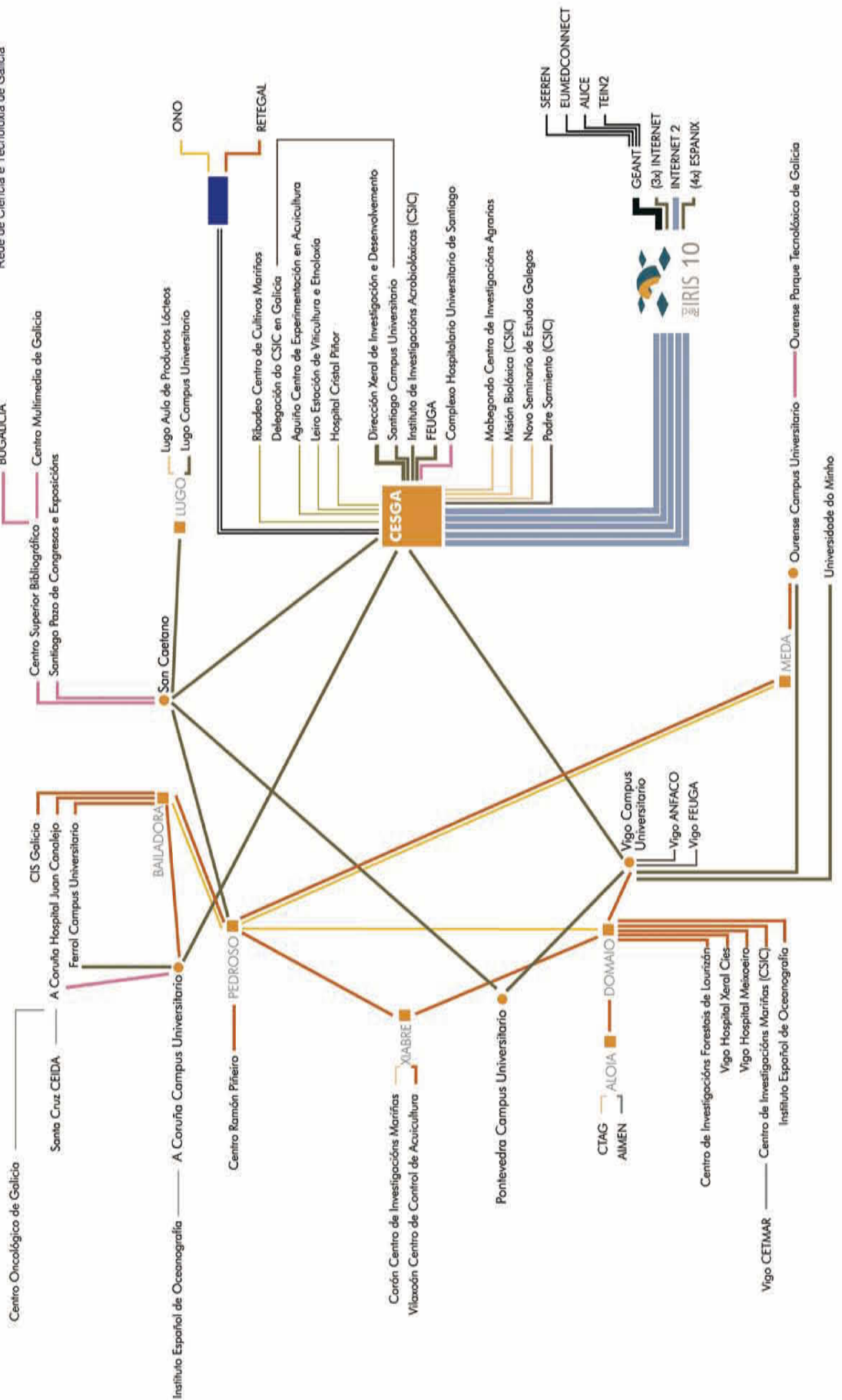
* Disconnected February 08

** 100% Conectivity provided on demand

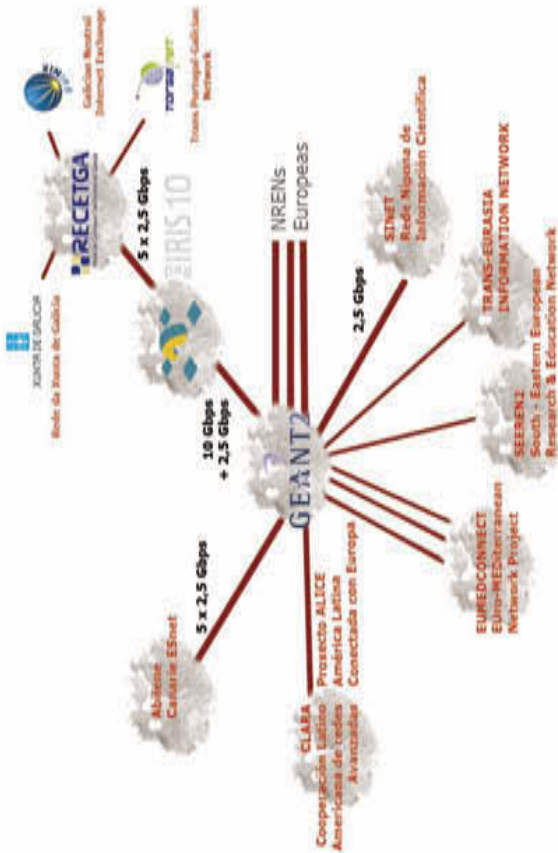
- Radio Enlace 4x2 Mbps
- Radio Enlace ATM a 34 Mbps
- Radio Enlace ATM a 155 Mbps
- RDSI [64 Mbps]
- Fibra Óptica [1 Gbps]
- Fibra Óptica [2.5 Gbps]
- Fibra Óptica [10 Gbps]
- Frame Relay [64 Kbps]
- Frame Relay [256 Kbps]
- Wireless [11/22 Mbps]
- FastEthernet [100 Mbps]

RECETGA

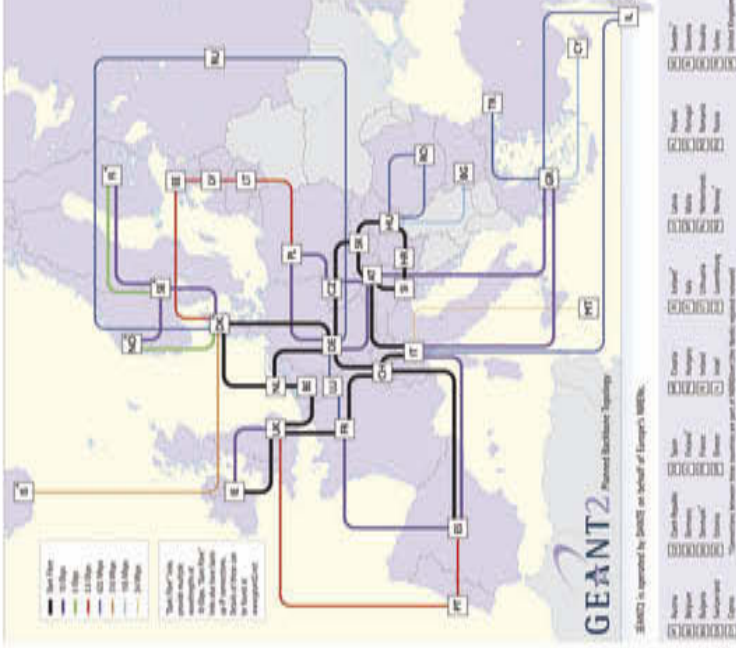
Rede de Ciencia e Tecnoloxía de Galicia



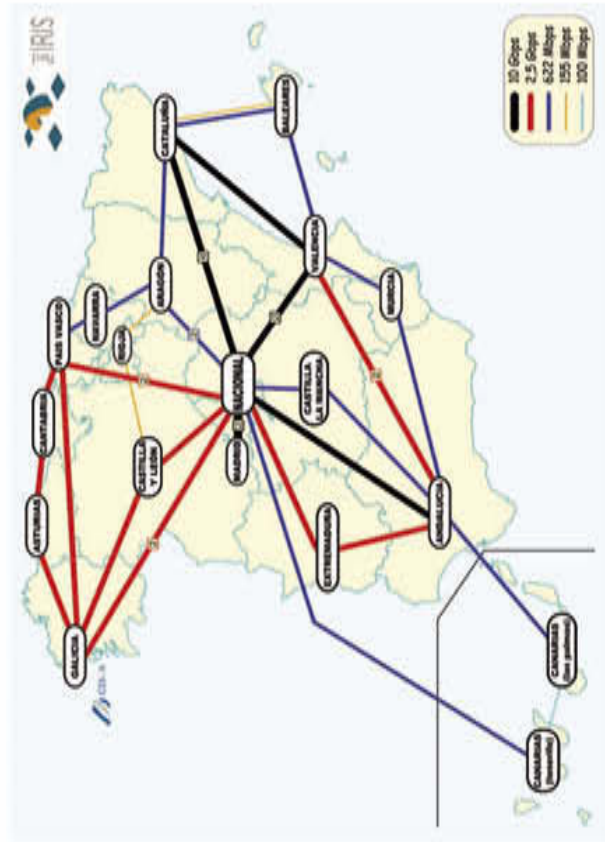
CONNECTIONS THROUGH GEANT



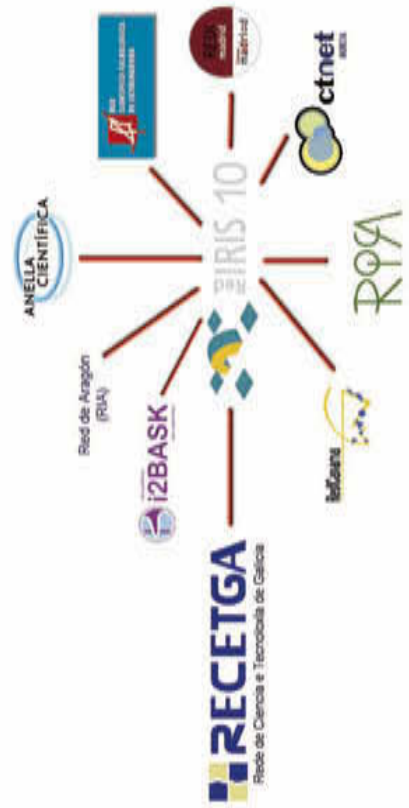
GEANT TOPOLOGY



RedIRIS TOPOLOGY



CONNECTIONS THROUGH REGIONAL NETWORKS





Support Infrastructures

CESGA'S support infrastructures

In order to guarantee 24 x 7 service to users and researchers at CESGA, computing servers, switching, and routing equipment have a support infrastructure available which provides the following resources.

ELECTRICAL SUPPLY

In order to support the increment in electrical power that the supercomputer requires, CESGA has:

- an external electrical supply line of 1.5 Mw,
- 10 electric circuit breakers,
- a 1,600 KVA transformer, complementary to the previous existing one with 630 KVA,
- two Systems of Uninterrupted Power Supply (UPS) of 400 KVA,
- two units adding up to 180 KVA, and
- an electricity generation group of 1,100 KVA and 8 tons of

weight. This group allows the entire installation to be maintained in operation during prolonged cuts in electrical supply.

COOLING

- Two chiller plants of 580 KW each, and
- 10 computer room air handlers (CRAH) of 120 KW, to dissipate the heat generated.

FIRE SUPPRESSION

- A state-of-the-art system for the detection and extinction of fires based on HFC227 gas.

DATA CENTRE ROOM

- The data centre room has a technical floor surface area of 340m².

EQUIPMENT	CHARACTERISTICS
ELECTRICAL SUPPLY	
General Circuit Breaker Board Remodeling	10 New circuit breaker boards (general distribution board, UPS distribution boards, 6 distribution boards in data centre)
Transformers	1.600 KVA 630 KVA
UPS	1 x 120 KVA 1 x 60 KVA
External Electrical Supply Line	1.5 Mw
Power Generator	1.100 KVA
COOLING	
Chilled Water Plants	2 x 580 Kw
CRAH	10 Units x 120 Kw
DATA CENTER ROOM	
Technical Flooring Surface Area	340 m ²
FIRE SUPPRESSION	
Fire Detection & Extinction System	Based on HFC227 Gas



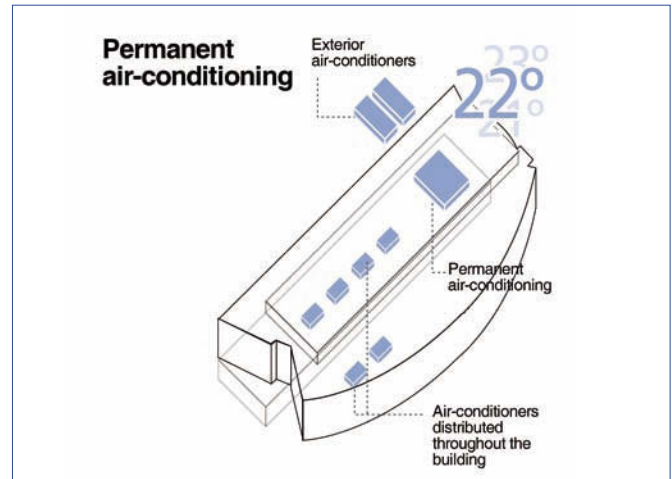
permanent air-conditioning

Large computers generate an enormous amount of heat. In order to maintain optimal climactic conditions (22° and 50% humidity), the building has two chiller plants of 580 KW each, with a total of 10 interior computer room air handlers.

Exterior water chiller plants.

Computer room air handlers (CRAH).

Air-conditioners distributed throughout the building.



Security – Electrical Power Supply

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

Transformer

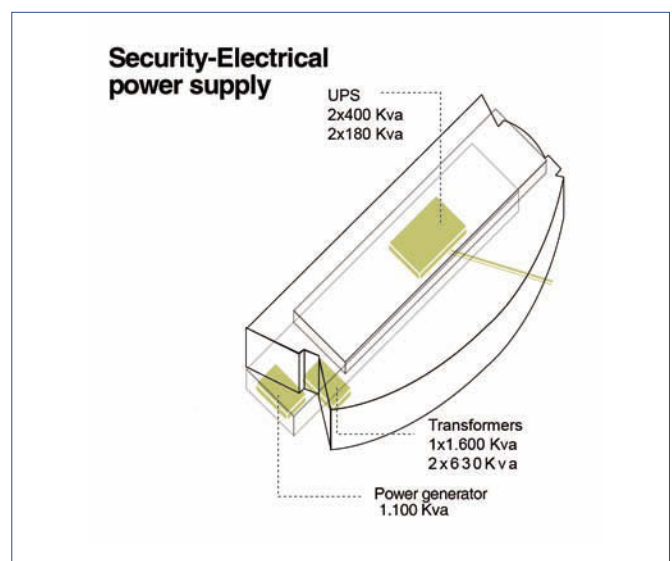
(1,600 Kva+630 KVA)

Power generator

(1,100 KVA)

UPS

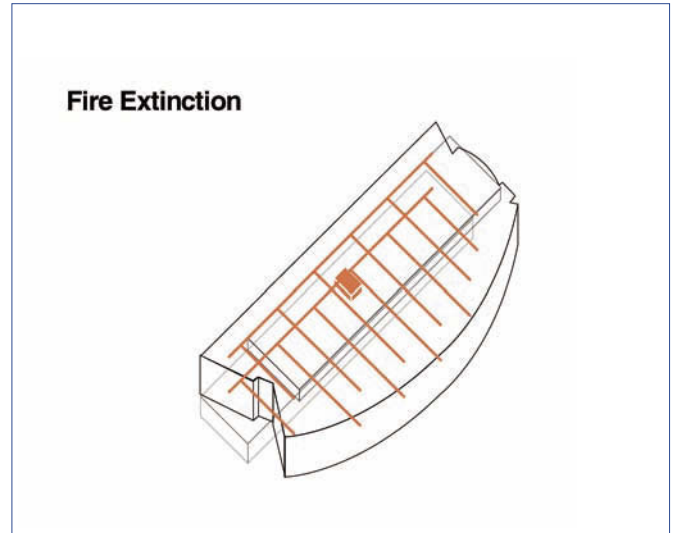
(2x400 KVA+180 KVA)



Fire Suppression

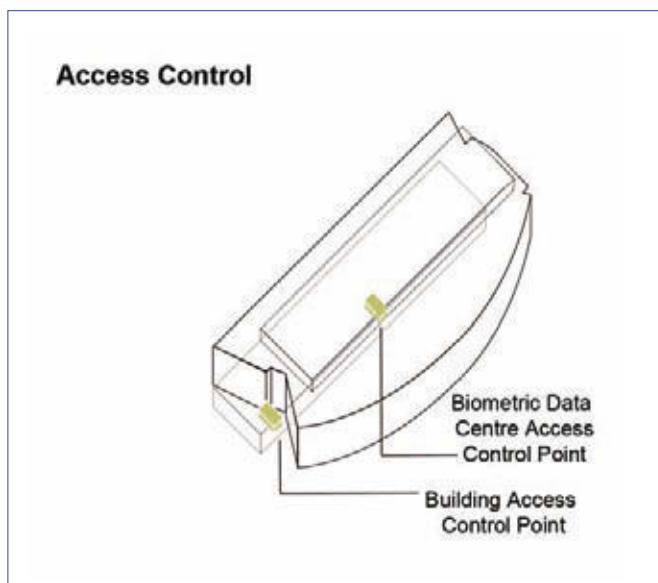
A system of smoke detectors activates the alarm and initiates the gas (HFC227) extinction system when necessary. This gas rapidly displaces the oxygen in the rooms and prevents combustion.

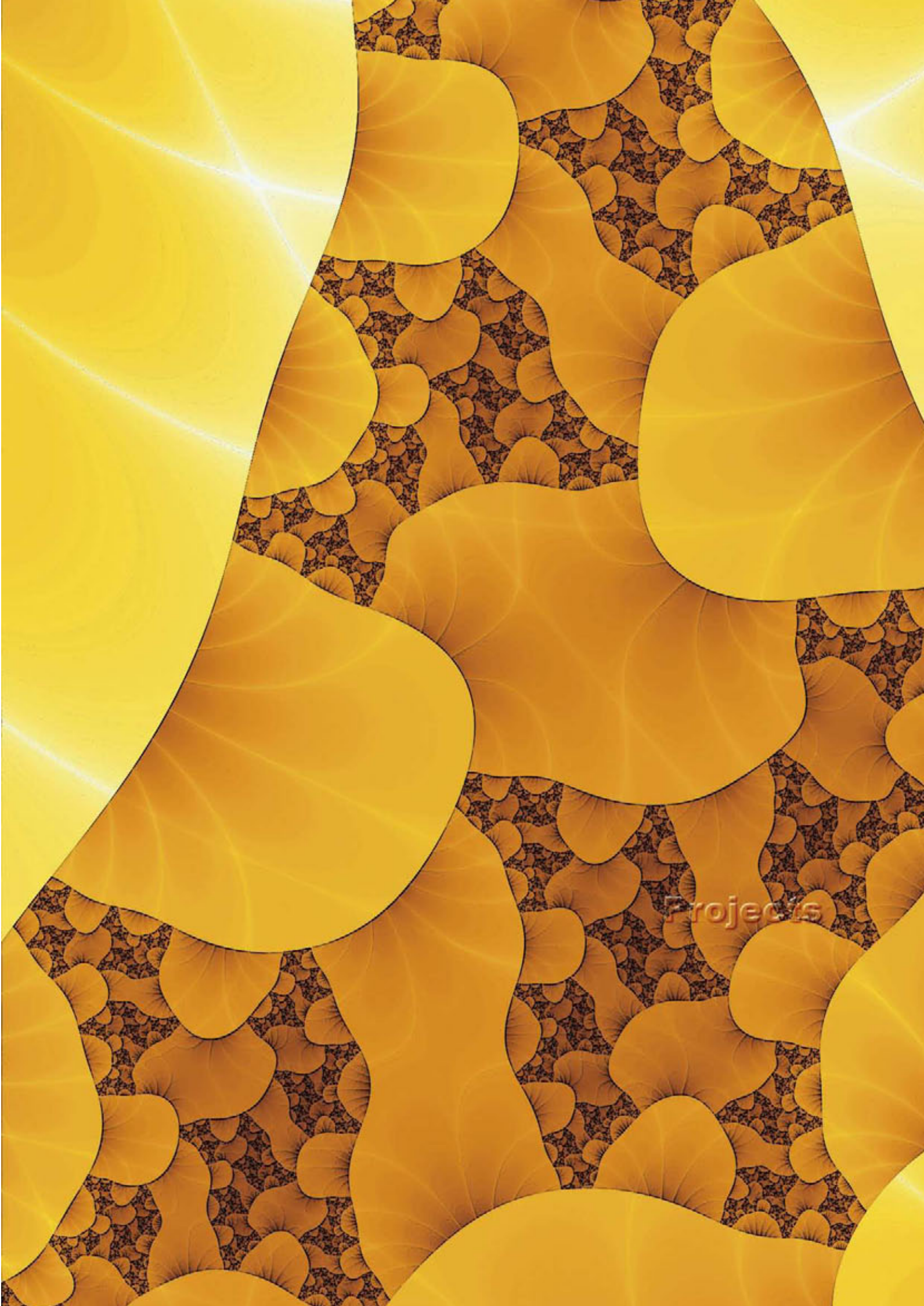
- UPS room
- Extinction room
- Storage room
- Air-conditioning rooms
- Power generator room
- Electricity transformer centre (transformers)



Access Control

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





Projects

Research, technological development & innovation projects in which CESGA actively participated in 2008

During 2008, CESGA's activity in RTD and Innovation Projects was very intense, with notable results. In total, CESGA directed or collaborated in more than 40 proposals for regional, national, or international projects.

The achievement in 2008 of two European Union VII Framework Programme projects and the continuation of a project under the PROFIT programme are all noteworthy. In addition, the success rate of project proposals resolved this year was very high (73%). All of that was accomplished while constantly attending to the development of the projects in progress such as EGEE, e-IMRT, or int.eu.grid, in which important goals were achieved.

The GIS, e-Learning & Collaboration Tools, and Technology Transfer & e-Business departments increased their activity in projects in 2008. These departments have entered joined new project consortiums and have successfully continued work in projects in progress.

Activity regarding the creation and participation in regional, national, and international networks has been equally important. In the following pages a list of the research, technological development and innovation projects in which CESGA participated in 2008 is detailed.

AREA	PROJECTS
Computing	19
Network Communications	4
Colaboration Tools & e-Learning	3
Geographical Information Systems	4
Technology Transfer & e-Business	4
Other	4
TOTAL	38
GRANT SOURCE	PROJECTS
European Commission	10
Spanish Government	7
Galician Regional Government	17
Industry	4
TOTAL	38
Thematic Networks, Technological Platforms	19

COMPUTING

Enabling Grid for E-SciEnce III (EGEE III)

Partners: CERN, JKU, KFKI-RMKI, CESNET, II SAS, JSI, CYFRONET, SRCE, FOM, VUB, FZK, SWITCH, CNRS, CCGV, INFN, ED, TRUST-IT, UH.HIP, CSC, SIGMA, VR-SNIC, RRC KI, GRNET, IPP BAS, UCY, TAU, ICI, IPB, TUBITAK, LIP, IFAE, TCD, STFC, DANTE, KEK, ASGC, KISTI, CNU, UNIMELB, WISCONSIN SYSTEM, RENCI, BT-IC.

Coordinator: B. Jones, CERN

Principal Researcher: I. López Cabido, CESGA

Financing: European Commission: Information Society Technologies Programme.

Project Code: INFISO-RI-222667

Budget: 218,000.00 €

Period: 2008-2010

Objectives: This is the third phase of the deployment of a global GRID infrastructure accessible to researchers and businesses 24 hours a day. The objective is to provide researchers with access to important computational resources, independent of their geographical location.

Improvement of Memory Usability and Performance (HP UPC)

Partners: CESGA, UDC, USC

Coordinator: I. López Cabido, CESGA

Principal Researcher: I. López Cabido, CESGA

Financing: Research Contract (Subject to an Agreement of Confidentiality)

Project Code: HP-001

Budget: 84,007.00 €

Period: 2008-2011

Objective: To improve the usability and productivity of UPC.

Hardware Counters Use to improve Memory Performance (HP Counters)

Partners: USC, UDC, HP, and CESGA

Coordinator: C. Fernández Sánchez, CESGA

Principal Researcher: C. Fernández Sánchez, CESGA

Financing: Research Contract (Subject to an Agreement of Confidentiality)

Project Code: HP-002

Budget: 91,903.00 €

Period: 2008-2011

Objective: To improve memory performance.

EELA2

Partners: IBBM, IFLP/UNLP-CONICET, III-LIDI / UNLP, INIFTA / UNLP-CONICET, INNOVARED (NREN), INSIBO / UNT, LINTI / UNLP, LISiDi / UNS, UBA, CBPF, CCE / USP, CEFET-RJ, FCM / UERJ, FIOCRUZ, IF / USP, IME, INCOR, INPE, LNCC, ON, RNP (NREN), SPRACE / UNESP, UFCG, UFF, UFJF, UFMS, UFRGS, UFRJ, UFSM, UnB, UNILASALLE, UNISANTOS, CEAZA-USERENA, CMM-UCHILE, PUC, REUNA, UDEC, UFRO, UTALCA, UTFSM, UVALPARAISO, UNIANDES, UNIV. ANTIOQUIA, INAMHI / INOCA, IPGP, INFN, UNAM, CIP, IGP, PUCP, SENAMHI, UNT, UPCH, USMP, U. AVEIRO, U. MINHO, U. PORTO, CRMPA (INFN third party), DOCEBO (Italy), GFI (Spain), INSA (Spain), MAAT (Spain), CESGA, CIEMAT, DGSP / CSISP, DTIS-LVG, DVA, RED.ES (NREN), SATSI, UC, UCM, UEX, UPV, ULA, USB.

Coordinator: Bernard Maréchal, CETA-CIEMAT / UFRJ (Spain/ Brazil)

Principal Researcher: I. López Cabido, CESGA

Financing: The European Commission - VII Framework Programme

Project Code: EU-FP7-223797

Budget: 66,000.00 €

Period: 2008-2010

Objective: To construct a grid infrastructure that is scalable and has high quality and production capacity based on the existing EELA e-infrastructure installation grid. The new grid will be capable of providing 24 hour a day access to distributed computing, storage, and network resources for an ample spectrum of applications for the European and Ibero-American research communities.

Support Technicians II

Partners: CESGA

Coordinator: C. Fernández Sánchez, CESGA

Principal Researcher: C. Fernández Sánchez, CESGA

Financing: The Ministry of Science and Innovation

Project Code: PTA2007-0375-I

Budget: 54,000.00 €

Period: 2008-2011

Objectives: Support Technicians II, Ministry of Science and Innovation.

Development of the Second-level (Tier-2) Spanish Centre for the processing of Particles IV

Partners: USC and CESGA

Coordinator: J. J. Saborido Silva, University of Santiago de Compostela, USC

Principal Investigator: C. Fernández Sánchez, CESGA

Financing: The Ministry of Science and Innovation

Project Code: FPA2007-66437-Co2-02

Budget: 13,797.00 €

Period: 2007-2010

Objective: The launching of a GRID infrastructure for CERN's LHCb experiment.

int.eu.grid

Partners: IFCA, LIP (Portugal), Poznanskie Centrum superkomputerowo Sieciowe (Poland), Forschungszentrum Karlsruhe (Germany), UAB, CYFRO-NET AGH (Poland), GUP (Austria), Trinity College (Ireland), II SAS (Slovak Republic), ICM (Poland), BIFI (Spain), HLRS (Germany) and CESGA

Coordinator: J. Marco de Lucas, Instituto de Física de Cantabria, IFCA-CSIC

Principal Researcher: C. Fernández Sánchez, CESGA

Financing: The European Commission - VI PM-EU I3

Project Code: 031857

Budget: 114,000.00 €

Period: 2006-2008

Objectives: To launch, maintain, and operate a quality GRID infrastructure in order to provide service to communities of researchers with interactive applications that have a high computational demand.

Enabling Grid for E-SciEnce II (EGEE-II)

Partners: AGSC, BME, BT-IC, CEA, CERN, CESGA, CESNET,

CGG Services, CIEMAT, CKSC, CNES, CNR-ITB, CNRS, CRSA, CSC, CSIC, CYFRONET, DANTE, DESY, DFN, DKRZ, ELETTRA, ELSAG DATAMAT, ENEA, ETHZ(CSCS), FhG/SCAI, FOM, FZJ, FZK, GARR, Glasgow, GRNET, GSI, HEALTHGR ID, ICI, IHEP, IISAS, IMPB RAS, Imperial, INFN, IPB, IPP-BAS, ITEP, JINR, JKU, JSI, KFKI-RMKI, KIAM RAS, KISTI, KTH, LIP, MTA SZTAKI, MTW, NIIF, Oxford, PIC, PNPI, PSNC, RED.ES, RENCI, RRC KI, RUG, SARA, SINP MSU, SRCE, STFC, SWITCH, TAU, TCD, TID, Trust-IT, TUBITAKULAKBIM, UChicago, UCM, UCY, UEDIN, UH-HIP, UiB, UIBK, UKBH, ULB, UNICAL, UNILE, UNIMAN, UNINA, UNIZAR, UPV, USCUvA, UW, UWisc-Madison, VR.

Coordinator: Bob Jones, CERN

Principal Researcher: I. López Cabido, CESGA

Financing: Information Society Technologies Programme (EU)

Project Code: INFISO-RI-031688

Budget: 182,530.00 €

Period: 2006-2008

Objective: This is the second phase of the deployment of a global GRID infrastructure that is available to researchers and businesses 24 hours a day. The objective is to provide researchers with access to important computing resources independent of their geographic location.

Development of 2nd and 3rd level Spanish Centres (Tier-2 and Tier-3) for the processing of experimental data (Particles III)

Partners: USC and CESGA

Coordinator: J.J. Saborido Silva, Universidade de Santiago, USC

Principal Researcher: C. Fernández Sánchez, CESGA

Financing: Ministry of Science and Innovation

Project Code: FPA2005-07761-Co2-02

Budget: 11,550.60 €

Period: 2005-2008

Objectives: The launching of a GRID infrastructure in Spain for the CERN-LHCd experiment.

The Consolidation and Structure of Competitive Research Units of the Galician I+D+i System (unid-inv-08)

Partners: CESGA

Coordinator: J. García Tobío, CESGA

Principal Researcher: J. García Tobío, CESGA

Financing: Xunta de Galicia

Project Code: INCITEo8ENA704088ES

Budget: 128,295.00 €

Period: 2010/2008-21/11/2008

Objectives: Aid for research group consolidation.

Moving CSEGA forward as a Research Centre of Excellence (NextCESGA)

Partners: CESGA

Coordinator: J. García Tobío, CESGA

Principal Researcher: J. García Tobío, CESGA

Financing: European Commission, VII Framework Programme

Project Code: FP7-203135

Budget: 138,316.00 €

Period: 2008-2009

Objectives: To produce a SWOT Analysis (Strengths, Weaknesses, Opportunities, and Threats) of CESGA and to define an Action Plan to move CESGA forward as a research centre of excellence.

BEinGRID. Business experiment for the improvement of IMRT planning (Intensity-modulated Radiotherapy) using on demand GRID services with service level agreements (SLAs)

Partners: Over 100 research groups from Universities, Research & Technology Centres

Coordinator: Santiago Ristol, ATOS Origin

Principal Researcher: A. Gómez Tato, CESGA

Financing: Galician Regional Government, Xunta de Galicia

Project Code: PGIDITo4CS0137030PR

Budget: 54,600.00 €

Period: 2008-2009

Objective: The proposed business experiment is designed to integrate the solution in a GRID environment, adding a service-level agreement and security from beginning to end. These aspects will support the common components of BEinGRID, permitting possible providers to obtain more computing resources in order to confront periods of peak demand. The final objective of the project is to offer BEinIMRT services to many European hospitals based on a pay-per-use or a flat rate payment system.

SmartLM. Grid-friendly software licensing for location independent application execution

Partners: Noesis Solutions NV, Belgium, L.M.S.-Systems BVBA, Belgium, Intes-Ingenieurgesellschaft Fuer Technische Software MBH, Germany, Gridcore AB, Sweden, L.M.S.

International NV, Belgium, Cineca Consorzio Interuniversitario, Italy, Fundación Centro Tecnológico de Supercomputación de Galicia, Spain, The 451 Group Limited, United Kingdom, Forschungszentrum Juelich GMBH, Germany, T-Systems Solutions for Research GMBH, Germany, ANSYS Germany GMBH, Germany, LMS Numerical Technologies, Belgium, Fraunhofer-Gesellschaft Zur Foerderung der Angewandten Forschung E.V, Germany.

Coordinator: J. Martrat, ATOS

Principal Researcher: A. Gómez Tato, CESGA.

Financing: European Commission – VII PM

Project Code: 216759

Budget: 153,323.75 €

Period: 2008-2010

Objectives: SmartLM will provide a concession of generic, flexible licenses for a new virtualisation technology service oriented toward those business models through the limits of the organisation.

Finis Terrae Socio-economic Impact Study (ICTS-Impacto)

Partners: CESGA

Coordinator: J. García Tobio, CESGA

Principal Researcher: A. Gomez Tato, CESGA

Financing: Ministry of Science and Innovation

Project Code: CAC-2007-54

Financing: 68,000.00 €

Period: 2007-2008

Objectives: This is a socio-economic analysis of the impact of the installation of Finis Terrae.

Qualified Electronic Signature Infrastructure – IfeC

Partners: Aldaba Servicios Profesionales, Aldaba Soluciones y Proyectos SL, UVIGO, and CESGA

Coordinator: J.A. Castelao Boo, Aldaba Servicios Profesionales

Principal Researcher: A. Gómez Tato, CESGA

Financing: Centre for Technological and Industrial Development (CDTI) and the Government of Galicia (Xunta de Galicia)

Project Code: FIT-360000-2007-14

Budget: 19,978.70 €

Period: 2007-2008

Objectives: This study of the design and development of a Qualified Electronic Signature Infrastructure (IFeC), sustained on the Management of Privileges Infrastructure (PMI)

and a Time Seal Authority (TSA), permits its easy inclusion in applications that require authorisation control such as in management environments of corporate authorisations.

g-fluxo

Partners: CESGA

Coordinator: J. López Cacheiro, CESGA

Principal Researcher: J. López Cacheiro, CESGA

Financing: Regional Government of Galicia, Xunta de Galicia

Project Code: 07SIN001CT

Budget: 49,220.00 €

Period: 2007-2009

Objectives: This is a utility for the development of work flows for distributed computing that permits the use of different applications and existing computing resources at CESGA or that are accessible by way of the GRID as a unique environment.

Qualified Electronic Signature Infrastructure (ISEC)

Partners: Aldaba Servicios Profesionales, Aldaba Soluciones y Proyectos SL, UVIGO, and CESGA

Coordinator: A. Gómez Tato, CESGA

Principal Researcher: A. Gómez Tato, CESGA

Financing: Xunta de Galicia

Project Code: 07SIN012CT

Budget: 147,338.00 €

Period: 2007-2009

A Virtual Laboratory for the National Oceanographic Remote Sensing Network (RETELAB)

Partners: USC, AZTI, ICCM, and CESGA

Coordinator: J.M. Cotos Yáñez, Universidade de Santiago (USC)

Principal Researcher: I. López Cabido, CESGA

Financing: Spanish Ministry of Science and Innovation

Project Code: ESP2006-13778-CO4

Budget: 114,950.00 €

Period: 2006-2009

Objectives: The development of a collaborative and distributed work environment that constitutes a virtual laboratory for the development of interdisciplinary projects related to oceanographic remote sensing.

Advanced Planning Systems for Radiotherapy by means of Computing Environments (e-IMRT)

Partners: CESGA, USC, and UVIGO

Coordinator: A. Gómez Tato, CESGA

Principal Researcher: A. Gómez Tato, CESGA

Financing: Regional Government of Galicia, Xunta de Galicia

Project Code: PGDIT05SIN00101CT

Budget: 38,775.00 €

Period: 2005-2008

Objectives: The e-IMRT project has produced new remote services for the planning of radiotherapy treatments that require high computational capacity. The services developed include a verification system of treatment plans based on Monte Carlo techniques as well as a search service designed to search for optimal plans for a treatment.

Support technicians for R&D infrastructures. Technicians: MCYT

Partners: CESGA

Coordinator: I. López Cabido, CESGA

Principal Researcher: I. López Cabido, CESGA

Financing: Ministerio de Ciencia e Innovación

Budget: 210,823.20 €

Period: 2005-2008

Objectives: Grant for hiring research infrastructure support technicians.

INGENIO MATHEMATICA (i-MATH)

Partners: Universidad de Almería, Universidad de Cádiz, Universidad de Granada, Universidad de Jaén, Universidad de Málaga, Universidad de Sevilla, Universidad de Oviedo, Universidad de Zaragoza, Universidad de Islas Baleares, Universidad de La Laguna, Universidad de Las Palmas de Gran Canaria, Universidad de Cantabria, Universidad de Castilla - La Mancha, Universidad de León, Universidad de Burgos, Universidad de Salamanca, Universidad de Valladolid, ICREA, Universidad de Barcelona, Universidad de Lleida, Universidad, Autónoma de Barcelona, Universidad Politécnica de Cataluña, Universidad de Girona, Universidad de Extremadura, Universidad de Santiago de Compostela, Universidad de A Coruña, Universidad de Vigo, Universidad de Alcalá, Universidad de Autónoma de Madrid, CSIC, INTA, Universidad Carlos III de Madrid, Universidad Complutense de Madrid, Universidad Nacional de Educación a Distancia,

Universidad Politécnica de Madrid, Universidad Rey Juan Carlos, Universidad de Murcia, Universidad de Navarra, Universidad Pública de Navarra, Universidad del País Vasco, Universidad de la Rioja, Universidad de Alicante, Universidad Jaume I de Castellón, Universidad Miguel Hernández de Elche, Universidad Politécnica de Valencia, and Universidad de Valencia.

Coordinator: M. A. López-Cerdá, Universidad de Alicante

Principal Researcher: A. Gómez Tato, CESGA

Financing: Ministerio de Ciencia e Innovación

Project Code: CSD2006-00032

Budget: 7,500,000.00 €

Period: 2006-2011

Objectives: This Ingenio-Consolider Project is designed to quantitatively and qualitatively increase the presence of Mathematics in science, technology, and innovation.

NETWORK COMMUNICATIONS

OPERA OBERTA

Partners: USC, UVIGO, UDC, UMINHO, and CESGA.

Coordinator: Liceu de Barcelona

Principal Researcher: Spanish Ministry of Education

Period: Indefinite

Objectives: The live multicast of operas from the Liceo in Barcelona to the participating universities, to be used as educational resources.

A distributed system for the massive synthesis of interactive TV channels using real time coding in Gpus

Partners: UDC, CESGA

Coordinator: V. M. Gulías Fernández, UDC.

Principal Researcher: López Cabido, CESGA.

Financing: Regional Government of Galicia, Xunta de Galicia.

Project Code: (PGIDIT07TIC005105PR).

Budget: 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 network transmission.

Platform for the Analysis of Telecommunications Services – PASITO

Partners: RedIRIS, CESCA (Centre de Supercomputació de Catalunya) CESGA (Centro de Supercomputación de Galicia), CICA (Centro Informático Científico de Andalucía), I2BASK (Red Académica Vasca), Universidad del País Vasco (UPV/EHU), Fundación I2CAT, Grupo de Red del IMDEA (Instituto Madrileño de Estudios Avanzados), Universidad Autónoma de Madrid (UAM), Universidad Carlos III de Madrid (UCIII), Universidad de Granada (UGR), Universidad de Murcia (UMU), Universidad Politécnica de Cataluña (UPC), Universidad Politécnica de Madrid (UPM), Universidad Politécnica de Valencia (UPV), and Universidad de Vigo (UVIGO).

Coordinator: RedIRIS

Principal Researcher: I. López Cabido, CESGA

Financing: Ministerio de Industria, Turismo y Comercio.

Budget total: 705,000.00 €

Periodo: 2008 – 2009.

Objectives: The launching of a national communications network for the testing of new services.

GEOGRAPHIC INFORMATION SYSTEMS

GIS Archaeological Patrimony 2008 - GIS-Patrimo8

Partners: Xunta de Galicia and CESGA

Coordinator: F. Landeira Vega, CESGA

Principal Researcher: F. Landeira Vega, CESGA

Financing: Regional Government of Galicia, Xunta de Galicia

Budget: 4,708.00 €

Period: 2008

Objectives: The development of tools and technical assistance in GIS for the Archaeological Service of the office of the Director General for Patrimony.

The generation of GIS contents for Project Terra - GIS-TERRA

Partners: IDEGA and CESGA

Coordinator: F. Landeira Vega, CESGA

Principal Researcher: F. Landeira Vega, CESGA

Budget: 11,875.00 €

Period: 11/04/2008-19/12/2008

Objectives: The generation of GIS contents for the educational material for Project Terra of the Galician Architects Professional Association.

Archaeological Patrimony - GIS-Patrimo7

Partners: Xunta de Galicia, CESGA

Coordinator: F. Landeira Vega, CESGA

Principal Researcher: F. Landeira Vega, CESGA

Financing: Xunta de Galicia

Budget: 10,930.00 €

Period: 2007-2008

Objectives: The elaboration of the 6th phase of a geographic information system applied to the management and analysis of cultural patrimony.

GIS-SIFI

Partners: CIS Madera and CESGA

Coordinator: X.F. Pedras Saavedra, CIS Madera

Principal Researcher: F. Landeira Vega, CESGA

Financing: Xunta de Galicia

Project Code: PGIDIT06RF000301CT

Budget: 28,750.00 €

Period: 2006-2009

Objectives: Elaboration of a geographic information system for the industrial forestry sector of Galicia.

GIS analysis of environmental risks - GIS-RIESGOS M.A.

Partners: CIS Deseño e Tecnoloxía, USC, and CESGA

Coordinator: J. Aneiros, CIS Deseño e Tecnoloxía

Principal Researcher: F. Landeira Vega, CESGA

Financing: Xunta de Galicia

Project Code: PGDIT05TAM00201CT

Budget: 51,260.00 €

Period: 2005-2008

Objectives: The development of a geographic information system for the study of possible areas of impact regarding various environmental risks.

E-LEARNING & COLLABORATION TOOLS

Standards based Intermediation System for the Search for Personalised Courses Using Semantic Technologies - eProcura

Partners: UVIGO and CESGA

Coordinator: M. J. Rodríguez Malmierca, CESGA

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: Xunta de Galicia

Project Code: 08SIN004CT

Budget: 109,494.95 €

Period: 2008-2011

Objectives: The design, development, and launch of an intermediation system specifically oriented toward the personalised search and localisation of courses that permits those in search of training to unveil all the offer available on the Web and to select that which is of real interest

Application of Pedagogical Competencies and Skills for Teachers – ICTeachers

Partners: Die Berater (Coordinator), Österreichische Computer Gesellschaft (Austria), Universidade de Santiago de Compostela (Spain), Centro de Supercomputación de Galicia (Spain), Westminster Business School, University of Westminster (U.K.), VIA University College-Læreruddannelsen i Århus (Denmark), y Nyugat-magyarországi Egyetem, Információs Társadalom Oktató és Kutató Csoport (Hungary).

Coordinator: M. Röhner, die Berater

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: European Commission - Lifelong Learning Programme

Project Code: 141882-2008-LLP-AT-COMENIUS-CM

Budget: 22,792.00 €

Period: 2008-2010

Objectives: This project is designed to improve the ICT competencies and skills that Primary and Secondary Teachers have (at a European level) for which the main goal is to promote ICT use in primary and secondary education and, as a consequence, improve the quality of teaching and learning.

Standards based e-Learning Services Integration – SUMA2

Partners: Tecsidel, CESGA, Germinus, ATOS Origin, OpenTrends, GEC, UPCNet, Inter On Line, IOL, UOC, UVIGO, and UFV.

Coordinator: P. Artiga Calvo, Tecsidel S.A

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: Spanish Ministry of Industry, Tourism and Commerce (Plan Avanza)

Project Code: TSI-020301-2008-9

Budget: 12,887.00 €

Period: 2008-2009

Objectives: Services of integration for e-learning based on standards. This is a strategic project of the e-learning work group of the INES technological platform.

T-Maestro

Partners: UVIGO and CESGA

Coordinator: M.J. Rodríguez Malmierca, CESGA

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: Regional Government of Galicia, Xunta de Galicia

Project Code: 07TIC02CT

Budget: 108.054,00 €

Period: 2007-2010

Objectives: An intelligent tutor for the production of personalised learning contents adaptable to T-learning and M-learning on MHP and DVB-H.

Parents as family vocational adviser for children - PARENTS

Partners: Academy of Management (Poland), University of Oradea (Romania), Die Berater (Austria), Training 2000 (Italy), Asociació Baobab (Spain), and CESGA (Spain)

Coordinator: Academy of Management

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: European Commission, Socrates-Leonardo Programme

Project Code: 134247-LLP-2007-1-PL-Grundtvig-GMP

Budget: 39,681.00 €

Period: 2007-2009

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

Red Latinoamericana de Capacitacion para la Industria Lactea - REDLECHE

Partners: USC, FEPAL y CESGA

Coordinator: J.M. Dónega, USC

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: Collaboration Agreement with the Galician Regional Government, Xunta de Galicia

Budget: 5,514.00 €

Period: 2007-2009

Objectives: Skill building for the Latin American dairy industry.

Youth Employment Support - YES

Partners: Die Berater (Austria), Local Mission Agenais and Albret (France), Glotta Nova (Slovenia), Further Training Centre for the Saxonian Economy (Germany), Transfer

(Slovakia), Reflexion Foundation (Netherlands), Meter Silesia (Czech Republic), and CESGA (Spain).

Coordinator: Die Berater

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: European Commission, Socrates-Leonardo Programme

Project Code: LLP-LdV/TOI/2007/AT/0003

Budget: 29,248.00 €

Period: 2007-2009

Objectives: The design and provision of a support system based on ICT such as specific e-learning training for SME in order to try to improve the incorporation of youth who have not finished their studies into the workplace. This will include the analysis and the evaluation of e-learning models and will adequate the ITC to this context.

Standards based e-Learning Services Integration - SUMA

Partners: Tecsidel, CESGA, Germinus, ATOS Origin, OpenTrends, GEC, UPCNet, Inter On Line, IOL, UOC, UVIGO, UFV

Coordinator: P Artiga Calvo, Tecsidel S.A

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: Spanish Ministry of Industry, Tourism, and Commerce (Plan Avanza)

Project Code: FIT-350503-2007-8

Budget: 13,313.00 €

Period: 2007-2008

Objectives: Integration of e-Learning services based on standards. This is a strategic project of the e-learning work group of the INES technological platform.

E-intervention

Partners: CESGA, USC, and UVIGO

Coordinator: A. Gómez Tato, CESGA

Principal Researcher: A. Gómez Tato, CESGA

Financing: Galician Regional Government, Xunta de Galicia

Project Code: PGIDIT05TIC00101CT

Budget: 70,000.00 €

Period: 2006-2009

Objectives: The development of a technological platform for at-home gerontological attention.

Flexible and creative educational environments – EFELCREN

Partners: USC (Spain), Trinity College (Ireland), Centre of Information Technology (Lithuania), Ca'Foscari University

of Venice (Italy), Haslev Seminarium (Denmark), Euneos Corporation (Finland), and CESGA (Spain)

Coordinator: B. Cebreiro López, USC

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: European Commission, Socrates-Comenius Programme

Project Code: 226552-CP-1-2005-1-ES-COMENIUS-C21

Budget: 54,625.00 €

Period: 2005-2008

Objectives: The analysis and development of training proposals for flexible and creative educational environments in primary and secondary education. This will be accomplished by the use of the new ICT and the identification of new teaching strategies. Within the project, we also contemplate the creation of e-learning materials as well as making those resources available to teachers.

e-learning opportunities for adult patients during hospitalisation in health-care institutions - e-HOSPITAL

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

Coordinator: H Bienzle, Die Berater

Principal Researcher: M. J. Rodríguez Malmierca, CESGA

Financing: European Commission, Socrates-Grundtvig Programme

Project Code: 225761-CP-1-2005-1-AT-GRUNDTVIG-G1

Budget: 42,415.00 €

Period: 2005-2008

Objectives: The analysis of the application of e-learning techniques to adult patients hospitalised for long periods of time and to the production of guides and tools for teachers that work in this environment.

TECHNOLOGY TRANSFER & E-BUSINESS

Improving regional policies related to innovation and the knowledge economy priority – ICHNOS PLUS

Partners: ANCITEL SARDEGNA, CESGA, VYSOCYNA, NORTH AEGEAN REGION, TARTU SCIENCE PARK, RUDA SLASKA INCUBATOR

Coordinator: P. P. Falco, Ancitel Sardegna

Principal Researcher: R. Basanta Cheda, CESGA

Financing: INTERREG

Project Code: 0415C1 – ICHNOS PLUS

Budget: 198,000.00 €

Period: 2008-2010

Objectives: The basic objectives of ICHNOS PLUS are the optimisation of the application of this model to the three regions that are working on ICHNOS as well as the effectiveness of the transfer and deployment in other European regions.

VINDEIRA: Strategic associative action to improve the VG-CMMI software processes

Partners: SUMMA, Servicios de Ingeniería y Consultores SA, Brújula Telecom SA, AT4.Net Internet y Comunicación SL, ALTIA Consultores, Bahía Software SL, IGALIA SL, Aldaba Servicios Profesionales, LAMBDASTREAM SL, SATDATA Telecom SL, 2mares demil SL, Shylex Telecomunicaciones SL, Optare Solutions SL, Factoría de Software y Multimedia SL, and CESGA

Coordinator: R. Basanta Cheda, CESGA

Principal Researcher: R. Basanta Cheda, CESGA

Financing: Ministerio de Industria, Turismo y Comercio

Project Code: FIT-340502-2007-10

Budget: 62,700.00 €

Period: 2007-2008

Objectives: This is an associative strategic action orientated to technological excellence in the development of software by means of quality certification models (CMMI, SPICE).

Optimum design of the architecture of livestock exploitations' integral veterinary control system - XesveTIC

Partners: COMPUTER-3 S.L., CESGA, and AGACA

Coordinator: C. Diaz Carrodeaguas, COMPUTER-3, S.L.

Principal Researcher: R. Basanta Cheda, CESGA

Financing: Galician Regional Government, Xunta de Galicia

Project Code: 07MRU029E

Budget: 5,282.00 €

Period: 2007-2009

Objectives: This is an optimum design for the architecture of an integral veterinary control system for livestock operations.

Joint Cooperatives Management – CoopTIC

Partners: Galician Association of Agrarian Cooperatives, Computer-3 y CESGA

Coordinator: Computer-3, S.L

Principal Researcher: R. Basanta Cheda, CESGA

Financing: Galician Regional Government, Xunta de Galicia

Project Code: PGIDITo6RAGO25E

Budget: 24,000.00 €

Period: 2006-2008

Objectives: The objective is to conduct research in order to determine the optimal design of the architecture of a system that permits product tracing for agricultural cooperatives.

VG-CMMI-SPICE

Partners: CESGA, SUMMA, Servicios de Ingeniería y Consultores S.A., Brújula Telecom S.A., AT4.Net Internet y 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., and Factoría de Software e Multimedia S.L.

Coordinator: R. Basanta, CESGA.

Principal Researcher: R. Basanta, CESGA.

Financing: Spanish Ministry of Industry, Tourism, and Commerce.

Total Budget: 670,754.00 €

Budget CESGA: 62,802.00 €

Period: 2007 - 2009

RESEARCH NETWORKS & TECHNOLOGICAL PLATFORMS IN WHICH CESGA ACTIVELY PARTICIPATED IN 2008

CAPAP-H

High Performance Computing Network on heterogeneous parallel architectures

Members: 13 research groups from Spanish Universities and CESGA

Coordinator: Enrique S. Quintana-Ortí, Universidad Jaime I de Castellón

Financing: Ministerio de Ciencia e Innovación

URL: <http://capap-h.uji.es/>

Objectives: The objectives include the facilitation of the exchange and transfer of knowledge and experiences among the different research groups interested in CAPAP-H in a way that will promote cooperation among them. Another is to assist with the consolidation and dissemination of existing knowledge concerning CAPAP-H. A third objective is to promote the development and use of new techniques and methodologies that make CAPAP-H possible, principally along those lines in which the Partners are researching.

Another objective is to optimise and to organise individual efforts in order to identify and reach the most ambitious objectives, such as, consolidating the community that works in this environment in a way that will augment their specific weight at an international level, in order to later obtain its own identity in the European Research Space.

Another goal is to tighten the relations between the participating groups in the network as well as other public and private organisations, national or international, that collaborate in the development of publications, projects, conferences, and seminars.

CyTED-Grid

Grid Technology for Iberamerican Project of Science and Technology for Development

Members: UCM, UAB, UDELAR, UH, UNLP, UNA, UDEA, UNAM, UNSA, UMAG, ESPOL, UPV, UDC, ULA, UNEB, UOC, UFCG, UNSL, UP, USB, and CESGA

Coordinator: Francisco Tirado Fernández, Universidad Complutense de Madrid

Financing: The Iberamerican Project of Science and Technology for Development (CYTED)

URL: www.cytetedgrid.org

Objectives: The creation of a human and technological infrastructure among those different Latin American groups that are potential users of GRID technology, that are dedicated to the field of computing, and that have experience in the area of scientific applications. The construction of a new GRID network as support for different applications for analysis up to the point that the available solutions are valid and the new developments that will provide the necessary functionality are proposed.

eBSN

European e-Business Support Network

Members: Over 160 Business Associations, University based research groups, Industries, Government bodies, Technology Centers throughout Europe.

Coordinator: Iordana Eleftheriadou, European Commission

Financing: European Commission

URL: <http://ec.europa.eu/enterprise/e-bsn/>

Objectives: eBSN was founded in order to improve cooperation and raise synergies within the European space of commercial community policy. eBSN activities focus on the creation of networks and the exchange of best practices. More concrete

objectives are listed below.

- Organise meetings of managers in order to adopt decisions in the field of business with the objective of sharing information and discussing the orientation to enlighten strategic policies,
- Provide a platform for the coordination of policies among European Union members,
- Provide a "one-stop-shop" in order to obtain information about initiatives and regional, national, and European financing possibilities for SME, and
- Organise special meetings of governmental experts as a platform for sharing practical experience and to identify future challenges.

Red Española de e-Ciencia

Spanish e-Science Network

Members: ACUALSA/UAL, ADE/UJ, ARCO/UNEX, ARCOS/UC3M, ArTeCS/UCM, ATC/UCBIFI/UNIZAR, BSC, CESA, CESGA, CeSViMa, CETA-UAA/CIEMAT, CETA-USE/CIEMAT, CFM/CSIC-EHU, CGG/CEIT, CICA, CIEMAT, CNB/CSIC, CNDS/UPC, DELi/DEUSTO, DIPC/UPV, DPCS/UOC, e-CA, EEC/UNEX, ESAC-CSG/ESA, ETSF/UPV, F2cat, GAC/UDC, GAC/UMA, GAC/USC, GACSO/UAB, GASDS/UCM, GB/CIPF, GB/UPVLC, GCC/INTA, GCOC/UPVLC, GEA/UNEX, GFA/UGR, GFAE/USC, GFAE/UB, GFTAE/UGR, GFTS/FATRONIK, GGC-IFIC/CSIC, GGE/UEVEG, GGRID/UPNA, GHPC-CTI/CSIC, GIDS/UPM, GMA/UC, GMI/UPVLC, GMT/UPVLC, GQMA/UPVLC, GQT/UPV, GQTC/UEVEG, GRTC/US, GRV/EUVE, GRyCAP/UPVLC, GTC/UPVLC, i2BASK, I3A/UNIZAR, IFAE/UAB, IFCA-GRID/CSIC, IFISC/CSIC, IMDEA-Networks, IMDEA-Software, IRAM/UGR, ISG/UPV, LabGP/IBMCP, LMFC/UPM, LNF/CIEMAT, MICINN, MTC-LABSIS/USC, NEIKER, OEG/UPM, PIC, PRHLT/UPVLC, PURG/UEVEG, QCyCAR/UCLM, RAAP/UCLM, REBIUN, RedIRIS, RETICS/UCLM, SAVIE/UPVLC, SBG, SCompBio/CNIO, SDBG/ESI, SGI/IZO/EHU, SPAS/UAH, TIC/CIEMAT

Coordinator: Vicente Hernández García, Universidad Politécnica de Valencia

Financing: Spanish Ministry of Science and Innovation

URL: <http://www.e-ciencia.es/>

Objective: The Spanish e-Science Network is designed to organise, coordinate, and move e-Science forward in Spain, as well as to constitute a tool that is complementary to projects, infrastructure programmes, and other resources within the e-Science environment. The general objectives are listed below.

- To have an e-Science infrastructure coordinated among di-

fferent institutions that facilitates user access from different areas of science to supercomputing and GRID infrastructure resources.

-To improve Spanish participation in European e-Science projects.

-To improve scientific excellence by means of access to e-Infrastructures.

-To create an e-Science culture by way of training, dissemination, and promotion of the e-Science concept.

-To consolidate scientific relations with European countries, particularly with Portugal, and with other non-European countries of strategic interest for Spain.

eMOV

Spanish Platform of Wireless Communications

Members: Over 150 Industrial Companies, Professional Associations, Universities, and Research and Technology Centres.

Coordinator: Luis Jorge Romero, Telefonica

Financing: Spanish Ministry of Industry, Tourism and Commerce, Ministry of Education and CDTI.

URL: <http://www.idi.aetic.es/emov/>

Objectives: The objective of the Spanish Platform of Wireless Communications (eMOV) is to contribute to the strengthening of the agents who play a role in the development of mobile and wireless systems and services. In the end, this should have the effect of improving the economic situation of the sector in terms of the creation of employment and the generation of wealth, as well as to contribute to raising productivity and well-being through the adoption of mobile systems and services in other sectors and in Spanish society as a whole.

GIS-REDIX

Geographic Information Systems Galician Research Network

Members: Laboratorio del Territorio (LaboraTe) – Universidad de Santiago de Compostela, Instituto de Biodiversidad Agraria y Desarrollo Rural (IBADER), Arquitectura de Computadores- Universidad de A Coruña, Arquitectura de Computadores - Universidad de Santiago de Compostela, Videalab – Universidad de A Coruña, Laboratorio de Ingeniería Cartográfica (CartoLab) – Universidad de A Coruña, Investigación Socio-espacial SIG-T-Universidad de Santiago de Compostela, Sprawl City-Universidad de A Coruña, SITGA, and CESGA.

Financing: Galician Regional Ministry of Education, Xunta de Galicia

Coordinator: U. Fra Paleo, Universidad de Santiago de Compostela

URL: <http://sit.usc.es/redix/index.html>

Objectives: REDIX is a network of research groups and organisations interested in the development, dissemination, and application of the GIS to science, technology, and research methodologies.

GRIDCHEM

Grid Computing in Chemistry

Members: Research institutions from 18 European states.

Coordinator: Hans Peter Luthi, Physical Chemistry Laboratory - ETH Zurich

Financing: COST (European Cooperation in Science and Technology)

URL: http://w3.cost.esf.org/index.php?id=189&action_number=D37

Objectives: One objective is to facilitate the creation and utilisation of distributed computing infrastructures (Grid) in chemistry with the goal of taking chemical computational models and simulations to new frontiers of complexity and to a new time-to-solution regime. This will stimulate innovation in the creation and manipulation of chemical knowledge. The fields of application take on traditional chemistry, material science, molecular biology, and environmental chemistry. The presence of chemistry in the network will also have an impact on the development of middleware and the creation and availability of network infrastructures. The final objective is to facilitate and accelerate the transition of researchers to the computational science infrastructure of the XXI century, which should in turn make European Computational Chemistry much more competitive.

Mathematica Network - Consulting and Computing of Galicia

Members: 14 research groups in applied mathematics and computing from Galician Universities and Technology Centres.

Coordinator: Wenceslao González Manteiga, USC.

Financing: Galician Regional Ministry of Education, Xunta de Galicia

URL: <http://matematica.nodo.cesga.es/content/view/13/27/>

Objectives: Promote research and working relationships among members, as well as transfer of math and computing methods and technology to industry and administrations.

INES

Spanish Technological Platform of Software and Services

Members: 136 Spanish Telecom Companies, Industries, Business Associations, Technology Centres, and Universities.

Coordinator: Santiago Ristol, Atos Origin

Financing: Spanish Ministry of Industry, Tourism, and Commerce

URL: www.ines.org.es

Objectives: The objective is to define a strategic research programme adapted to Spanish necessities and capacities, including proposals for unique, scientific and technologic strategic projects setting medium and long term goals.

INSME

International Small and Medium Enterprise Network

Members: Members from 5 continents: governmental bodies, international organizations, international non-profit organisations and representatives of 36 networks and their intermediaries that work in the field of innovation and the transfer of technology to PYMES.

Coordinator: Paolo Anselmo, Italian Business Angels Network (IBAN)

Financing: OECD. UNIDO.

URL: <http://www.insme.org>

Objectives: To create a permanent forum for the promotion and strengthening of multilateral dialogue between stakeholders.

- To develop "North-South" interaction and cooperation.
- To facilitate knowledge exchange and the arousal of synergies and economies of scale.
- To indirectly support the competitiveness of the SME at local, national, and international levels.

RED-GHPC

Galician High Performance Computing Network

Members: Grupo de Antenas-Universidad de Vigo, Grupo de Arquitectura de Computadores-Universidad de A Coruña, Grupo de Arquitectura de Computadores - Universidad de Santiago de Compostela, Grupo de Física de la Atmósfera y el Océano- Universidad de Vigo, Grupo de Física no Lineal-Universidad de Santiago de Compostela, Grupo Integrado de

Ingeniería-Universidad de A Coruña, Grupo Laboratorio de Sistemas - Universidad de Santiago de Compostela, Grupo de Métodos Matemáticos y Simulación Numérica en Ingeniería y Ciencias Aplicadas-Universidad de A Coruña, Grupo de Química Teórica y Computacional-Universidad de Santiago de Compostela, Grupo de Resolución Numérica de Ecuaciones en Derivadas Parciales-Universidad de Santiago de Compostela, Centro de Investigación e Información Ambiental (CINAM), and Centro de Supercomputación de Galicia (CESGA)

Coordinator: Ramón Doallo, UDC

Financing: Galician Regional Ministry of Education, Xunta de Galicia

URL: <http://ghpc.udc.es/>

Objectives: The Galician Thematic network of High Performance Computing (Red G-HPC) is designed to put in contact and to propitiate collaboration among groups and research centres of the University System of Galicia (USG) and users of HPC technologies (High Performance Computing). The Red G-HPC network has two fundamental purposes:

1. To promote interdisciplinary research collaboration among groups integrated in the network, as well as other research groups or companies that may be interested in research and/or in the development of technologies that require supercomputing or other HPC techniques.
2. The organization of training courses, conferences, seminars, or workshops that help to disseminate knowledge concerning HPC technologies.

REDOAPA

Thematic Network for Designs and Objects for Learning

Members: Universidad a Distancia de Madrid, Universidad Complutense de Madrid, Universidad de Alcalá, Universidad de Alicante, Universidad de Almería, Universidad de Barcelona, Universidad de Cádiz, Universidad de Castilla La Mancha, Universidad de Mondragón, Universidad de Murcia, Universidad de Oviedo, Universidad de Sevilla, Universidad de Valladolid, Universidad de Vigo, Universidad del País Vasco, Universidad Francisco de Vitoria, Universidad Politécnica de Madrid, Universidad Pontificia de Salamanca, Universitat Oberta de Catalunya.

Coordinator: S. Sánchez, Universidad de Alcalá de Henares

Financing: Ministry of Education and Science

URL: <http://www.cc.uah.es/ie/projects/redaopa/>

Objectives: REDAOPA began in 2004 with the objective of continuing the annual multidisciplinary meetings that were

initiated in the SPDECE'04 symposium. The thematic network strives for permanence in order to continue the provision of support for the different aspects associated with electronic teaching and learning with an emphasis on the reutilisation of resources. Actually, aspects of interest for the network members are, among others:

- The reusability of open educational resources,
- The sharing of designs for learning, a step beyond that of the contents,
- The codification and classification of theories of instructional design, and
- The creation of models of quality for digital educational resources.

RGB

Galician Bioinformatics Network

Partners: Medicina Genómica-Universidad de Santiago de Compostela, Grupo de Poblaciones Genéticas y Cyto-Genética-Universidad de Vigo, Grupo de investigación de Sistemas Complejos-Universidad de Santiago de Compostela, Grupo de Bio-Farmacia- Universidad de Santiago de Compostela, Grupo de MathBioinfo-Universidad de Santiago de Compostela, Grupo de Red de Neuronas Artificiales y Sistemas Adaptativos-Centro de Informática Médica y Diagnóstico Radiológico-Universidad de A Coruña, CESGA

Coordinator: A. Pazos Sierra, UDC

Financing: Galician Regional Ministry of Education, Xunta de Galicia

URL: <http://rgb.cesga.es/>

Objectives: The RGB is an initiative that has the objective of structuring and integrating research and teaching activities in Bioinformatics that take place in Galicia.

VINDEIRA

The Galician ICT Technological Platform

Members: Over 90 members from industry, ICT business associations, business angels, universities and technology centres.

Coordinator: A. Rodríguez del Corral, R Cable

Financing: Regional Government of Galicia, Xunta de Galicia.

URL: <http://www.vindeira.org/>

Objectives: Vindeira is defined as a meeting point for all agents associated with the ICT sector in Galicia and whose future depends in great measure on the capacity to maintain

and create competitive advantages by means of the development of research and innovation activities. The probabilities of maintaining a sustainable and prosperous ICT industry in Galicia are practically nonexistent without a strategy of innovation that is appropriate in a sector which is particularly globalised such as ICT.

The platform was born of a spirit that is open to the integration of all of agents involved in technological development and in the exploitation of the Galician ICT with a desire for continuity into the future.

NESSI

European Software and Services Initiative Network

Members: 366 members of which 81 are large ITC companies, 91 are SME, 180 are academic institutions, 22 are partners of which 18 are from industry, 3 are from the academic world, and one is from the open source community.

Coordinator: V. Pevtschin, Software AG

Financing: European Commission

URL: <http://www.nessi-europe.com/>

Objective: NESSI's is fundamentally service oriented. Many definitions of service exist in many different contexts. However, all are based on the same principle: the consumer of services is not the owner of the services and for that reason it is not necessary for them to be concerned about the aspects generally associated with property, such as infrastructure, technology, integration, and maintenance. They only have to select a service that satisfies their business needs. Businesses concentrate more and more on activities that can have competitive advantages. They are able to obtain certain support capacities as a service to specialised providers. In this context, NESSI will transform the EU economy by means of business models that are Service Oriented.

RETGALIA

Galician Technological Centre Network

Members: 21 technological centres of Galicia

Coordinator: Javier García Tobío, CESGA

Financing: Galician Regional Government, Xunta de Galicia

URL: <http://www.retgalia.org>

Objective: To coordinate the Technological Centres that operate in Galicia in a way that all potentialities will be taken advantage of, thereby contributing to the achievement of total quality in the Galician system of innovation. The intention is to also support the development of specific actions for

dissemination of knowledge, information, and promotion of science and technology as well as the offering of services to businesses.

NEURONA

Galician Technological Platform Network

Members: 14 technological platforms of Galicia

Coordinator: Salustiano Mato de la Iglesia, Dirección Xeral I+D+i, Xunta de Galicia

Financing: Xunta de Galicia

URL: www.redeneurona.org

Objective: The strategic objectives of Neurona are:

- To establish a meeting forum for the exchange of information and experiences among the agents associated with the Galician Technological Platforms.
- To promote and facilitate collaboration between agents of the Galician Technological Platforms in order to develop joint research projects.
- To create a unique institutional image of Research, Development, and Innovation in Galicia for the key sectors of the Galician economy.

Elearningeuropa.info

Members: European Union e-Learning community and stakeholders.

Coordinator: Maria José Rodríguez Malmierca (CESGA)

Financing: European Commission

URL: <http://www.elearningeuropa.info>

Objective: To promote innovation in e-learning throughout the lifetime.

PTAG

Audiovisual Industry Technology Platform

Members: The Galician Audiovisual Technological Platform is composed of businesses that are active in strengthening RTD and innovation, universities, technology centres, and other entities committed to technological progress in the audiovisual industry of Galicia, as well as managers of policies and grant programs, and the business associations related with the sector.

Coordinator: Xunta de Galicia / Galician Audiovisual Cluster

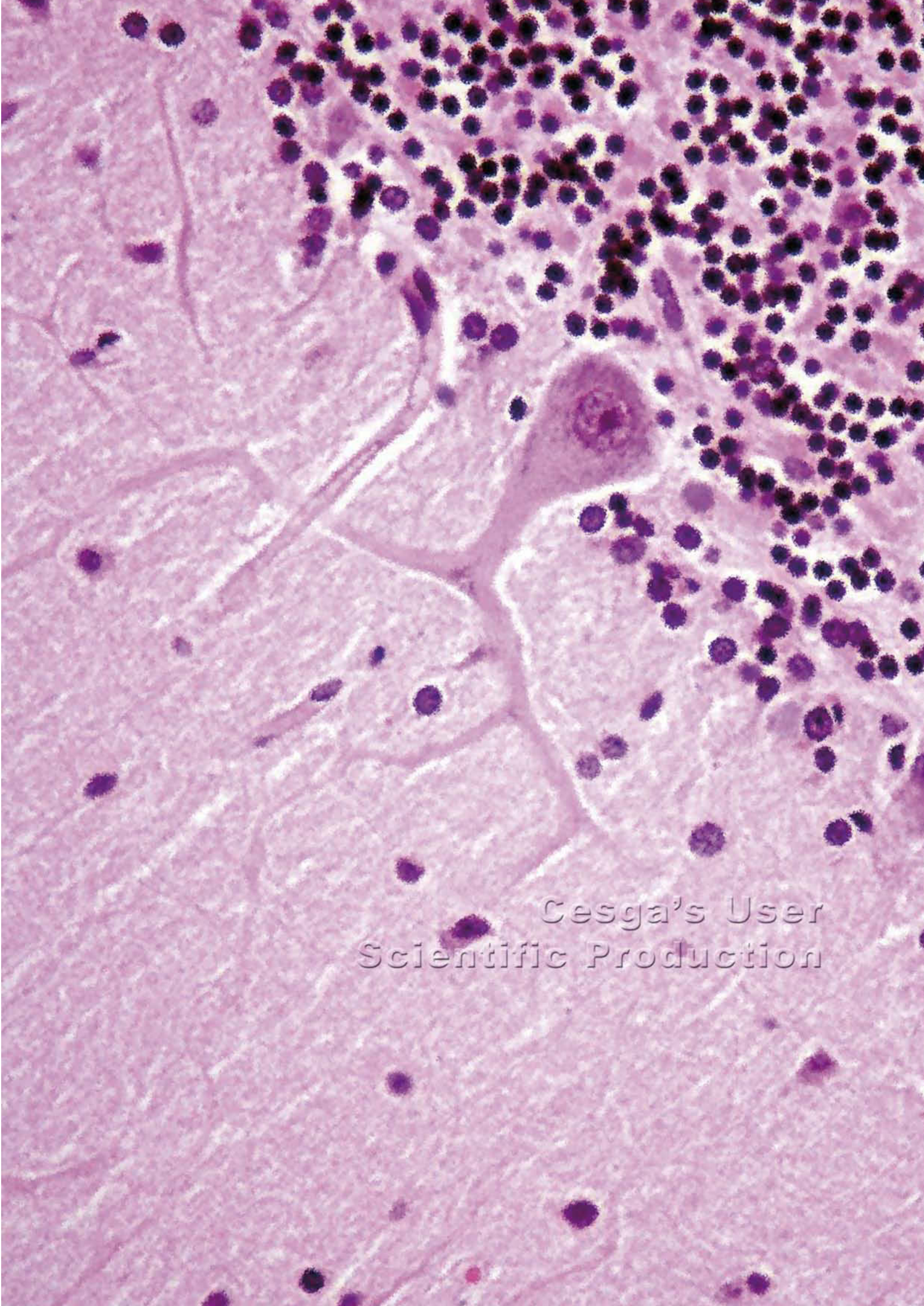
Financing: Xunta de Galicia

URL: <http://www.idea.org.es/?q=gl/node/121>

Objective: The Technological Platform i+dea is an open work

forum for the Galician audiovisual industry and research entities and other organisations related to their scientific and technological progress. The strategic objectives are presented below.

- To elaborate a consensual vision of the priorities of the RTD of the sector.
- To develop a work program that will stimulate technological advancement in the sector and exploit new business opportunities.
- To achieve better collaboration, coherence, and critical mass in RTD activities that are promoted for the sector.
- To insert the strategic objectives of the sector into the organisations and forums of influence regarding RTD material.



Cesga's User
Scientific Production

Contribution of CESGA services to the scientific production of the User Community 2002-2007

At the beginning of each year, CESGA sends out a request to its users regarding their production. The request is that they report their scientific results regarding the use of the computing resources during the past two years. This year, 2008, was the second year in which we also indicated that they declare the status of their articles, that is, whether they had been submitted or if they were in process during the year prior to being published in order to maintain the method from 2007 to 2008. The result is that the scientific production of CESGA users continues to grow at an important rate, in spite of the fact that the impact of putting Finis Terrae into production will probably not be completely reflected until 2010 when the memory of the current year will be published. It is also important to highlight the increase in the scientific production of CESGA itself, mainly in the areas related to computing into which much effort was directed.

In spite of the continuous growth in the scientific production of CESGA users, in 2008 the Centre concentrated efforts on the analysis of the quality of the publications by means of bibliographic studies.

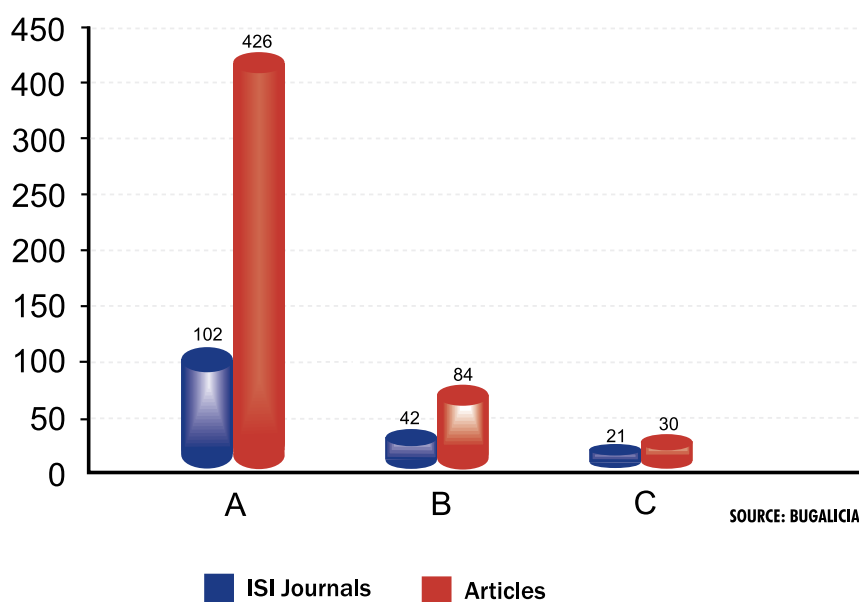
The first of these studies was conducted by BUGALICIA, the Consortium of University Libraries in Galicia, classifying and analysing all of the scientific publications reported by the users between 2002 and 2007. During this period, the scientific production in ISI publications multiplied by 3.18 (from 45 to 143 articles). The most outstanding conclusions are listed below.

1. Of the 582 publications, 550 were published in journals that are included in the ISI list.
2. Of those, the majority were published in journals with high impact: 426 articles in Category A journals.
3. The area in which most arti-

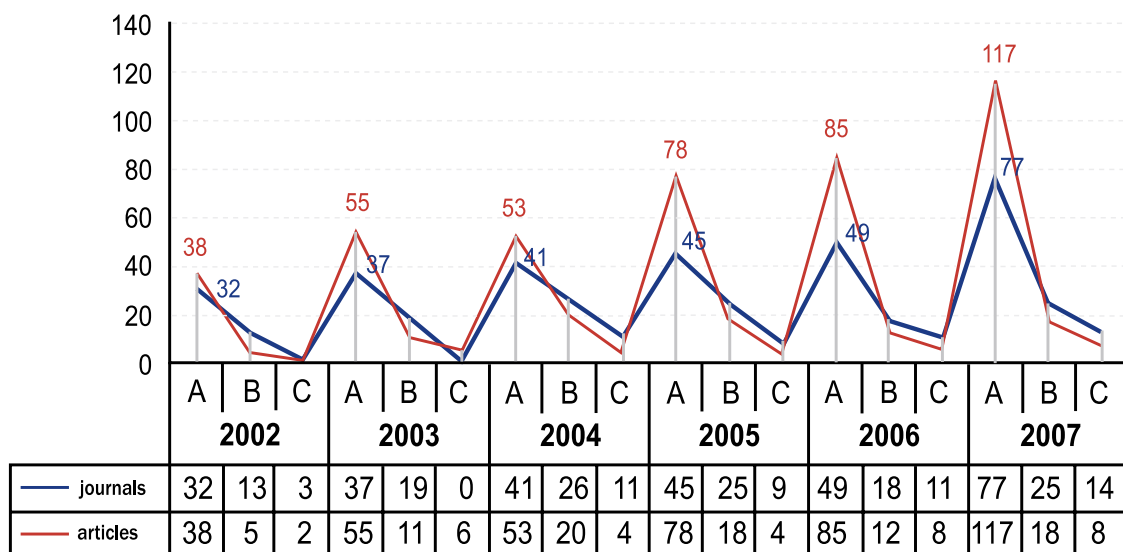
cles were produced was Physics, Atomic, Molecular, and Chemistry.

The second study attempted to define an indicator of the quality or the impact of the users' scientific production that would permit CESGA to measure the results of the utilisation of resources over time. The indices that exist, such as the H index, are not intended to measure multidisciplinary infrastructures in which both the users and the areas in which they work vary with time. For this reason, in a collaborative work with BUGALICIA and the University of Santiago Department of Statistics and Operative Investigation, a proposal of indices was designed and elaborated that concerns the normalisation of the impact for each area, that is, each journal fits into a knowledge area and is assigned a value between 0 and 1. Two indices were defined. One index concerns impact and the journals with most impact in the specific area of knowledge are assigned a 1 while journals with less impact are assigned a 0. The other concerns the order of the journal within the list. In either case, CESGA users' scientific production was very high for the period 2002-2007 as compared with the national average (above 0.80 over 1).

**CESGA'S USERS SCIENTIFIC PRODUCTION 2002-2007
ARTICLE DISTRIBUTION PER JOURNAL TYPE (A,B,C)**

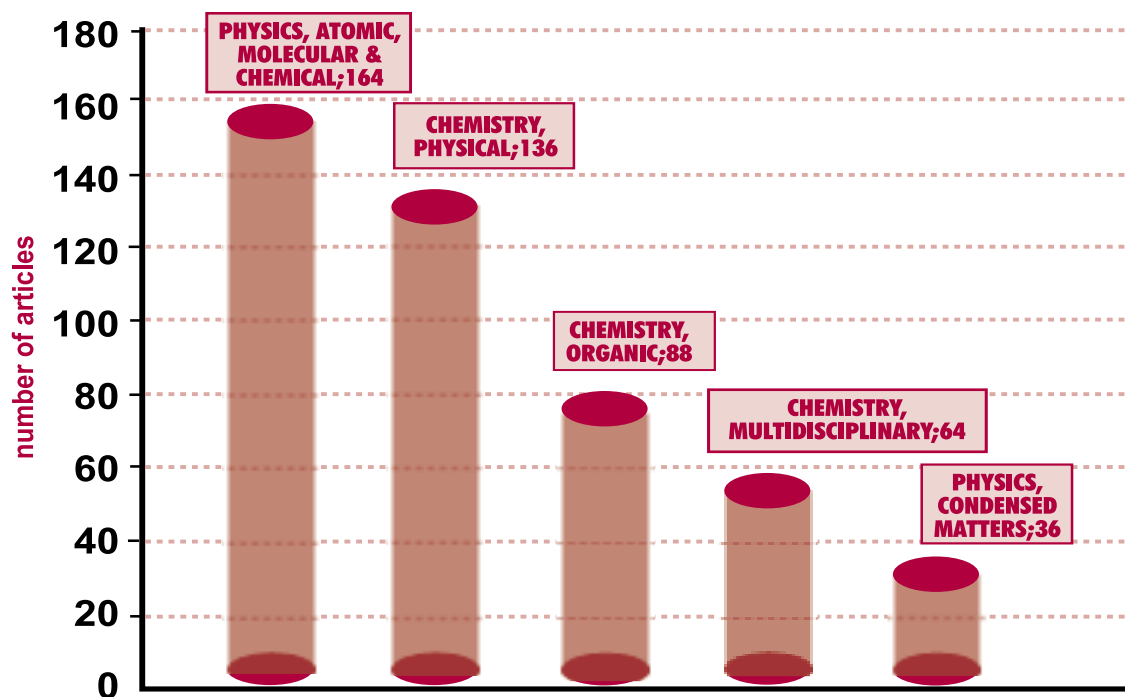


**CESGA'S USERS SCIENTIFIC PRODUCTION 2002-2007
ARTICLE & JOURNAL DISTRIBUTION PER TYPE (A,B,C) AND YEAR**



SOURCE: BUGALICIA

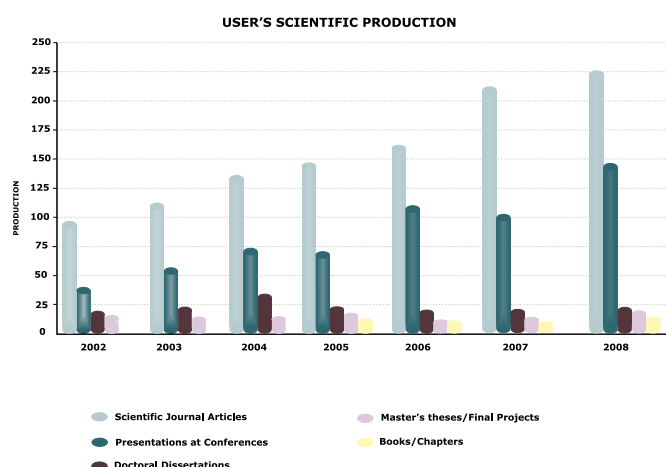
**CESGA'S USERS SCIENTIFIC PRODUCTION 2002-2007
ISI CATEGORIES SHOWING THE HIGHEST PRODUCTION**



SOURCE: BUGALICIA

scientific production reported by CESGA'S users in 2008

The data summarising the scientific production reported by users is presented in the following tables. The production reported has steadily increased since CESGA first started collecting this information from its users.



	2004	2005	2006	2007	2008
Percentage of users declaring production	78,57%	87,40%	74,43%	85,26%	72,99%
Percentage of hours consumed by users declaring production	90,01%	98,32%	94,65%	99,45%	98,30%

DISTRIBUTION OF SCIENTIFIC PRODUCTION PER YEAR

	2002	2003	2004	2005	2006	2007	2008
SCIENTIFIC ARTICLES	93	107	134*	147	154	208	225
ACCEPTED / IN PRESS	4	8	20	16	26	19	21
SUBMITTED	16	29	26	27	23	24	31
PUBLISHED	73	70	91	104	105	165	173
PRESENTATIONS IN CONFERENCES	42	52	72*	65	105	101	148
PRESENTATIONS	33	40	53	37	53	46	60
POSTERS	9	12	35	28	52	47	88
DOCTORAL THESES	17	21	32	24	18	18	20
DEFENDED	9	4	5	9	10	11	10
PRESENTED	0	0	0	0	3	5	1
IN PROCESS	8	17	27	15	5	2	9
MASTERS THESES GRADUATE PROJECTS	12	9	12	14	5	10	14
DEFENDED	6	4	5	13	3	8	10
IN PROCESS	6	5	7	1	2	2	4
BOOKS / CHAPTERS	NA	NA	NA	5	4	3	9
ACCEPTED / IN PRESS	NA	NA	NA	4	1	1	1
SUBMITTED	NA	NA	NA	1	0	2	0
PUBLISHED	NA	NA	NA	0	3	0	8
TOTAL	169	194	256	260	301	351	416

* 8 PUBLICATIONS & 16 CONFERENCES WITH AUTHORS FROM MORE THAN ONE INSTITUTION

DISTRIBUTION OF SCIENTIFIC PRODUCTION DECLARED

	CSIC	UDC	USC	UVIGO	TOTAL
SCIENTIFIC ARTICLES	79	24	77	37	217
ACCEPTED/IN PRESS	12	1	5	1	19
SUBMITTED	12	6	9	1	28
PUBLISHED	55	17	63	35	170
PRESENTATIONS IN CONFERENCES	40	17	44	28	129
PRESENTATIONS	21	6	11	8	46
POSTERS	19	11	33	20	83
IN PREPARATION	—	—	—	—	—
DOCTORAL THESES	7	6	5	—	18
DEFENDED	5	2	2	—	9
PRESENTED	—	1	3	—	4
IN PROCESS	2	3	—	—	5
MASTERS THESES / GRADUATE PROJECTS	—	7	2	1	10
DEFENDED	—	5	2	1	8
IN PROCESS	—	2	—	—	2
BOOKS / CHAPTERS	3	3	—	2	8
ACCEPTED/ IN PRESS	1	—	—	—	1
PUBLISHED	2	3	—	2	7
OTHERS	—	—	—	—	—
SUBMITTED	—	—	—	—	—
PUBLISHED	—	—	—	—	—
IN PROCESS	—	—	—	—	—
	129	57	128	68	382

CESGA AND SERGAS NOT INCLUDED

scientific production reported by CESGA'S users

In the following pages a detailed account of the products reported by users is provided.

SPANISH NATIONAL RESEARCH COUNCIL (CSIC)

Scientific Articles Published



REHMMAN H, ARIAS-PALOMO E, HADDERS MA, SCHWEDE F, LLORCA O, BOLJL. 2008. Structure of Epac2 in complex with a cyclic AMP analogue and RAP1B. *Nature*. 455:124-127.

TORREIRA E, JHA S, LÓPEZ-BLANCO JR, ARIAS-PALOMO E, CHACÓN P, CAÑAS C, AYORA S, DUTTA, LLORCA O. 2008. Architecture of the pontin/reptin complex, essential in the assembly of several macromolecular complexes. *Structure*. 16(10): 1511-1520.

FERNÁNDEZ A, CORZANA F, BUSTO JH, PEREGRINA JM, AVENOZA A. 2008. Non-natural Amino Acids as Modulating Agents of the Conformational Space of Model Glycopeptides. *Chemistry-A European Journal*, 14, 23: 7042-7058.

GARCÍA-VELAA. 2008. Highly delocalized orbiting resonances. *J. Chem. Phys.* 129, 094307.

BUSSERY-HONVAULT B, DAYOU F, ZANCHETA. 2008. Long-range multipolar potentials of the 18 spin-orbit states arising from the C(P-3)+OH(X (2)Pi) interaction. *J.Chem.Phys.*, 129: 234302.

IUGA C, HERNÁNDEZ-LAGUNA A, SAINZ-DÍAZ C.I, VIVIER-BUNGE A. 2008. Theoretical Study of the Reaction between OH Radicals and Formaldehyde adsorbed on Small Silica Clusters. *Journal of Physical Chemistry C*, 112, 4590 – 4600.

CAMPOS-MARTÍNEZ J, HERNÁNDEZ M.I, BARTOLOMEI M. 2008. Interactions and Collision Dynamics in O-2 + O-2. *Theoretical Chemistry and Physics*, 18, 387-401 (2008)

CEDRIC TASSEL, JOSE MIGUEL PRUNEDA, NAOAKI HAYASHI, TAKASHI WATANABE, ATSUSHI KITADA, YOSHIHIRO TSUJIMOTO, HIROSHI KAGEYAMA, KAZUYOSHI YOSHIMURA, MIKIO TAKANO, MASAKAZU NISHI, KENJKI OHYAMA, MASAICHIRO MIZUMAKI, NAOMI KAWAMURA, JORGE

IÑIGUEZ, ENRIC CANADELL. 2009. CaFeO2: A New Type of Layered Structure with Iron in a Distorted Square Planar Coordination. *Journal of the American Chemical Society*, 2009 131 (1), 221-229.

D.BEN ABDALLAH, K .HAMMAMI, F. NAJAR, N. JAIDANE, Z. BEN LAKHDAR, M. L. SENENT. 2008. Low temperature rate constants for rotational excitations and de-excitations of C3 (1S) by collisions with He (1S). C. Chambaud and M.Hochlaf, *ApJ*, 686: 379-383.

QUIÑONERO D, FRONTERA A, DEYA P.M, ALKORTA I, ELGUERO J. 2008. Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators. *Chem.Phys. Lett.* 460, 406-410.

OLGUIN D.R, VILLA M, SENENT M.L, MORA-DELGADO M.A. 2008. Ethane internal rotation vibrational Hamiltonian. *Journal of Mexican Chemical Society*, 52(1):98-102.

MOLINA-MONTESE, DONAIOD, HERNANDEZ-LAGUNAA, SAINZ-DIAZ C.I, PARINELLO M. 2008. DFT research on the dehydroxylation reaction of Pyrophyllite 1. Ab initio Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, 112: 7051 – 7060.

MOLINA-MONTES E, DONAIO D, HERNANDEZ-LAGUNA A, SAINZ-DIAZ C.I. 2008. DFT research on the dehydroxylation reaction of Pyrophyllite II. Characterization of reactants, intermediates and transition states along the reaction paths. *Journal of Physical Chemistry A*, 112: 6373 - 6383.

MOLINA-MONTES E, TIMON V, HERNANDEZ-LAGUNA A, SAINZ-DIAZ C.I. 2008. The Fe3+ substitution effects on the dehydroxylation mechanisms in phyllosilicates by quantum mechanical methods. *Geochimica et Cosmochimica Acta*, 72: 3929-3938.

ENRIQUE MARCOS, RAMON CREHUET, JOSEP M. ANGLADA. 2008. Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. *J. Chem. Theory Comput.*, 4 (1):49-63.

- ENRIQUE MARCOS, RAMON CREHUET, JOSEP M. ANGLADA. 2008. Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. *J. Chem. Theory Comput.*, 4 (1), 49-63 DOI: 10.1021/ct700220z.
- F. BLANCO, I. ALKORTA, J. ELGUERO, V. CRUZ, B. ABARCA, R. BALLESTEROS. 2008. [1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ring-chain isomerization. *Tetrahedron*, 64, 11150-11158.
- F. BLANCO, I. ALKORTA, J. ELGUERO. 2008. The Structure of Alkali Metal Derivatives of Azoles: N- Σ versus n Structures. *J. Phys. Chem. A*, 112, 7682-7688.
- F. BLANCO, M. SOLIMANNEJAD, I. ALKORTA, J. ELGUERO. 2008. Inverse hydrogen bonds between XeH₂ and hydride and fluoride derivatives of Li, Be, Na and Mg. *Theor. Chem. Acc.* 121, 181-186.
- F. DANIEL, J. CERNICHARO. 2008. Solving radiative transfer with line overlaps using Gauss-Seidel algorithms. *A&A* 488, 1237-1247.
- F. DAYOU, P. LARREGARAY, L. BONNET. 2008. A comparative study of the Si+O₂ -> SiO+O reaction dynamics from quasi-classical trajectory and statistical based methods. *J. Chem. Phys.*, 128: 174307.
- FERNANDEZ-TEJADA A, CORZANA F, BUSTO JH. 2008. Non-natural amino acids as modulating agents of the conformational space of model glycopeptides. *Chemistry-A European Journal* 14, 23: 7042-7058.
- FERNANDO BLANCO, IBON ALKORTA, JOSE ELGUERO, VICTOR CRUZ, BELEN ABARCA, RAFAEL BALLESTEROS. 2008. [1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ring-chain isomerisation. *Tetrahedron* 64, 11150-11158.
- FRAILE JM, GARCIAJI, JIMENEZ-OSES G. 2008. Surface confinement effects on enantioselective cyclopropanation. Reactions with supported chiral 8-oxazolinyquinoline-copper complexes. *Organometallics* 27, 10: 2246-2251.
- FRANKE KJ, SCHULZE G, HENNINGSEN N. 2008. Reducing the molecule-substrate coupling in C-60-based nanostructures by molecular interactions. *Physical Review Letters*. Volume: 100 Issue: 3 Article Number: 036807.
- HERRERA C.M, BAZAGA P. 2008. Population-genomic approach reveals adaptive floral divergence in discrete populations of a hawk moth-pollinated violet. *Molecular Ecology* 17, 5378-5390.
- ALKORTA I, BLANCO F, ELGUERO J. 2008. Theoretical study of racemization in chiral alkenylidene truxenes. *J. Phys. Org. Chem.* 21, 381-386.
- ALKORTA I, ELGUERO J, SOLIMANNEJAD M. 2008. Dihydrogen bond cooperativity in (HCCBeH)_n clusters. *J. Chem. Phys.* 129, 064115.
- MARTIN-GARCIA J.M, YLLANES D, PORTUGAL R. 2008. The Invar tensor package: differential invariants of Riemann. *Computer Physics Communications* 179 586-590, arXiv: 0802.1274.
- MARTIN-GARCIA J.M. 2008. xPerm: fast index canonicalization for tensor computer algebra. *Computer Physics Communications* 179, 597-603, arXiv: 0803.0862.
- PRUNEDA J.M, IÑIGUEZ J, CANADELL E, KAGEYAMA H, TAKANO M. Structural and electronic properties of SrFeO₂ from first principles. *Phys. Rev. B* 78. 115101 (2008)
- J. ORTEGA-CASTRO, N. HERNANDEZ-HARO, A. HERNANDEZ-LAGUNA, C.I. SAINZ-DIAZ. 2008. DFT calculation of crystallographic properties of dioctahedral 2:1 phyllosilicates. *Clay minerals*, 43: 351 - 361.
- J. REVUELTA, T. VACAS, M. TORRADO, F. CORZANA, M. MENENDEZ, C. GONZALEZ, J. JIMENEZ-BARBERO, A. BASTIDA, J. L. ASENSIO. 2008. NMR-Based Analysis of Aminoglycoside Recognition by the Resistance Enzyme ANT(4'): The Pattern of OH/NH₃⁺ Substitution Determines the Preferred Antibiotic Binding Mode and is Critical for Drug Inactivation. *Journal of the American Chemical Society*, 130, 15: 5086-5103.

- J. SACRISTAN, C. MIJANGOS. 2008. Influence of water content on Structure and Dynamics of Polyvinyl alcohol by means of Molecular dynamics simulations. *Journal of Chemical Physics* 129, 154907.
- J. SACRISTAN, C. MIJANGOS. 2008. A molecular dynamics Study of the Influence of Swelling Degree on the Structure and Dynamics of Polyvinyl alcohol Hydrogels. *Virtual Journal of Biological Physics Research*, 16, 9.
- JIMENEZ-OSSES, G; GARCIA, JI; SILVA, AMG. 2008. Mechanistic insights on the site selectivity in successive 1,3-dipolar cycloadditions to meso-tetraarylporphyrins. *Tetrahedron* 64, 34: 7937-7943.
- JOSEP M. ANGLADA. 2008. The Gas Phase HO-Initiated Oxidation of Furan: A Theoretical Investigation on the Reaction Mechanism. *The Open Chemical Physics Journal*, 1, 80-93.
- M .L. SENENT, R. RUIZ, R. DOMINGUEZ-GOMEZ, M. VILLA. 2009. Ab initio study of the far-infrared spectrum of ethyl methyl ether. *J.Chem.Phys.* 130 (6), 064101.
- M. AGUNDEZ, J. P. FONFRIA, J. CERNICHARO, J. R. PARDO, M. GUELIN. 2008. Detection of circumstellar CH₂CHCN, CH₂CN, CH₃CCH, and H₂CS. *A&A*, 479: 493-501.
- M. DOLORES DIAZ, MARIA DEL CARMEN FERNANDEZ-ALONSO, GABRIEL CUEVAS, F. JAVIER CAÑADA, JESUS JIMENEZ-BARBERO. 2008. On the role of aromatic-sugar interactions in the molecular recognition of carbohydrates: A 3D view by using NMR. *Pure and Applied Chemistry*, 80, 1827-1835.
- M. NSANGOU, M. L. SENENT, M. HOCHLAF. 2009. Theoretical investigations of the cyanogen anion. *Chem.Phys.*, 355: 164-168.
- MANZANO, H; DOLADO, JS, GRIEBEL, M. 2008. A molecular dynamics study of the aluminosilicate chains structure in Al-rich calcium silicate hydrated (C-S-H) gels. *Physica status solidi A-applications and materials science*, 205 - 6: 1324-1329.
- MARTINEZ J., CRUZ V., RAMOS J., GUTIERREZ-OLIVA S., MARTINEZ-SALAZAR J., TORO-LABBEA. 2008. On the nature of the active site in bis(imino)pyridyl iron, a catalyst for olefin polymerization. *Journal of Physical Chemistry C*, 112, 5023-5028.
- N. INOSTROZA, J. R. LETELIER, P. FUENTEALBA, M.L.SENENT. 2008. Theoretical ro-vibrational spectrum of CF⁺. *Spectrochim. Acta A*, 71: 798-802.
- N. INOSTROZA, M. HOCHLAF, M.L. SENENT, R. LETELIER. 2008. Ab initio characterization of the linear SiC₃ isomers. *Astronomy & Astrophysics*, 486 (3), 1047-1052.
- O.YAZIDI, A. BEN HOURIA, Z. BEN LAKHDAR, M .L. SENENT, M. HOCHLAF. 2008. Electronic structure and spectroscopy of MgO₂⁺ cation. *Chemical Physics*, 348: 215-226.
- R. DE NALDA, J. DURA, A. GARCIA-VELA, J.G. IZQUIERDO, J. GONZALEZ-VAZQUEZ, L. BAÑARES. 2008. A detailed experimental and theoretical study of the femtosecond A-band photodissociation of CH₃I. *J. Chem. Phys.* 128, 244309.
- R. RURALI, E. WACHOWICZ, P. HYLDGAARD, P. ORDEJON. 2008. Band bending and quasi-2DEG in the metallized beta-SiC(001) surface *Physica Status Solidi-Rapid Research Letters* 2, 218.
- REHMANN H, ARIAS-PALOMO E, HADDERS MA, SCHWEDE F, LLORCA O, BOS JL. 2008 Sep 4. Structure of Epac2 in complex with a cyclic AMP analogue and RAP1B. *Nature*;455(7209): 124-7.
- S. LOPEZ-LOPEZ, R. PROSMITI and A. GARCIA-VELA. 2008. Effect of the Excitation Energy on the (HI)₂ Nonadiabatic Photodissociation Dynamics. *J. Phys. Chem. A*, 112, 2762-2772.
- S. LOPEZ-LOPEZ, R. PROSMITI, A. GARCIA-VELA. 2008. Effect of the Excitation Energy on the (HI)₂ Nonadiabatic Photodissociation Dynamics. *J. Phys. Chem. A*, 112, 2762 (2008).

SOPHIE VANDENBUSSCHE, DOLORES DIAZ, MARIA CARMEN FERNANDEZ-ALONSO, WEIDONG PAN, STEPHANE P. VINCENT, GABRIEL CUEVAS, FRANCISCO JAVIER CAÑADA, JESUS JIMENEZ-BARBERO, KRISTIN BARTIK. 2008. Aromatic-Carbohydrate interactions: An NMR and Computational study of model systems. *Chemistry: an European Journal*, 14, 7570-7578.

TORREIRA E, JHA S, LOPEZ BLANCO JR, ARIAS-PALOMO E, CHACON P, CAÑAS C, AYORA S, DUTTA A, LLORCA O. 2008 Oct 8. Architecture of the pontin/reptin complex, essential in the assembly of several macromolecular complexes. *Structure*. 16(10):1511-20.

Z. ZHANG, S. A. McCALLUM, J. XIE, L. NIETO, F. CORZANA, J. JIMENEZ-BARBERO, M. CHEN, J. LIU, R. J. LINHARDT. 2008. Solution structures of chemoenzymatically synthesized heparin and its precursors. *Journal of the American Chemical Society*, 130, 39: 12998-13007.

ZHENQING ZHANG, SCOTT A. McCALLUM, JIN XIE, LIDIA NIETO, FRANCISCO CORZANA, JESUS JIMENEZ-BARBERO, MIAO CHEN, JIAN LIU, ROBERT J. LINHARDT. 2008. Solution Structures of Chemoenzymatically Synthesized Heparin and Its Precursors. *Journal of the American Chemical Society*, 130, 12998-13007.

Scientific Articles in-press

S. GARCIA-GIL, A. GARCIA, N. LORENTE, P. ORDEJON. Optimal strictly-localized basis sets for noble metal surfaces. *Physical Review B*.

REGLA AYALAA, ELIZABETH C. BERET, JOSE MANUEL MARTINEZ, RAFAEL R. PAPPALARDO, ADELA MUÑOZ-PAEZA, ENRIQUE SANCHES MARCOS. The proceedings of Actinide XAS workshop 2008. Nuclear Science Committee of the OECD/NEA. 2008.

J. C. CONESA. 2008. Surface anion vacancies on ceria: quantum modelling of mutual interactions and oxygen adsorption. *Catal. Today*.

GONZALEZ PEREZ, ADAN; SILVA LOPEZ, CARLOS; MARCO-CONTELLAS, JOSE; FAZA, OLALLA; SORIANO, ELENA; DE LERA, ANGEL. Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl) oxiranes: a dual role of the catalyst. *Journal of Organic Chemistry*.

HEGOI MANZANO, JORGE S. DOLADO, ANDRES AYUELA. Aluminum incorporation to silicate chains of C-S-H gel. *Journal of Physical Chemistry*.

HEGOI MANZANO, JORGE S. DOLADO, ANDRÉS AYUELA. Elastic properties of the main species present in Portland cement pastes. *Acta Materialia*

HEGOI MANZANO, JORGE S. DOLADO, ANDRES AYUELA. Structural, Mechanical and Reactivity Properties of Tricalcium Aluminate Using First-principles Calculations. *Journal of the American Ceramic Society*.

J. A. JIMENEZ MADRID, A. M. MANCHO. 2009. Distinguished trajectories in time dependent vector fields. *Chaos* 19.

J. A. JIMENEZ MADRID, ANA M. MANCHO. 2009. Distinguished trajectories in time dependent vector fields. *Chaos* 19, 013111. Published online.

J. SACRISTAN, C MIJANGOS. 2009. Chemical crosslinking of Poly Vinyl Alcohol and prediction of material properties by means of fully Atomistic Molecular dynamics Simulation. *Macromol. Theory Simul.*

M.P. DE LARA-CASTELLS, A. O. Mitrushchenkov, G. Delgado-Barrio y P. Villarreal. 2008. Using a Jacobi-Davidson "nuclear orbital" method for small doped ^3He clusters. *Few Body Systems*.

N. INOSTROZA, J. R. LETELIER, M.L. SENENT. 2008. On the Variational Solution of the Coupled Breathing Rotation-Vibration of a Spherical Top Molecule. *J. Math. Chem.* A 2596.

Presentations at Congresses/Conferences

2008 ECOLOGICAL SOCIETY OF AMERICA, ANNUAL MEETING.

Milwaukee, Wisconsin, (USA) 4th August 2008.

DANIEL B. STOUFFER. Is food-web stability greater than the sum of its parts?

37th INORGANIC REACTION MECHANISMS GROUP MEETING.

Barcelona (Spain), January 2008.

JOSÉ I. GARCÍA, GONZALO JIMENEZ-OSÉS, JOSÉ A. MAYORAL.

Performance of different functional in a difficult case reaction: Cu-catalyzed cyclopropanation of alkenes.

4th INTERNATIONAL MEETING ON MOLECULAR ELECTRONICS.

Grenoble, (France). 2008.

Manuel Cobián, F.D. Novaes, A. García, H. Ueba, P. Ordejón, N. Lorente. Electron transport simulations through organic adlayer on metal surfaces.

ARENA WORKSHOP ON SPECTROSCOPY ON DOMESTIC: FROM UV TO SUB-MILLIMETRIC WAVELENGTHS.

Granada, (Spain) 16-18th April 2008.

M. L. SENENT. Ab initio calculations of spectroscopic parameters.

BULLETIN OF THE 61st ANNUAL MEETING OF THE APS DIVISION OF FLUID DYNAMICS.

San Antonio, Texas (USA). November 2008.

A.M. MANCHO, J. A. JIMENEZ MADRID. Generalized fixed points and the Lagrangian structure of time dependent geophysical flows.

CONGRESO MEXICANO DE ECOLOGIA.

Mérida, Yucatán (México) November 2008.

MEDRANO MARTINEZ MONICA, GARRIDO SANCHEZ JOSE LUIS, CASTELLANOS MARIA CLARA, HERRERA MALIANI CARLOS M. Diferenciación local en rasgos vegetativos y florales en dos especies europeas del género *Aquilegia* (Ranunculaceae): una aproximación basada en técnicas genómicas.

ESPA-2008.

Mallorca (Spain) 2008.

R. PROSMITI, A. VALDÉS, L. GARCÍA-GUTIERREZ, L. DELGADO-TELLEZ, P. VILLARREAL, G. DELGADO-BARRIO. Ab initio ground and electronic excited states of van der Waals Hel₂ cluster.

ESPA-2008.

Mallorca (Spain) 2008.

R. PROSMITI. Ab initio Intermolecular Potentials and vibrational dynamics of Rg₂-dihalogen clusters.

EUROICE2008 AN EXPLORATORY WORKSHOP DE LA EUROPEAN SCIENCE FOUNDATION.

Granada, 1-4th October 2008.

N. HERNANDEZ HARO, V. TIMON, J. ORTEGA CASTRO, C.I.

SAINZ DIAZ, A. HERNANDEZ-LAGUNA. Theoretical study of ice films adsorbed on muscovite surface models.

IBER 2008, IX IBERIAN JOINT MEETING ON ATOMIC AND MOLECULAR PHYSICS.

Capuchos (Portugal) 7-9th September, 2008.

ALBERTO GARCÍA-VELA. Nonadiabatic photodissociation dynamics in (HI)₂ induced by intracluster collisions.

IBER-2008.

Capuchos (Portugal) 7-9th September, 2008.

G. DELGADO, R. PROSMITI, P. VILLARREAL, J.V. ALEMÁN, G. WINTER, J.S. MEDINA, B. GONZÁLEZ. Equilibrium molecular dynamics simulations of liquid water viscosities.

ICCMSE-2008: COMPUTATIONAL QUANTUM CHEMISTRY: FROM ATOMS AND MOLECULES TO CLUSTERS AND NANOOBJECTS.

Crete (Greece). 2008.

R. PROSMITI. HeI₂ vdW complex: ground and electronic excited surfaces for studying dynamics.

II ENCUESTRO HPC - CSIC.

Madrid (Spain) 3rd June, 2008.

M. L. SENENT. Cadenas carbonadas de interés astrofísico.

MaCoMuFi 2nd YEARLY MEETING.

Groningen (The Netherlands), 17-19th November, 2008.

JACEK C. WOJDEL. Magnetolectric response of compounds of the BiMO₃ family.

MOLEC XVII, EUROPEAN CONFERENCE ON DYNAMICS OF MOLECULAR COLLISIONS.

San Petersburgo (Rusia). 23-28th August, 2008.

ALBERTO GARCÍA-VELA. Nonadiabatic Photodissociation Dynamics in Small Molecules and Clusters.

MOLECULAR SPECTROSCOPY CONFERENCE.

Ohio State University, (USA) 2008.

M. L. SENENT, M. HOCHLAF, H. MASSÓS. Spectroscopy and structure of chains Type C_n, C_nH and C_nSi.

MOLECULAR SPECTROSCOPY CONFERENCE.

Ohio State University, (USA) 2008.

O.YAZIDI, A. BEN HOURIA, Z. BEN LAKHDAR, M. HOCHLAF, M. L. SENENT. Electronic structure and spectroscopy of the MgO₂⁺ cation.

MOLECULAR SPECTROSCOPY CONFERENCE.

Ohio State University, (USA) 2008.

R. RUIZ, M. L. SENENT, R. DOMÍNGUEZ-GÓMEZ, M. VILLA. CCSD(T) Study of the Far-Infrared spectrum of dimethyl-ether.

STRUCTURAL, ELECTRONIC AND TRANSPORT PROPERTIES OF QUANTUM WIRES.

Lyon (France) 2008.

FREDERICO D. NOVAES, S. GARCÍA, E. MACHADO, M. BRANDGYBE, A.J.R. DA SILVA, A. FAZZIO, E.Z. DA SILVA, P. ORDEJÓN. Impurities in metallic nanowires.

WORKSHOP DE PHYSIQUE MOLÉCULAIRE: COLLISIONS RÉACTIVE ET NON RÉACTIVE.

Tunisia, April 2008.

M.L. SENENT. Ab initio calculations for spectroscopy and astrophysics.

Posters at Congresses/Conferences

7th EUROPEAN CONFERENCE ON COMPUTATIONAL CHEMISTRY.

Venetia, (Italy). 11-15th September, 2008.

J.C. CONESA. Quantum modelling of adsorbing sites and adsorbed O₂ species on ceria.

WORKSHOP ON NONLINEAR PROCESSES IN OCEANIC AND ATMOSPHERIC FLOWS. Castro Urdiales, (Spain). 2- 4th July, 2008.

JOSÉ ANTONIO JIMENEZ MADRID, ANA M. MANCHO. Generalizing fixed points to aperiodic dynamical systems.

14th INTERNATIONAL WORKSHOP ON COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE: TOTAL ENERGY AND FORCE METHODS.

Trieste (Italy). 8-10th January, 2009.

LAURA ZOPPI, KIM BALDRIDGE, ALBERTO GARCÍA. Corannulene on Cu(111) surface: structure and properties using a first-principles theoretical approach.

14th INTERNATIONAL WORKSHOP ON COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE: TOTAL ENERGY AND FORCE METHODS.

Trieste (Italy) 8-10th January, 2009.

M. COBIAN, F.D. NOVAESA, H. UEBAB, A. GARCIA, P. ORDEJON C, N. LORENTEC. Electron transport simulations through organic ad layer on metal surfaces.

14th INTERNATIONAL WORKSHOP ON COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE: TOTAL ENERGY AND FORCE METHODS.

Trieste (Italy) 8-10th January, 2009.

OTTO E. GONZALEZ, JORGE IÑIGUEZ.

Pressure induced structural, electronic and magnetic effects in BiFeO₃.

3^a JORNADA DE JOVENES INVESTIGADORES DE ARAGON.

Zaragoza, (Spain). 10th December, 2008.

ISAURA OSPINO, OLGA CRESPO, CESAR DIEZ, MARIA, CONCEPCION GIMENO, ANTONIO LAGUNA, MIGUEL MONGE.

Estudio Fotofísico y Teórico de Complejos de Oro con el Anión [7,8-PPh₂-(7,8-C₂B₉H₁₉)]- como Ligando.

ESPA2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

D. MUÑOZ-SANTIBURCIO, C.I. SAINZ DIAZ, A. HERNANDEZ-LAGUNA.

Theoretical study of adsorption of nitroorganic compounds on smectite models.

ESPA2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

J. ORTEGA CASTRO, N. HERNANDEZ HARO, V. TIMON, C.I. SAINZ DIAZ, A. HERNANDEZ-LAGUNA. DFT study of strains and elastic properties of muscovite.

ESPA2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

N. HERNANDEZ HARO, V. TIMON, J. ORTEGA CASTRO, C.I. SAINZ DIAZ, A. HERNANDEZ-LAGUNA. DFT study of the adsorption of films of partially ordered water on muscovite surface models.

ESPA2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

VICENTE TIMON, NOEMI HERNANDEZ-HARO, JOAQUIN ORTEGA-CASTRO, CLARO I. SAINZ-DIAZ, ALFONSO HERNANDEZ-LAGUNA.

DFT band-gap study of Fe³⁺, Ga³⁺ and Ge⁴⁺ substitutions in 2:1 dioctahedral phyllosilicates.

IBER 2008, IX IBERIAN JOINT MEETING ON ATOMIC AND MOLECULAR PHYSICS.

Capuchos (Portugal). 7-9th September, 2008.

A. GARCIA-VELA. Highly Delocalized Orbiting Resonances in Ne-Br₂.

IBER 2008: 9th IBERIAN JOINT MEETING ON ATOMIC AND MOLECULAR PHYSICS. Capuchos (Portugal). 7-9th September, 2008.

M. BARTOLOMEI, E. CARMONA-NOVILLO, J. PEREZ RIOS, M. I. HERNANDEZ, J. CAMPOS-MARTINEZ, R. HERNANDEZ-

LAMONEDA. A theoretical study of the O₂-O₂ dimer: ab initio interaction potentials, bound states and scattering calculations.

MOLEC XVII, EUROPEAN CONFERENCE ON DYNAMICS OF MOLECULAR COLLISIONS. San Petersburg (Russia). 23-28th August, 2008.

ALBERTO GARCÍA-VELA. Highly Delocalized Orbiting Resonances in Ne-Br₂.

THE 14th TOTAL ENERGY WORKSHOP.

Trieste (Italy) 2009.

FREDERICO D. NOVAES, D. BILC, J. INIGUEZ, P. ORDEJON, P. GHOSEZ. Tunnelling across a ferroelectric barrier: a first-principles study.

THE 15th INTERNATIONAL WORKSHOP ON OXIDE ELECTRONICS.

Estes Park (USA) 2008.

FREDERICO D. NOVAES, D. BILC, J. INIGUEZ, P. ORDEJON, P. GHOSEZ. Tunnelling across a ferroelectric barrier: a first-principles study.

WORKSHOP NONLINEAR PROCESSES IN OCEANIC AND ATMOSPHERIC FLOWS.

Castro Urdiales, (Spain). July 2008.

J. AJIMENEZ-MADRID, A.M. MANCHO. Generalizing fixed points to aperiodic dynamical systems.

ANNUAL MEETING & WORKSHOP OF THE COST NETWORK D41 INORGANIC OXIDES: SURFACES AND INTERFACES.

Barcelona, (Spain). 16-18th October, 2008.

J.C. CONESA: Electron localization effects and dioxygen activation on defective CeO₂(111) surfaces.

GOSPEL WORKSHOP ON SURFACE/ADSORBED OXYGEN ON METAL OXIDES – ROLE IN GAS SENSING AND CATALYSIS.

Tübingen (Germany). 9-10th June 2008.

J.C. CONESA. Quantum modelling of adsorbing sites and adsorbed dioxygen species on ceria.

ACTINIDE XAS WORKSHOP 2008.

Paris, France, 2008.

R. AYALA, J.M. MARTINEZ, R.R. PAPPALARDO, A. MUÑOZ PAEZ, E. SANCHEZ MARCOS. Po (IV) Hydration: a Computational Study.

GORDON RESEARCH CONFERENCE ON THREE DIMENSIONAL ELECTRON MICROSCOPY.

Barga, Lucca (Italy). June 2008.

E. ARIAS-PALOMO, H. REHMANN, BOS, JL, O. LLORCA. EM structure of the Epac2-Rap-cAMP complex.

PhD Thesis (Defended)

ANGEL RIVERA CALZADA.

Biología estructural de la reparación de roturas de doble cadena en el ADN.

Centro de Investigaciones Biológicas. CSIC. Madrid 2008.

Thesis Director: Dr. Óscar Llorca Blanco.

ERNESTO ARIAS PALOMO.

Análisis estructural de proteínas reguladoras de GTPasas de la superfamilia Ras mediante microscopía electrónica.

Centro de Investigaciones Biológicas. CSIC. Madrid 2008.

Thesis Director: Dr. Óscar Llorca Blanco.

ESTHER MOLINA MONTE.

Investigación mecano-cuántica de las reacciones de deshidratación y deshidroxilación en filosilicatos 2:1 dioctaédricos.

Facultad de Ciencias de la Universidad de Granada. 15th May, 2008.

Thesis Directors: Alfonso Hernández Laguna, Claro Ignacio Sainz Díaz.

H. MASSÓ GONZALEZ.

Estudio espectroscópico ab initio de moléculas carbonadas. Cadenas C₄, C₅ y C₆.

Facultad de Ciencias de la Universidad Autónoma de Madrid, 14th March, 2008.

Director: M.L. Senent.

ERNESTO ARIAS PALOMO (Bioquímica y Biología Molecular)

Análisis estructural de proteínas reguladoras de GTPasas de la superfamilia Ras mediante microscopía electrónica.

Departamento de Bioquímica y Biología Molecular I.

Universidad Complutense de Madrid.

Defense: 21st November, 2008.

Books and Book Chapters Published

J. CAMPOS-MARTINEZ, M. BARTOLOMEI, E. CARMONA-NOVILLO, MARTA I. HERANDEZ, R. HERNANDEZ-LAMONEDA, F. DAYOU. 2008. Interactions and collision dynamics in O₂ + O₂ REF. In: Frontiers in Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics, 18. (Wilson, S.; Grout, P.J.; Maruani, J.; Delgado-Barrio, G.; Piecuch, P. Eds.), 387-401. Springer Netherland, ISBN: 978-1-4020-8706-6, DOI. 10.1007/978-1-4020-8707-3-18.

G. DELGADO-BARRIO, R. PROSMITI, P. VILLARREAL, G. WINTER, J.S. MEDINA, B. GONZALEZ, J.V. ALEMAN, J.L. GOMEZ, P. SANGRA, J.J. SANTANA, M.E. TORRES. 2008. Viscosity of liquid water via equilibrium molecular dynamics simulations. In: Progress in Theoretical Chemistry and Physics: Frontiers in Quantum Systems in Chemistry and Physics, Springer (The Netherlands), 18, 351-362 ISBN 978-1-4020-8706-6.

R. PROSMITI, A. VALDES, L. GARCIA-GUTIERREZ, L. DELGADO-TELLEZ, P. VILLARREAL, G. DELGADO-BARRIO. 2008. He₂vdW complex: {em Ab initio} potential energy surfaces for studying dynamics. AIP Conference Proceedings, in press.

UNIVERSIDADE DE SANTIAGO DE COMPOSTELA (USC)

Scientific Articles Published



A. MUÑOZ, C. DE LA CALLE, J. A. ALONSO, P. M. BOTTA, V. PARDO, D. BALDOMIR, J. RIVAS. 2008. Crystallographic and magnetic structure of SrCoO_{2.5} brownmillerite: Neutron study coupled with bandstructure calculations. Physical Review B, A 78: 054404-1, 054404-8. ISBN: 1098.

A. ZHUKOV, C. GARCIA, J.J. DELVAL, J. GONZALEZ, M. KNOBEL, D. SERANTES, D. BALDOMIR, V. ZHUKOVA. 2008. Studies of Fe-Cu microwires with nanogranular structure. Journal of Physics: Condensed Matter, A 21: 035301- 035306. ISBN: 10.1088/0953-8984/21.

- ALONSO MEIJIDE, J. M., CASAS MENDEZ, B., HOLLER, M. J., LORENZO FREIRE, S. 2008. Computing Power Indices: Multilinear extensions and new characterization. *European Journal of Operational Research* 188, 540-554.
- ANGEL PIÑEIRO, GERARDO PRIETO, JUAN M. RUSO. 2009. Surface films of short fluorocarbon-hydrocarbon diblocks studied by molecular dynamics simulations: Spontaneous formation of elongated hemimicelles. *Journal of Colloid and Interface Science* 329, 2: 351-356.
- ANTONIO FERNANDEZ-RAMOS, RUBEN MEANA-PAÑEDA. 2008. Mechanisms of Double Proton Transfer. Theory and Applications. Zorka Smedarchina, Willem Siebrand. *Zeitschrift für Physikalische Chemie* 222, 8-9:1291
- B. HERNANDO, J. L. SANCHEZ LLAMAZARES, J. D. SANTOS, LL. ESCODA, J.J. SUÑOL, R. VARGA, D. BALDOMIR, D. SERANTES. 2008. Thermal and magnetic field-induced martensite-austenite transition in Ni₅₀.₃Mn₃₅.₃Sn₁₄.₄ ribbons. *Applied Physics Letters*, A 92: 042504-1, 042504-4. ISBN: 0003-6951.
- B. HERNANDO, J.L. SANCHEZ LLAMAZARES, J.D. SANTOS, LL. ESCODA, J.J. SUÑOL, R.VARGA, D. BALDOMIR, D.SERANTES. 2008. Magnetocaloric effect in melt spun Ni₅₀.₃Mn₃₅.₅Sn₁₄.₄. *Applied Physics Letters*, A 92: 132507-1, 132507-3. ISBN: 0003-6951.
- C. MATEO-MATEO, C. VAZQUEZ-VAZQUEZ, M.C. BUJAN-NUÑEZ, M.A. LOPEZ-QUINTELA, D. SERANTES, D. BALDOMIR, J. RIVAS. 2008. Synthesis and characterization of CoFe₂O₄-PVP nanocomposites. *Journal of non-crystalline solids A*, 354: 5236-5237. ISBN: 0022-3093.
- C. VAZQUEZ-VAZQUEZ, M. LOVELLE, C. MATEO, M.A. LOPEZ-QUINTELA, M.C. BUJAN-NUÑEZ, D. SERANTES, D. BALDOMIR, J. RIVAS. 2008. Magnetocaloric effect and size dependence study of the magnetic properties of cobalt ferrite nanoparticles prepared by solthermal synthesis. *Physica Status Solidi(a)-Applications and Material Science*, A 205: 1358-1362. ISBN: ISSN: 1862-6300.
- CABALEIRO-LAGO, E. M.; PENA-GALLEGO, A.; RODRIGUEZ-OTERO. 2008. Study of the interaction in clusters formed by phenol and CH₃X (X=CN,F,Cl) molecules. *Journal of Chemical Physics* 128, 194311/1.
- CABALEIRO-LAGO E.M, RODRIGUEZ-OTERO J, PENA-GALLEGO. 2008. Characteristics of the interaction of azulene with water and hydrogen sulphide: A computational study A. *Journal of Chemical Physics* 129, 084305/1.
- CABALEIRO-LAGO, E.M.; RODRIGUEZ-OTERO, J.; PENA-GALLEGO. 2008. Computational Study on the Characteristics of the Interaction in Naphthalene••••(H₂X)_{n=1,2} (X = O, S) Clusters. A. *Journal of Physical Chemistry A*, 112, 6344.
- CARPENTE RODRIGUEZ, L., CASAS MENDEZ, B., GARCIA JURADO, I., VAN DEN NOUWELAND, A. 2008. Coalitional interval games for strategic games in which players cooperate. *Theory and Decision* Vol. 65, 3:253-269.
- CRISTINA NUÑEZ, RUFINA BASTIDA, ALEJANDRO MACIAS, MARTA MATO-IGLESIAS, CARLOS PLATAS-IGLESIAS, LAURA VALENCIA. 2008. A hexaaza macrocyclic ligand containing acetohydrazide pendants for Ln(III) complexation in aqueous solution. Solid-state and solution structures and DFT calculations. *Dalton Transactions* (29), 3841-3850
- D. BALDOMIR, D. SERANTES, M. PEREIRO, J. RIVAS, C. VAZQUEZ-VAZQUEZ, M.C. BUJAN-NUÑEZ, J.E. ARIAS. 2008. Role of magnetic anisotropy in the magnetocaloric effect for a superparamagnetic nanoparticle system: a Monte Carlo study. *Physica Status Solidi(a)-Applications and Material Science A*, 205: 1343-1348. ISBN: ISSN: 1862-6300.
- D. BALDOMIR, V. PARDO, S. BLANCO-CANOSA, F. RIVADULLA, J. RIVAS, A. PIÑEIRO, J.E. ARIAS. 2008. Pressure-induced metal insulator transition in MgV₂O₄. *Physica B, A*, 403: 1639-1641. ISBN: 0921-4526.
- D. SERANTES, D. BALDOMIR, M. PEREIRO, J. RIVAS, C. VAZQUEZ-VAZQUEZ, M.C. BUJAN-NUÑEZ, J. E. ARIAS. 2008.

Magnetic field-dependence study of the magnetocaloric properties of a superparamagnetic nanoparticle system: a Monte Carlo simulation. *Physica Status Solidi (a)-Applications and Material Science*, A 205: 1349-1353. ISBN: ISSN: 1862-6300.

D. SERANTES, D. BALDOMIR, M. PEREIRO, J. E. ARIAS, C. MATEO-MATEO, M. C. BUJAN-NUÑEZ, C. VAZQUEZ-VAZQUEZ, J. RIVAS. 2008. Interplay between the magnetic field and dipolar interaction on a magnetic nanoparticle system: a Monte Carlo study. *Journal of non-crystalline solids A*, 354: 5224-5226. ISBN: 0022-3093.

EDUARDO JARDON-VALADEZ, ALFREDO ULLOA-AGUIRRE, ANGEL PIÑEIRO. 2008. Modelling and molecular dynamics simulation of the human gonadotropin-releasing hormone receptor in a lipid bilayer. *Journal of Physical Chemistry* 112, 34: 10704-10713 Published: 2008

G. FERNANDEZ-GARCÍA, PEREZ-MUÑUZURI. 2008. Superdiffusive wave front propagation in a chemical active flow. *Eur. Phys. J. Special Topics* 165, 169-174.

G. FERNANDEZ-GARCIA, D. I. RONCAGLIA, V. PEREZ-VILLAR, A. P. MUÑUZURI, V. PEREZ-MUÑUZURI. 2008. Chemical-wave dynamics in a vertically oscillating fluid layer. *Physical Review E* 77, 026204.

HOPPE, C. E.; RIVADULLA, F.; LOPEZ-QUINTELA, M. A.; CARMEN BUJAN, M.; RIVAS, J.; SERANTES, D.; BALDOMIR, D. 2008. Effect of Submicrometer Clustering on the Magnetic Properties of Free-Standing Superparamagnetic Nanocomposites. *Journal of Physical Chemistry C*, A 34: 13099-13104. ISBN: 1932-7447.

J. BOTANA, M. PEREIRO, D. BALDOMIR, H. KOBAYASHI, J. E. ARIAS. 2008. Magnetic and electronic structure of nFe/3cr/nFe slabs (n = 1 → 6). *Thin Solid Films A*, 516: 5144-5149. ISBN: 0040-6090.

JAVIER LOPEZ CACHEIRO, BERTA FERNANDEZ, ANTONIO RIZZO, BRANISLAV JANSIK, THOMAS BONDO PEDERSEN. 2008. Theoretical pressure and dielectric second virial coefficients of CO-Ar. *Molecular Physics An International Journal in*

the Field of Chemical Physics, 106, 881. ISSN: 0026-8976

JESUS A. VARELA, SILVIA G. RUBIN, LUIS CASTEDO, CARLOS SAA. 2008. "Formal" and Standard Ruthenium-Catalyzed [2 + 2 + 2] Cycloaddition Reaction of 1,6-Diynes to Alkenes: A Mechanistic Density Functional Study. *Journal of Organic Chemistry* 73, 1320-1332.

JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO, ANGELES PEÑA-GALLEGO. 2008. Cation- π and anion- π interactions: Changes in aromaticity upon complexation. *Chemical Physics Letters* vol. 452, issue 1-3, pp. 49-53.

JORGE BOTANA, MANUEL PEREIRO, DANIEL BALDOMIR, JUAN ENRIQUE ARIAS, KRZYSZTOF WARDA, LESZEK WOJTCZAK. 2008. Magnetic-dependent structure in eight-atom gold clusters. *Journal of Applied Physics*, A 103: 07B716-1, 07B716-3. ISBN: 0021-8978.

JORGE CARBALLIDO-LANDEIRA, IGAL BERENSTEIN, PABLO TABOADA, VICTOR MOSQUERA, VLADIMIR K. VANAG, IRVING R. EPSTEIN, VICENTE PÉREZ-VILLAR, ALBERTO P. MUÑUZURI. 2008. Long-lasting dashed waves in a reactive microemulsion. *Physical Chemistry Chemical Physics*, 10, 1094-1096.

JOSE C. CLEMENTE, ARTHUR ROBBINS, PAULA GRAÑA, M. RITA PALEO, JUAN F. CORREA, M. CARMEN VILLAVERDE, F. JAVIER SARDINA, LAKSHMANAN GOVINDASAMY, MAVIS AGBANDJE-MCKENNA, ROBER MCKENNA, BEN DUNN, FREDY SUSSMAN. 2008. Design, synthesis, evaluation and crystallographic based structural studies of HIV-1 protease inhibitors with reduced response to the V82A mutation. *J. Med. Chem.*, 51, 852-860.

M. ALDEGUNDE, A. J. GARCIA LOUREIRO, K. KALNA. 2008. Development of a 3D Parallel Finite Element Monte Carlo Simulator for Nano-MOSFETs. *Lect. Notes Comput. Sc.* vol. 4818, pp. 115-122.

M. M. G. ALEMANY, LUIS TORTAJADA, XIANGYANG HUANG, MURILO L. TIAGO, L. J. GALLEGO, JAMES R. CHELIKOWSY. 2008. Role of dimensionality and quantum confinement

- in p-type semiconductor indium phosphide quantum dots. *Physical Review B*, 78, 233101.
- M. MERCED MONTERO-CAMPILLO, JESUS RODRIGUEZ-OTERO, ENRIQUE CABALEIRO-LAGO. 2008. Theoretical Study of the [2+2+2+1] Cycloaddition Mechanism of Eneynes and Carbon Monoxide Catalyzed by Rhodium. *Journal of Physical Chemistry A*, 112, 2423-2427
- M. OTERO-LEAL, F. RIVADULLA, M.GARCIA-HERNANDEZ, A. PIÑEIRO, V. PARDO, D. BALDOMIR, J.RIVAS. 2008. Effect of spin fluctuation on the thermodynamic and transport properties of the itinerant ferromagnet CoS₂. *Physical Review B*, A 78: 180415-1, 180415-4. ISBN: 1098.
- M. PEREIRO, D. BALDOMIR, J. BOTANA, J.E. ARIAS, K.WARDA, L.WOJTCZAK. 2008. Biomedical applications of small silver clusters. *Journal of Applied Physics A*, 103: 07A315-1, 07A315-3. ISBN: 0021-8978.
- M.ALDEGUNDE, A.J.GARCÍA LOUREIRO, A.MARTINEZ, K.KALNA. 2008. Tetrahedral elements in self-consistent parallel 3D Monte Carlo simulations of MOSFETs. *Journal of Computational Electronics*. vol. 7, issue 3, pp. 201-204.
- M.ALDEGUNDE, N. SEOANE, A.J.GARCIA LOUREIRO, P.V.SUSHKO, A.L.SHLUGER, J.L.GAVARTIN, K.KALNA, A. ASENOV. 2008. Atomistic mesh generation for the simulation of nanoscale metal-oxide-semiconductor field-effect transistors. *Physical Review E*. Vol. 77, issue 5, pp. 056702.
- M.C. BUJAN-NUÑEZ, N. FONTAÍÑA-TROTIÑO, C. VAZQUEZ-VAZQUEZ, M.A. LOPEZ-QUINTELA, Y. PIÑEIRO, D. SERANTES, D. BALDOMIR J. RIVAS. 2008. Influence of the nanoparticle size on the blocking temperature of interacting systems: Monte Carlo simulations. *Journal of non-crystalline solids A*, 354:5222-5223. ISBN: 0022-3093.
- M.M.G. ALEMANY, XIANGYANG HUANG, MURILO L. TIAGO, L. J. GALLEGO, JAMES R. CHELIKOWSKY. 2008. Ab initio calculations for p-type doped bulk indium phosphide. *Solid State Communications*, 146, 245.
- MOLINA-RUIZ, R., SAIZ-URRA, L., RODRIGUEZ-BORGES, J.E., PEREZ-CASTILLO, Y., PEREZ-GONZALEZ, M., GARCIA-MERA, X. CORDEIRO, M.N.D.S. 2009. Toward the Rational Design of New Potent Cytotoxic Compounds: A TOPological Sub-structural Molecular Design (TOPS-MODE)-QSAR approach for modeling the antiproliferative activity against murine leukemia tumor cell line (L1210). *Bioorg Med Chem*, 17, 537-547.
- MONTERO-CAMPILLO, M. M.; CABALEIRO-LAGO, E. M.; RODRIGUEZ-OTERO. 2008. A Density Functional Theory Study of Rhodium-Catalyzed Hetero-[5+2]-cycloaddition of Cyclopropyl Imine Derivatives and Alkynes. *Journal of Physical Chemistry A*, 112, 9068.
- MONTERO-CAMPILLO, M. M.; CABALEIRO-LAGO, E. M.; RODRÍGUEZ-OTERO. 2008. A Theoretical Study of Pericyclic Rearrangements Catalyzed by Lithium. *Journal of Physical Chemistry A*, 112, 5218.
- MONTERO-CAMPILLO, M. M.; RODRIGUEZ-OTERO, J.; CABALEIRO-LAGO, E. M. 2008. On the mechanism of rhodium-catalyzed [6+2] cycloaddition of 2-vinylcyclobutanones and alkenes. *Tetrahedron*, 64, 6215.
- MORALES-HELGUERA, A., RODRIGUEZ-BORGES, J.E., FERNANDEZ, F., GARCIA-MERA, X. CORDEIRO, M.N.D.S. 2007. Probing the Anticancer Activity of Nucleoside Analogues: A QSAR Model Approach Using an Internally Consistent Training Set. *Journal of Medicinal Chemistry*, 50, 1537-1545.
- N. SEOANE, A.J. GARCIA LOUREIRO, M. ALDEGUNDE. 2008. Optimization of linear systems for 3D parallel simulation of semiconductor devices: Application to statistical studies. *International Journal of Numerical Modelling: Electronic Networks, Devices and Fields*. On line.
- PATRICIA MARTINEZ-BESCOS, FERNANDO CAGIDE-FAGIN, LUIS F. ROA, JUAN CARLOS ORTIZ-LARA, KRZYSZTOF KIERUS, LIDIA OZORES-VITURRO, MARTA FERNANDEZ-GONZALEZ, RICARDO ALONSO. April 23, 2008. Synthesis, structure, and E-Z isomerisation of beta-(hetero) aryl-alpha-nitro-alpha, beta-enals. *J. Org. Chem.* 73 (10), pp 3745-3753.

- R. C. LONGO, A. VEGA, S. BOUARAB, J. FERRER, M. M. G. ALEMANY, L. J. GALLEG0. 2008. Possibility of collinear magnetic order in frustrated free-standing Fe₂Cr₄ clusters. *Physical Review B*, 77, 212406.
- R. C. LONGO, A. VEGA, S. BOUARAB, J. FERRER, M. M. G. ALEMANY, L. J. GALLEG0. 2008. Possibility of collinear magnetic order in frustrated free-standing Fe-Cr clusters. *Physical Review B*, 77: 212406-ss.
- R. C. LONGO, M. M. G. ALEMANY, A. VEGA, J. FERRER. L. J. GALLEG0. 2008. Engineering the magnetic structure of Fe clusters by Mn alloying, *Nanotechnology* 19, 245701.
- R. C. LONGO, M. M. G. ALEMANY, J. FERRER, A. VEGA, L. J. GALLEG0. 2008. 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*, 128, 114315.
- R. C. LONGO, M. M. G. ALEMANY, J. FERRER, A. VEGA, L. J. GALLEG0. A density-functional study of the possibility of non-collinear magnetism in small Mn clusters using SIESTA and the generalized gradient approximation to exchange and correlation. *Journal of Chemical Physics*, 128: 114315-ss.
- R. VALIN, A. J. GARCIA LOUREIRO, N. SEOANE, M. ALDEGUNDE, C. SAMPEDRO, A. GODOY, F. GAMIZ. 12/11/2008. Parallel Implementation of a 2D DGSOI Monte Carlo Simulator Using OpenMP. DCIS 2008.
- R. VALIN, N. SEOANE, M. ALDEGUNDE, A. J. GARCIA LOUREIRO. 17/09/2008 Simulación Monte Carlo de dispositivos semiconductores en entornos HPC y HTC. *Jornadas de Paralelismo*, Castellón. pp. 139-144.
- R. C. LONGO, M. M. G. ALEMANY, A. VEGA, J. FERRER, L. J. GALLEG0. 2008. Engineering the magnetic structure of Fe clusters by Mn alloying. *Nanotechnology*, 19: 245701-ss.
- RODRIGUEZ-OTERO, J.; CABALEIRO-LAGO, E. M.; PENA-GALLEG0. 2008. Comment on A Theoretical Investigation of the Interactions between Water molecules and Ionic Liquids. *A. Journal of Physical Chemistry B*, 112, 13465.
- RODRIGUEZ-OTERO, J.; MONTERO-CAMPILLO, M. M.; CABALEIRO-LAGO, E. M. 2008. Density Functional Theory Study of Ruthenium (II)-Catalyzed [2+2+2] Cycloaddition of 1,6-Diynes with Tricarbonyl Compounds. *Journal of Physical Chemistry A*, 112, 8116.
- S. BLANCO-CANOSA, F. RIVADULLA, A. PIÑEIRO, V. PARDO, D. BALDOMIR, D. I. KHOMSKII, M. M. ABD-ELMEGUID, M. A. LÓPEZ-QUINTELA, J. RIVAS. 2009. Enhanced Dimerization of TiOCl under Pressure: Spin-Peierls to Peierls Transition. *Physical Review Letters*, A 102: 056406-1, 056406-4. ISBN: 0031-9007.
- SAIZ-URRA, L., PEREZ-CASTILLO, Y., PEREZ-GONZALEZ, M., MOLINA-RUIZ, R., CORDEIRO, M. N. D. S., RODRIGUEZ-BORGES, J. E. GARCIA-MERA, X. 2009. Theoretical Prediction of Antiproliferative Activity against Murine Leukemia Tumor Cell Line (L1210). 3D-Morse Descriptor and its Application in Computational Chemistry. *QSAR & Combinatorial Science*, 28 (1), 98-110.
- SILVIA PORTO, JOSE MANUEL SECO, JUAN FELIX ESPINOS, EMILIO QUIÑOIA, RICARDO RIGUERA. 2008. Resin-bound Chiral Derivatizing Agents for Assignment of Configuration by NMR Spectroscopy. *Journal of Organic Chemistry*, 73, 5714-572.
- V. PARDO, P. M. Botta, D. BALDOMIR, J. RIVAS, A. PIÑEIRO, C. DE LA CALLE, J. A. ALONSO, J. E. ARIAS. 2008. Electronic structure of the antiferromagnetic phase of Sr₂Co₂O₅. *Physica B*, A 403: 1636-1638. ISBN: 0921-4526.
- V. PARDO, S. BLANCO-CANOSA, F. RIVADULLA, D. I. KHOMSKII, D. BALDOMIR, HUAWU, J. RIVAS. 2008. Homopolar Bond Formation in ZnV₂O₄ Close to a Metal-Insulator Transition. *Physical Review Letters*, A, 101: 256403-1, 256403-4. ISBN: 0031-9007.
- VAZQUEZ LOPEZ, M.; VAZQUEZ, M. E.; GOMEZ-REINO, C.; PEDRIDO, R.; BERMEJO, M. R. 2008. A metallo-supramolecular approach to a half-subtractor. *New Journal of Chemistry*, 32, 1473-1477.

VICTORIA LEIRO, JOSE MANUEL SECO, EMILIO QUIÑOIA, RICARDO RIGUERA. 2008. Assigning the configuration of amino alcohols by NMR: a single derivatization method. *Organic Letters*, 10, 2733-2736.

VICTORIA LEIRO, JOSE MANUEL SECO, EMILIO QUIÑOIA, RICARDO RIGUERA. 2008. Cross Interaction between Auxiliaries: The Chirality of Amino Alcohols by NMR. *Organic Letters*, 10, 2729-2732

Scientific Articles In-Press

CRISTINA NUÑEZ, MARTA MATO-IGLESIAS, RUFINA BASTIDA, ALEJANDRO MACIAS, PAULO PEREZ-LOURIDO, CARLOS PLATAS-IGLESIAS, LAURA VALENCIA. 2008. Solid-State and Solution Structure of Lanthanide(III) Complexes with a Flexible Py-N6 Macrocyclic Ligand. *European Journal of Inorganic Chemistry*.

HUBERT CYBULSKI, PIORT S. ZUCHOWSKI, BERTA FERNANDEZ, JOANNA SADLEJ. 2008. The water-nitric oxide intermolecular potential-energy surface revisited. *Journal of Chemical Physics*, accepted.

JOSE MARIA ALONSO MEIJIDE, JESUS MARIO BILBAO, BALBINA CASAS MENDEZ, JULIO R. FERNANDEZ. 2008. Weighted multiple majority games with unions: generating functions and applications to the European Union. *European Journal of Operational Research*.

LORENZO FREIRE, S.; CASAS MENDEZ, B.; HENDRICKX, R. 2009 The two-stage constrained equal awards and losses rules for multi-issue allocation situations. Aceptado en TOP, An Official Journal of the Spanish Society of Statistics and Operations Research.

SANCHEZ-PEDREGAL, V.; SANTAMARIA-FERNANDEZ, R.; NAVARRO-VAZQUEZ, A ; Residual Dipolar Coupling of Freely Rotating Groups in Small molecules. Stereochemical Assignment and Side-Chain Conformation of 8-Phenylmenthol. *Organic Letters*.

Presentations at Congresses/Conferences

FISES2008.

Salamanca, (Spain). 27-29th March, 2008.

GUILLERMO FÉRNANDEZ GARCIA, VICENTE PEREZ MUÑUZURI, V. PEREZ-VILLAR. Experimento de Faraday en medio activo. Difusión anómala.

12th INTERNATIONAL ELECTRONIC CONFERENCE ON SYNTHETIC ORGANIC CHEMISTRY (ECSOC-11).

Santiago de Compostela, (Spain). 1st to 30th November, 2008.

SAIZ-URRA, L., PEREZ-CASTILLO, Y., PEREZ-GONZALEZ, M., MOLINA RUIZ, R., CORDEIRO, M.N.D.S., RODRIGUEZ-BORGES, J.E, GARCIA-MERA, X. Theoretical Prediction of Antiproliferative Activity against Murine Leukemia Tumor Cell Line (L1210). 3D-Morse Descriptors and its Application in Computational Chemistry.

19th IUPAC INTERNATIONAL CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY (ICPOC-19).

Santiago de Compostela, (Spain). 13-18th July, 2008.

BEGOÑA PAMPIN, FERNANDO FERNANDEZ, AMALIA ESTEVEZ, RAQUEL G. SOENGAS, FREDY SUSSMAN, JUAN C. ESTEVEZ, RAMON J. ESTEVEZ. Synthetic and "in silico" approaches for the study of stereocontrolled generation of five member carbocycles and heterocycles from carbohydrates through chiral templates.

AGU 2008 FALL MEETING.

San Francisco, (USA). 15-19th December, 2008.

ALEXANDRE RIOS ENTENZA, GONZALO MIGUEZ MACHO. Regional Climate Simulations of the Hydrological Cycle in the Iberian Peninsula with WRF model. .

EGU (EUROPEAN GEOSCIENCES UNION) GENERAL ASSEMBLY.

Vienna, (Austria). 13-18th April 2008.

LUCIA GESTAL SOUTO, GONZALO MIGUEZ MACHO. A high resolution calculation of the climatology water table depth and the climatology soil moisture profile for Europe: does the water table matter?

ESPA 2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

ANGELIKA BARANOWSKA, BERTA FERNÁNDEZ RODRÍGUEZ, ANTONIO RIZZO, BRANISLAV JANSIK. The CO-Ne van der Waals complex intermolecular potential energy surface, polarizability and virial coefficients.

ESPA 2008.

Palma de Mallorca, (Spain). 2-5th September, 2008.

SILVIA BOUZON, BERTA FERNANDEZ RODRIGUEZ, HENRIK KOCH, PETER FELKER, Ground state benzene-argon intermolecular potential energy surface.

I XORNADA GALEGA DE BIOINFORMATICA.

A Coruña, (Spain). 4th April 2008.

P. BROCOS, N. DIAZ-VERGARA, A. VILLA, A. E. MARK, A. PIÑEIRO. Potential of mean force calculations for the formation of native cyclodextrins-based complexes.

IV BIENAL DEL GERMN/ I REUNION IBERICA DE RMN.

Seville, (Spain). 4th September, 2008.

ARMANDO NAVARRO-VÁZQUEZ. A general toolkit for computation of NMR properties: development and applications.

MARCH MEETING (OF THE AMERICAN PHYSICAL SOCIETY).

New Orleans, (USA) March, 2008.

M.M.G. ALEMANY, XIANGYANG HUANG, MURILO L. TIAGO, L. J. GALLEGO, JAMES R. CHELIKOWSKY. Ab initio calculations for the electronic properties of zinc-doped indium phosphide nanowires.

XI ENCUENTRO PEPTIDICO IBERICO.

Santiago de Compostela, (Spain). 6-7th March, 2008.

FREDY SUSSMAN, M. CARMEN VILLAVERDE, JUAN C. ESTEVEZ, RAMON J. ESTEVEZ. Predicting the folding properties of homooligomers of cyclopentane beta-amino acids.

XIX JORNADAS DE PARALELISMO. 2008.

Castellón, (Spain). 17th, 18th & 19th September, 2008.

A. J. GARCIA LOUREIRO, M. ALDEGUNDE, N. SEOANE. Paralelización de un simulador de arrastre-difusión con correcciones cuánticas aplicado al estudio de transistores MOSFET. pp. 127-132.

Posters at Congresses/Conferences

22nd GENERAL CONFERENCE OF THE CONDENSED MATTER DIVISION OF THE EUROPEAN PHYSICAL SOCIETY.

Roma, (Italy). 25-29th August, 2008.

JESUS CARRETE, JUAN CARLOS REBOREDO, LUIS MIGUEL VARELA. Transition between Non-Gaussian and Gaussian Stock Market Behaviour after Informational Shocks: Complex Network Analysis.

8th ANNUAL MEETING OF THE EUROPEAN METEOROLOGICAL SOCIETY.

Amsterdam, (Netherlands). October 2008.

MARTINEZ, A.; MIGUEZ-MACHO, G. Regional Model climatic simulation of Western Europe and the Iberian Peninsula for the Ensembles Project emissions scenario.

17th INTERNATIONAL SYMPOSIUM ON SURFACTANTS IN SOLUTION.

Berlin, (Germany) 18-22nd August, 2008.

P. BROCOS, A. PIÑEIRO, A. AMIGO, J. GRACIA-FADRIQUE. Revisiting positive aneotropy.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain). 13-18th July, 2008.

ENRIQUE M. CABALEIRO-LAGO, JESUS RODRIGUEZ-OTERO, ANGELES PEÑA-GALLEGO. A computational study of the interaction of indole analogs with h₂O and h₂S.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain). 13-18th July, 2008.

JORGE A. CARRAZANA-GARCIA, ENRIQUE M. CABALEIRO-LAGO, JESUS RODRIGUEZ-OTERO. Computational study of the interaction of water and hydrogen sulfide with fused benzene rings.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain). 13-18th July, 2008.

JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO,

ANGELES PEÑA-GALLEGO, M. M. MONTERO-CAMPILLO. A DFT Study of the interaction of Ferrocene with Lithium cation.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain). 13-18th July, 2008.

M. MERCED MONTERO-CAMPILLO, JESÚS RODRÍGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO. On the mechanism of Ru(II)-catalyzed [2+2+2] cycloaddition of 1,6-diyne and tricarbonyl compounds: A DFT study.

22nd GENERAL CONFERENCE OF THE CONDENSED MATTER DIVISION OF THE EUROPEAN PHYSICAL SOCIETY (CMD22).

Roma, (Italy). 25-29th August, 2008.

ROBERTO LONGO, MANUEL ALEMANY, ANDRES VEGA JAIME FERRER, LUIS GALLEGU. Engineering the magnetic structure of Fe clusters by Mn alloying.

6th CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA 2008).

Palma de Mallorca (Spain) 2-5th September, 2008.

J.J. NOGUEIRA, E. MARTINEZ NUÑEZ, J.M.C. MARQUES, A. VAZQUEZ. Chemical dynamics simulations of silyl ions scattering off a fluorinated self-assembled monolayer surface.

ECSOC 2008.

Lugo, (Spain). 1st-30th November, 2008.

ENRIQUE M. CABALEIRO-LAGO, JESUS RODRIGUEZ-OTERO, ANGELES PEÑA-GALLEGO, M. MERCED MONTERO-CAMPILLO. Study of the interaction between aniline and CH₃CN, CH₃Cl and CH₃F.

ECSOC 2008.

Lugo, (Spain). 1st-30th November, 2008.

JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO, ANGELES PEÑA-GALLEGO, M. MERCED MONTERO-CAMPILLO. Study of the Lithium Cation-Ferrocene Interaction by DFT Calculations: An In-Depth Analysis of the Existence of a Planetary System.

ECSOC 2008.

Lugo, (Spain). 1st-30th November, 2008.

M. MERCED MONTERO-CAMPILLO, JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO. Selectivity of the Ru(II)-Catalyzed [2+2+2] Cycloaddition of 1,6-Diyne and Tricarbonyl Compounds.

ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA) 2008.

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

ANGELES PEÑA-GALLEGO, DANIELA JOSA, ENRIQUE CABALEIRO-LAGO, JESUS RODRIGUEZ-OTERO. Study of the effects of cations on the inversion barrier and aromaticity of phosphole.

ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA) 2008.

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

CEILA FONG-PADRÓN, JESÚS RODRÍGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO, AMÉRICA GARCÍA. A theoretical study of the mechanism of imidazole formation catalyzed by the ionic liquid [Hbim]BF₄.

ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA) 2008.

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

DANIELA JOSA, ANGELES PEÑA-GALLEGO, JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO. Theoretical study of the aromaticity of phospholes.

ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA) 2008.

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

VALENTINA ERASOVA, JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO, ANGELES PEÑA-GALLEGO. An ab initio and DFT study of the mechanism of the unimolecular elimination of α,β -unsaturated aldehydes in the gas phase.

ESPA 2008, THE 6th CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA).

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

CEILA FONG PADRON, JESUS RODRIGUEZ OTERO, ENRIQUE

M. CABALEIRO LAGO, AMERICA GARCIA. A Theoretical study of the mechanism of Imidazole formation catalyzed by the Ionic liquid [HBIM]BF₄.

ESPA 2008.

Palma de Mallorca (Spain). 2nd to 5th September, 2008.

SILVIA BOUZÓN, BERTA FERNÁNDEZ, HENRIK KOCH, PETER FELKER. Ground State Benzene-Argon Intermolecular Potential Energy Surface.

I XORNADA GALEGA DE BIOINFORMÁTICA.

A Coruña, (Spain). 4th April, 2008.

P. BROCOS, N. DIAZ-VERGARA, A. VILLA, A. E. MARK, A. PIÑEIRO. Potential of mean force calculations for the formation of native cyclodextrins-based complexes.

INTERNATIONAL CONFERENCE ON SIMULATION OF SEMICONDUCTOR PROCESSES AND DEVICES (SISPAD 2008).

Hakone (Japan) 2008.

M. ALDEGUNDE, A.J. GARCIA LOUREIRO, A. MARTINEZ, K.KALNA. 3D Monte Carlo Simulation of Tri-Gate MOSFETs Using Tetrahedral Finite Elements. pp. 153-156.

INTERNATIONAL WORKSHOP ON OPERATIONS RESEARCH.

Madrid, (Spain). June, 2008.

LUISA CARPENTE, BALBINA CASAS, JAVIER GOZALVEZ, NATIVIDAD LLORCA, MANUEL PULIDO, JOAQUIN SANCHEZ-SORIANO. Bankruptcy problems with non linear utilities of the agents.

IV BIENAL DEL GERMN/ I REUNION IBERICA DE RMN.

Seville, (Spain), 2008.

R. SANTAMARIA-FERNANDEZ, V. SANCHEZ-PEDREGAL, A. NAVARRO-VAZQUEZ. May external alignment be described by a single tensor? Quinine as a test study.

IV BIENAL GERMN/ I REUNION IBERICA DE RMN.

Seville, (Spain), 2008.

V. SANCHEZ-PEDREGAL, R. SANTAMARIA-FERNANDEZ, A. NAVARRO-VAZQUEZ. Using Free Rotating Groups in RDC analysis of Small Molecules.

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY. New Orleans, (USA). March, 2008.

L. J. GALLEGO, M. M. G. ALEMANY, R.C. LONGO, D.J. GONZALEZ, L. E. GONZALEZ MURILO, L. TIAGO, JAMES R. CHELIKOWSKY. Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of liquid lead.

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY. New Orleans, (USA). March, 2008.

R. C. LONGO, M. M. G. ALEMANY, J. FERRER, A. VEGA, L. J. GALLEGO. Ab initio study of the possibility of noncollinear magnetism in small Mn clusters.

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY. New Orleans, (USA). March, 2008.

ROBERTO C. LONGO, MANUEL ALEMANY, JAIME FERRER, ANDRES. VEGA, LUIS J. GALLEGO. Ab initio study of the possibility of noncollinear magnetism in small Mn clusters.

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY. New Orleans, (USA) 2008.

ROBERTO C. LONGO, MANUEL ALEMANY, LUIS J. GALLEGO, D. J GONZALEZ, L.E. GONZALEZ, MURILO L. TIAGO, JAMES R. CHELIKOWSKY. Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of liquid Pb.

THE 2nd GENERAL CONFERENCE OF THE CONDENSED MATTER DIVISION OF THE EUROPEAN PHYSICAL SOCIETY. Roma, (Italy) 2008.

R.C. LONGO, M. M. G. ALEMANY, A. VEGA, J. FERRER, L. J. GALLEGO. Engineering the magnetic structure of Fe clusters by Mn alloying.

THE XIV INTERNATIONAL SYMPOSIUM ON SMALL PARTICLES AND INORGANIC CLUSTERS.

Valladolid, (Spain), 2008.

M.M.G. ALEMANY, LUIS TORTAJADA, XIANGYANG HUANG, MURILO L. TIAGO, L. J. GALLEGO, JAMES R. CHELIKOWSKY. The role of dimensionality and quantum confinement in p-type semiconductor nanomaterials: a first-principles study based on a real-space implementation of DFT.

WATOC 2008.

Sydney (Australia) 14-19th September, 2008.

ENRIQUE M. CABALEIRO-LAGO, JESÚS RODRÍGUEZ-OTERO, ANGELES PEÑA-GALLEGO. Computational study of the solvent effect upon the interaction between guanidinium cation and aromatic systems.

WATOC 2008.

Sydney (Australia) 14-19th September, 2008.

JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO, ANGELES PEÑA-GALLEGO. Theoretical Study of the Solvent Effect on the Interaction between Pyridinium Cation and Benzene.

XXXIV CONGRESSO DEI CHIMICI TEORICI DI ESPRESSIONE LATINA.

Cetraro (Italia). 3rd to 8th July, 2008.

M. MERCED MONTERO-CAMPILLO, JESUS RODRIGUEZ-OTERO, ENRIQUE M. CABALEIRO-LAGO. Estudio teórico de la cicloadición [2+2+2] de 1,6-dianos y compuestos tricarbonílicos catalizada por rutenio.

PhD Thesis Defended

GUILLERMO FERNANDEZ GARCIA.

"Estructura espacio-temporal en sistemas de reacción-difusión-advección".

Universidad de Santiago de Compostela, (Spain). October, 2008.

Directors: V. Pérez Villar and V. Pérez Muñuzuri.

M. MERCED CAMPILLO.

"Estudio teórico de reacciones pericíclicas catalizadas por litio y cicloadiciones multicomponente catalizadas por rodio y rutenio".

Universidad de Santiago de Compostela, (Spain). December 2008.

Directors: Jesús Rodríguez Otero, Enrique M. Cabaleiro Lago.

Graduate Thesis and Final Projects

CRISTINA JACOME RODRIGUEZ.

"Implementación de algoritmos para la optimización de turnos y rutas de cosechadoras en una cooperativa agraria".

Technical Engineering in Computer Systems. December, 2008.

Director: María Luisa Carpena Rodríguez.

LUIS TORTAJADA LAVIN.

"Estudio del confinamiento cuántico tridimensional de los estados electrónicos en nanocristales de InP puros y dopados con Zn utilizando técnicas de simulación ab initio".

Faculty of Physics. Universidad de Santiago de Compostela. 12th September 2008.

RAÚL VALÍN FERREIRO.

"Paralelización con OpenMP de un simulador Monte Carlo de dispositivos DGSOI₂".

Universidad de Santiago de Compostela, May 2008.

Directors: Antonio Jesús García Loureiro, Natalia Seoane Iglesias.

Books and Book Chapters Published

SAAVEDRA, S.; MENDEZ, M.R.; SOUTO, J.A.; BERMUDEZ, J.L.; VELLON, M.; COSTOYA, M. 2008. Regional transport of tropospheric ozone: a case study in the northwest coast of Iberian Peninsula. *Air Pollution Modeling and its Application XIX*, (Ed. Springer), ISBN 978-1-4020-8451-5, pp. 667-668, 2008.

UNIVERSIDADE DA CORUÑA (UDC)



Scientific Articles Published

ANAARDA, RAQUEL GONZALEZ-SOENGAS, M. ISABEL NIETO, CARLOS JIMENEZ, JAIME RODRIGUEZ. 2008. Total Synthesis of (-)-Dysithiazolamide. *Organic Letters*, 11, 2175-78.

CARLOS TEIJEIRO BARJAS, GUILLERMO LOPEZTABOADA, JUAN TOURIÑO DOMINGUEZ, BASILIO B. FRAGUELA RODRIGUEZ, RAMON DOALLO BIEMPICA, JOSE CARLOS MOURIÑO

- GALLEGO, ANDRES GOMEZ TATO, IGNACIO LOPEZ CABIDO. 2008. "Evaluación del Rendimiento de las Comunicaciones Colectivas en UPC". XIX Jornadas de Paralelismo (JPo8) - Castellón (Spain), 2008.
- CRISTINA NUÑEZ, RUFINA BASTIDA, ALEJANDRO MACIAS, MARTA MATO-IGLESIAS, CARLOS PLATAS-IGLESIAS, LAURA VALENCIA. 2008. A hexaaza macrocyclic ligand containing acetohydrazide pendants for Ln(III) complexation in aqueous solution. Solid state and solution structures and DFT calculations. *Dalton Transactions*, 3841-3850.
- D. R. RAMOS, M. V. GARCIA, M. CANLE L., J. A. SANTABALLA, P. G. FURTMÜLLER, C. OBINGER. 2008. Myeloperoxidase-catalyzed chlorination: the quest for the active species. *Journal of Inorganic Biochemistry* doi:10.1016/j.jinorgbio.
- DAVID ESTEBAN-GOMEZ, CARLOS PLATAS-IGLESIAS, ANDRES DE BLAS, LUIGI FABBRIZZI, TERESA RODRIGUEZ-BLAS. 2008. Protonated Macrobicyclic Hosts Containing Pyridine Head Units for Anion Recognition. *Chemistry European Journal*, 14, 5829-5838.
- DOLORES ABELLA, VICTOR BLANCO, ELENA PIA, MARCOS CHAS, CARLOS PLATAS-IGLESIAS, CARLOS PEINADOR, JOSE M. QUINTELA. Stereoselective Self-Assembly of Atropisomeric Pd(II) Metallo-cycles with Quinoline Moieties Induced by an Aromatic Guest. *Chemical Communications*, 2879-2881.
- GUILLERMO L. TABOADA, JUAN TOURIÑO, RAMON DOALLO. November 2008. Java Fast Sockets: Enabling High-speed Java Communications on High Performance Clusters. *Computer Communications*, Vol. 31, No. 17, pp. 4049-4059
- JAVIER JESUS POZA, CARLOS JIMENEZ, JAIME RODRIGUEZ. 2008. J-Based Analysis and DFT-NMR Assignments of Natural Complex Molecules: Application to 3 β , 7-Hydroxy-5,6-epoxycholestanes. *European Journal of Organic Chemistry*, 3960-69.
- JAVIER JESUS POZA, ROGELIO FERNANDEZ, FERNANDO REYES, JAIME RODRIGUEZ, CARLOS JIMENEZ. 2008. Isolation, Biological Significance, Synthesis, and Cytotoxic Evaluation of New Natural Parathiosteroids A-C and Analogues from the Soft Coral *Paragorgia* sp. *Journal of Organic Chemistry*, 73, 7978-84.
- KRISTINA DJANASHVILI, CARLOS PLATAS-IGLESIAS, JOOPA. PETERS. 2008. The structure of the lanthanide aquo ions in solution as studied by ¹⁷O NMR spectroscopy and DFT calculations. *Dalton Transactions*, 602-607.
- LOIČ CHARBONNIÈRE, SAMIR MAMERI, PASCAL KADJANE, CARLOS PLATAS-IGLESIAS, RAYMOND ZIESSEL. 2008. Tuning the Coordination Sphere around Luminescent Lanthanide Complexes for Anion Sensing. *Inorganic Chemistry*, 47, 3748-3762.
- MARINA GONZALEZ-LORENZO, CARLOS PLATAS-IGLESIAS, MARTA MATO-IGLESIAS, DAVID ESTEBAN-GOMEZ, ANDRES DE BLAS, TERESA RODRIGUEZ-BLAS. 2008. Conformation Study of Lanthanide (III) complexes of N-(2-salicylal-dimino-benzyl)-1-aza-18-crown-6 by using X-ray and ab Initio Methods. *Polyhedron*, 27, 1415-1422.
- MARTA MATO-IGLESIAS, ADRIAN ROCA-SABIO, ZOLTÁN PÁLINKÁS, DAVID ESTEBAN-GOMEZ, CARLOS PLATAS-IGLESIAS, EVA TOTH, ANDRES DE BLAS, TERESA RODRIGUEZ BLAS. 2008. A New Structural Entry for the Design of MRI Contrast Agents Based on a 1, 7-Diaza-12-crown-4 Platform Containing Picolinate Pendants. *Inorganic Chemistry*, 47, 7840-7851.
- OLGA BLANCO, CRISTINA PATO, MARIA RUIZ, VICENTE OJEA. 2008. Access to pyrrolidine imino sugars via tin(II)-mediated aldol reactions of bislactim ethers: synthesis of 2,5-dideoxy-2,5-imino-D-glucitol. *Organic & Biomolecular Chemistry* 6: 3967-3969.
- R. G. SOENGAS, M. LARROSA, M. BALADO, J. RODRIGUEZ, M. L. LEMOS, CARLOS JIMENEZ. 2008. Synthesis and Biological Activity of Analogues of Vanchrobactin, a Siderophore from *Vibrio anguillarum* serotype O2. *Organic Biomolecular Chemistry*, 6, 1278-87.

RAQUEL FERREIROS-MARTINEZ, DAVID ESTEBAN-GOMEZ, CARLOS PLATAS-IGLESIAS, ANDRES DE BLAS, TERESA RODRIGUEZ-BLAS. 2008. Zn(II), Cd(II) and Pb(II) complexation with pyridinecarboxylate containing ligands. Dalton Transactions, 5754-5765 (2008).

RUIZ, MARIA; RUANOVA, TANIA M.; BLANCO, OLGA; NUNEZ, FATIMA; PATO, CRISTINA; OJEA, VICENTE. 2008. Diastereoselective Synthesis of Piperidine Imino Sugars Using Aldol Additions of Metalated Bislactim Ethers to Threose and Erythrose Acetonides. Journal of Organic Chemistry, 73(6), 2240-2255.

E. FERNANDEZ-BLANCO, J. DORADO, N. PEDREIRA. July 2008. Artificial cell systems based in Gene Expression Protein effects. Advancing Artificial Intelligence through Biological Process Applications. A. Porto, W. Buño, A. Pazos. Information Science Reference. Pp 146-164.

Scientific Articles In-Press

DANIEL R. RAMOS, RAQUEL CASTILLO, MOISES CANLE L., M. VICTORIA GARCIA, JUAN ANDRES, J. ARTURO SANTABALLA. 2008. A Theoretical Study on the Mechanism of the Base-promoted Decomposition of (N-Cl),N-methylethanolamine. Organic & Biomolecular Chemistry DOI: 10.1039/paperno.

Presentations at Congresses/Conferences

XIX JORNADAS DE PARALELISMO.

Castellón, (Spain). September 2008.

C. TEIJEIRO, G. LOPEZ, J. TOURIÑO, B. B. FRAGUELA, R. DOALLO, J. C. MOURIÑO, A. GOMEZ, I. LOPEZ. "Evaluación del Rendimiento de las Comunicaciones Colectivas en UPC".

18th EUROPEAN CONFERENCE ON ARTIFICIAL INTELLIGENCE ECAI 2008.

Patras, (Greece). 21-25th July, 2008.

DANIEL RIVERO, JULIAN DORADO, JUÁN RABUÑAL, ALEJANDRO PAZOS. Automatic Recurrent ANN development for signal classification: detection of seizures in EEGs. ISBN: 978-1-58603-891-5. 142-146.

NINTH TETRAHEDRON SYMPOSIUM.

Berkeley, CA, (USA) 22-25th July 2008.

MARTA LARROSA, RAQUEL G. SOENGAS, JAIME RODRIGUEZ, CARLOS JIMENEZ. Synthesis of vanchrobactin analogue-antibiotic quinolone conjugates used as Trojan horse against vibriosis.

PROCEEDINGS OF THE INTERNATIONAL WORKSHOP ON SCALABLE TOOLS FOR HIGH-END COMPUTING (STHEC 2008), HELD IN CONJUNCTION WITH THE 22nd INTERNATIONAL CONFERENCE ON SUPERCOMPUTING (ICS08), pp. 1-12.

Kos (Greece), June 2008.

GABRIEL RODRIGUEZ, MARIA J. MARTIÍN, PATRICIA GONZALEZ, JUAN TOURIÑO, RAMON DOALLO, A compiler-assisted tool for portable checkpointing of message-passing applications.

XIX JORNADAS DE PARALELISMO.

Castellón, (Spain). September, 2008.

MARTA LOUREIRO, GABRIEL RODRIGUEZ, PATRICIA GONZALEZ, MARIA J. MARTIN, JOSE C. MOURIÑO, TERESA SANCHEZ. "Tolerancia a fallos en aplicaciones reales utilizando CPPC". pp. 323-328. ISBN 978-84-8021-676-0.

Posters at Congresses/Conferences

19th INTERNATIONAL CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

D. R. RAMOS, M. CANLE L., M. V. GARCIA, J. ANDRES, J. A. SANTABALLA. A Joint Experimental-Computational Approach To Concurrent Reaction Mechanisms.

19th INTERNATIONAL CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

E. CARRO, M. CANLE L., J. A. SANTABALLA. In vitro Study of the Mechanism of Intracellular Oxidation of Uracil by Hypochlorous Acid.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

LUIS F. RVÁZQUEZ. Theoretical Study on the Glycine Synthesis Reaction in Cometary and Interstellar Ices Analogues. A Novel Mechanistic Model to Understand the Abiotic Synthesis of Amino Acids.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

LUIS F. R VÁZQUEZ. Theoretical Study on the Imine Synthesis Reaction in Cometary and Interstellar Ices Analogues. A Mechanistic Model to Understand the Abiotic Synthesis of Amino Acids Precursor.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

LUIS F. R VAZQUEZ. Theoretical Study on the Sulphide Oxydation by Hypochlorous Acid in Aqueous Media: A Novel Mechanism.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 13-18th July, 2008.

VICENTE OJEA, MARIA RUIZ, OLGA BLANCO, CRISTINA PATO. Diastereoselective Aldol Additions of Tin(II) Azaenolates to Matched 2,4-Ethylidene-D-Erythroses.

2nd EUCHEMS CHEMISTRY CONGRESS.

Turín (Italy) 16th September, 2008.

MARIA RUIZ, OLGA BLANCO, CRISTINA PATO, VICENTE OJEA. Diastereoselective Synthesis of 2,5-Dideoxy-2,5-imino-D-glucitol.

8th INTERNATIONAL PEROXIDASE SYMPOSIUM.

Tampere (Finland) 20-24th August 2008.

DANIEL R. RAMOS, PAUL G. FURTMÜLLER, CHRISTIAN OBINGER, M. CANLE L., M. V. GARCÍA, J.A. SANTABALLA. Compound II Revisited.

EUROMAR 2008: MAGNETIC RESONANCE FOR THE FUTURE.

Saint Petersburg, (Russia). 6-11th July 2008.

M. ISABEL NIETO, J. RODRIGUEZ, C. JIMENEZ. J-Based Analysis in 1,2 and 1,3 Acyclic Nitrogen Containing Chiral Systems.

IV IBERIAN CARBOHYDRATE MEETING. IX JORNADAS DE CARBOHIDRATOS.

Santiago de Compostela (Spain). 1st September, 2008.

OLGA BLANCO, CRISTINA PATO, MARIA RUIZ, VICENTE OJEA. Diastereoselective Synthesis of 2,5-Dideoxy-2,5-iminogalactitol.

NINTH TETRAHEDRON SYMPOSIUM.

Berkeley, CA, (USA) 22-25th July, 2008.

MARTA LARROSA, RAQUELG. SOENGAS, JAIME RODRIGUEZ, CARLOS JIMENEZ. Synthesis of vanchrobactin analogue-antibiotic quinolone conjugates used as Trojan horse against vibriosis.

PhD Thesis Defended

GABRIEL RODRIGUEZ.

Compiler-assisted checkpointing of message-passing applications in heterogeneous environments.

Universidade de A Coruña. December 2008.

Directors: María J. Martín, Patricia González.

JAVIER JESUS POZA.

"Síntesis de 6-Hidroximino esteroides con diferentes posiciones oxigenadas en los anillos A y/o B y fluoradas en C-5 como potentes agentes antitumorales".

Universidade da Coruña, June, 2008.

Directors: Carlos Jiménez, Jaime Rodríguez.

PhD Thesis Presented

MANUELA. PEITEADO PEITEADO,

"Estudios fotofísicos y fotoquímicos sobre el aminoácido aromático N-fenilglicina"

Graduate Thesis

DAMIAN ALVAREZ MALLON.

"Análisis Técnico de Rendimiento de Sistemas HPC".

Computer Architecture Group, Department of Electronics and Systems,

Universidad de A Coruña. 24th September, 2008.

Director: Andrés Gómez Tato.

Mentor: Guillermo López Taboada.

EDUARDO MARTINEZ PARDEIRO.

"Implementación da Técnica de Partición en Bloques no Compilador GCC".

Engineering and Computer Systems.

Directors: Manuel Carlos Arenaz Silva and Basilio B. Fraguela Rodríguez

JOSE MANUEL ANDION FERNANDEZ.

"Diseño e Implementación de nuevas Operaciones Colectivas para el Lenguaje de Programación Paralela UPC".

Department of Electronics and Systems. Universidad de A Coruña. September, 2008. Directors: Guillermo López Taboada, Juan Touriño Domínguez.

JORGE GONZALEZ DOMINGUEZ.

"Diseño en Implementación de una Biblioteca de Computación Matricial Densa y Dispersa para el Lenguaje de Programación Paralela UPC".

Computer Architecture Group, Department of Electronics and Systems, Universidad de A Coruña. September, 2008.

Mentors: Juan Touriño Domínguez, María José Martín Santamaría.

NOHAVEIGUELA BLANCO.

"Optimización de Redes Neurogliales Artificiales".

School of Informatics. Universidad de A Coruña, 2008.

Mentored work (DEA).

OSCAR IBAÑEZ PANIZO.

"Aplicación de Redes Neurogliales Artificiales a Clasificación y Predicción".

School of Informatics. Universidad de A Coruña, 2008.

Mentored Work (DEA).

ÓSCAR IBAÑEZ PANIZO.

"Sistemas Conexionistas y Modelos Computacionales Neurobiológicos".

Diploma of Advanced Studies. Universidad de A Coruña.

Mentor: Juan Ramón Rabuñal Dopico.

Books and Book Chapters Published

M. GESTAL, J. DORADO, E. FERNANDEZ-BLANCO. December 2008. "Redes de Neuronas Artificiales y Computación Evolutiva". *Tecnologías de la Información y las Comunicaciones en Ingeniería Civil*. Pp 41-64. Foundation Alfredo Brañas.

DANIEL RIVERO, DAVID PERISCAL. 2008. *Evolving Graphs for ANN Development and Simplification*. In: *Encyclopaedia of Artificial Intelligence* Ref. ISBN: 978-1-59904-849-9 (Hershey, New York). CL Volume: II. Pages: 618-624.

UNIVERSIDADE DE VIGO (UVIGO)

Scientific Articles Published



KEN S. FELDMAN, D. KEITH HESTER II, CARLOS SILVA LOPEZ, OLALLA NIETO FAZA. 2008. *Allenyl Azide Cycloaddition Chemistry. Photochemical Initiation and CuI Mediation Leads to Improved Regioselectivity*. *Org. Lett.* 10 (8), pp 1665–1668.

ALVAREZ, ROSANA; PEREZ, MARTIN; NIETO FAZA, OLALLA; DE LERA, ANGEL R. 2008. *Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway*. *Organometallics*, 27(14), 3378–3389. CODEN: ORGND7 ISSN: 0276-7333. CAN 149:128960 AN 2008:662319

ALVAREZ, ROSANA; PEREZ, MARTIN; NIETO FAZA, OLALLA; DE LERA, ANGEL R. *Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway*. *Organometallics* (2008), 27(14), 3378–

3389. CODEN: ORGND7 ISSN: 0276-7333. CAN 149:128960 AN 2008:662319

BELEN VAZ, RAQUEL PEREIRA, MARTIN PEREZ, ROSANA ALVAREZ, ANGEL R. DELERA. 2008. Stereoselective Stille Coupling of Enantiopure Haloallenes and Alkenylstannanes for the Synthesis of Allenyl Carotenoids. *Experimental and Computational Studies. Journal of Organic Chemistry*, 73 (17) 6541.

CARLOS SILVA LOPEZ, CARLOS PEREZ-BALADO, PAULA RODRIGUEZ-GRAÑA, ÁNGEL R. DE LERA. 2008. Mechanistic insights into the stereocontrolled synthesis of hexahydropyrrolo[2,3-b]indoles by electrophilic activation of tryptophan derivatives. *Organic Letters* 10 (1), pp. 77-80.

CARLOS SILVA LOPEZ, OLALLA NIETO FAZA, ANGEL R. DE LERA. 2008. Characterization of the switch in the mechanism of an intramolecular Diels-Alder reaction. *Journal of Organic Chemistry* 73 (2), pp. 467-473.

CARLOS SILVA LOPEZ, ROSANA ALVAREZ, MARTA DOMINGUEZ, OLALLA NIETO FAZA, ANGEL R. DE LERA. 2009. Complex Thermal Behaviour of 11-cis-Retinal, the Ligand of the Visual Pigments. *J. Org. Chem.*, 74 (3), pp 1007-1013

J.R. FLORES, A.B. GONZALEZ. 2008. The role of the excited electronic status on the C++H₂O reaction. *Journal of Chemical Physics*, 128, 144310.

J.R. FLORES. 2008. New benchmarks of the second-order correlation energies of Ne and Ar through the finite element method. *International Journal of Quantum Chemistry*, 108, 2172.

KEN S. FELDMAN, D. KEITH HESTER II, CARLOS SILVA LOPEZ, OLALLA NIETO FAZA. 2008. Allenyl azide cycloaddition chemistry. Photochemical initiation and CuI mediation leads to improved regioselectivity. *Organic Letters* 10 (8), pp. 1665-1668.

KEN S. FELDMAN, MALLIGA R. IYER, CARLOS SILVA LOPEZ, OLALLA NIETO FAZA. 2008. Allenyl azide cycloaddition chemistry: Exploration of the scope and mechanism of cyclopent-

tennelated dihydropyrrole synthesis through azatrimethylenemethane intermediates. *Journal of Organic Chemistry* 73 (13), pp. 5090-5099.

KEN S. FELDMAN, MALLIGA R. IYER, CARLOS SILVA LOPEZ, OLALLA NIETO FAZA. 2008. Allenyl Azide Cycloaddition Chemistry: Exploration of the Scope and Mechanism of Cyclopentennelated Dihydropyrrole Synthesis through Azatrimethylenemethane Intermediates. *Journal Org. Chem.* 73 (13), pp 5090-5099

L. ESTEVEZ, R.A. MOSQUERA. 2008. Where is the positive charge of flavylum cations? *Chemical Physics Letters*, 451 (1-3), pp. 121-126

L. ESTEVEZ, R.A. MOSQUERA. 2008. Molecular structure and antioxidant properties of delphinidin. *The Journal of Physical Chemistry A* 112 (42), pp. 10614-10623

L. LANDESA, J.M. TABOADA, F. OBELLEIRO, J.L. RODRIGUEZ, C. MOURIÑO, A. GOMEZ. Solution of very large integral-equation problems with single level FMM. *Microwave and Optical Technology Letters*.

M. M. PIÑEIRO, C. A. CERDEIRINA, M. MEDEIROS. 2008. Thermodynamic response functions of fluids: A microscopic approach based on NpT Monte Carlo. *Journal of Chemical Physics*. 129 (1), 014511/1, 014511/10.

M. N. LORENZO, J.J. TABOADA, I. IGLESIAS, I. ALVAREZ. 2008. The role of stochastic forcing on the behavior of Thermohaline circulation. *Annals of the New York Academy of Sciences*. ISBN: 1-57331-732-2 doi: 10.1196/annals.1446.002. Volume: 1146. Pages: 60-86.

MARCOS MANDADO, ANA M. GRAÑA, IGNACIO PEREZ-JUSTE. 2008. Aromaticity in spin-polarized systems: Can rings be simultaneously alpha aromatic and beta antiaromatic? *The Journal of Chemical Physics*. 129 164114.

MARCOS MANDADO, JOSE M. HERMIDA-RAMON, CARLOS M. ESTEVEZ. 2008. Molecular tweezers as receptors for anio-

ns: An energetic and topological study. *Journal of Molecular Structure: THEOCHEM* 854, 1–9.

NAHOUM, VIRGINIE; LIPSKI, ALEXANDRA; QUILLARD, FABIEN; GUICHOU, JEAN-FRANCOIS; BOUBKIK, YVAN; PEREZ, EFREN; GERMAIN, PIERRE; DE LERA, ANGEL R.; BOURGUET, WILLIAM. 2008. Nuclear receptor ligand-binding domains: reduction of helix H12 dynamics to favour crystallization. *Acta Crystallographica, Section F: Structural Biology and Crystallization Communications*, F64(7), 614-616. CODEN: ACSFCL ISSN: 1744-3091. AN 2008:821065

NAHOUM, VIRGINIE; PEREZ, EFREN; GERMAIN, PIERRE; RODRIGUEZ-BARRIOS, FATIMA; MANZO, FABIO; KAMMERER, SABRINA; LEMAIRE, GERALDINE; HIRSCH, OLIVER; ROYER, CATHERINE A.; Gronemeyer, Hinrich; de Lera, Angel R.; Bourguet, William. 2007. 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. CODEN: PNASA6 ISSN: 0027-8424. CAN 148:161787 AN 2007:1285460

O. NIETO FAZA, C. SILVA LOPEZ, A.B. GONZALEZ PEREZ, M. PEREZ RODRIGUEZ, Á. RODRIGUEZ DE LERA. 27 Oct 2008. Torquoselectivity in the electrocyclic ring-opening of cyclopropyl anions. *Journal of Physical Organic Chemistry Published Online*.

O. NIETO FAZA, C. SILVA LÓPEZ, A. B. GONZALEZ PEREZ, M. PEREZ RODRIGUEZ, Á. RODRIGUEZ DE LERA. 2008. Torquoselectivity in the electrocyclic ring-opening of cyclopropyl anions. *Journal of Physical Organic Chemistry* 999. 1099-1395 PN: 0894-3230

OLALLA NIETO FAZA, CARLOS SILVA LOPEZ, ADAN B. GONZALEZ PEREZ, MARTIN PEREZ RODRIGUEZ, ANGEL RODRIGUEZ DE LERA. 2008. Torquoselectivity in the electrocyclic ring-opening of cyclopropyl anions. *Journal of Physical Organic Chemistry* (DOI 10.1002/poc.1455)

P. LENAIN, M. MANDADO, R.A MOSQUERA, P. BULTINCK. 2008. Interplay between hydrogen bond formation and mul-

ticenter n-electron derealization: Intermodular hydrogen bonds. *The Journal of Physical Chemistry A* 112 (34), pp. 7898-7904

P. LENAIN, M. MANDADO, R.A MOSQUERA, P. BULTINCK. 2008. Interplay between hydrogen-bond formation and multicenter n-electron delocalization: Intramolecular hydrogen bonds. *The Journal of Physical Chemistry A* 112, (42), pp. 10689-10696.

ROSANA ALVAREZ, MARTIN PEREZ, OLALLA NIETO FAZA, ANGEL R. DE LERA. 2008. Associative Transmetalation in the Stille Cross-Coupling Reaction to Form Dienes: Theoretical Insights into the Open Pathway. *Organometallics*, 27 (14), pp 3378–3389

ROSANA ALVAREZ, MARTIN PEREZ, OLALLA NIETO FAZA, ANGEL R. DE LERA. 2008. Associative Transmetalation in the Stille Cross-Coupling Reaction Form Dienes: Theoretical Insights into the Open Pathway. *Organometallics*, 27, 3378.

VAZ, BELEN; PEREIRA, RAQUEL; PEREZ, MARTIN; ALVAREZ, ROSANA; DE LERA, ANGEL R. 2008. Stereoselective Stille Coupling of Enantiopure Haloallenes and Alkenylstannanes for the Synthesis of Allenyl Carotenoids. *Experimental and Computational Studies. Journal of Organic Chemistry*, 73(17), 6534-6541. CODEN: JOCEAH ISSN: 0022-3263. CAN 149:332487 AN 2008:939256

VAZ, BELEN; PEREIRA, RAQUEL; PEREZ, MARTIN; ALVAREZ, ROSANA; DE LERA, ANGEL R. 2008. Stereoselective Stille Coupling of Enantiopure Haloallenes and Alkenylstannanes for the Synthesis of Allenyl Carotenoids. *Experimental and Computational Studies. Journal of Organic Chemistry*, 73(17), 6534-6541. CODEN: JOCEAH ISSN: 0022-3263. CAN 149:332487 AN 2008:939256 CAPLUS

YAN XUGUANG; PEREZ, EFREN; LEID, MARK; SCHIMERLIK, MICHAEL I.; DE LERA, ANGEL R.; Deinzer, Max L. 2007. Deuterium exchange and mass spectrometry reveal the interaction differences of two synthetic modulators of RXR.alpha. LBD. *Protein Science*, 16(11), 2491-2501. CODEN: PRCIEI ISSN: 0961-8368. CAN 148:92225 AN 2007:1283971

M.N. LORENZO, J.J. TABOADA, I. IGLESIAS, I. ALVAREZ. 2008. The role of stochastic forcing on the behaviour of the Thermohaline circulation. *Annals of the New York Academy of Sciences*. Volume 1146, Issue 1, 60-86, Trends and Directions in Climate Research.

Scientific Articles In-Press

MARTIN PEREZ-RODRIGUEZ, ATAUALPA A. C. BRAGA, MAX GARCIA-MELCHOR, MONICA H. PÉREZ-TEMPRANO, JUAN A. CASARES, GREGORI UJAQUE, ANGEL R. DE LERA, ROSANA ALVAREZ, FELIU MASERAS, PABLO ESPINET. 2008. C-C Reductive Elimination in Palladium Complexes, and the Role of Coupling Additives. A DFT Study Supported by Experiment. *Journal of the American Chemical Society*.

Presentations at Congresses/Conferences

EFFECTS OF CLIMATE CHANGE ON THE WORLDS OCEANS INTERNATIONAL SYMPOSIUM.

M.N. Gijón, (Spain. May 2008).

LORENZO I. IGLESIAS, J.J. TABOADA. Influence of colored noise in the ocean coupling on the thermohaline circulation.

18th EUROPEAN CONFERENCE ON THERMOPHYSICAL PROPERTIES, ECTP.

Pau, France, 31st August to 4th September, 2008.

AURIANE KNORST-FOURAN, THOMAS LAFITTE, BRUNO MENDOBOURE, CHRISTELLE MIQUEU, D. BESSIÈRES, J. M. MÍGUEZ, MANUEL M. PIÑEIRO. Interfacial properties of methane confined in a slit pore: comparison of Monte Carlo simulation and a Gradient Theory - SAFTVR approach.

19th IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela, (Spain). 13-18th July, 2008.

OLALLA NIETO FAZA, ADAN GONZALEZ PEREZ, MARTIN PEREZ RODRIGUEZ, CARLOS SILVA LOPEZ, ANGEL R. DE LERA. Torquoselectivity in the electrocyclic ring-opening of cyclopropyl anions.

INTERNATIONAL CONFERENCE ON ELECTROMAGNETICS IN ADVANCE APPLICATIONS.

Torino, (Italy) 2007.

A. BERMUDEZ, C. LOPEZ, R. RODRIGUEZ, P. SALGADO. A finite element method for the eddy current problem in terms of the current density. Application to nondestructive testing. ICEAA'07. pp. 277-280, ISBN 1-4244-0767-2.

PROCEEDINGS OF IBERGRID 2008.

Oporto (Portugal), 12-14th May, 2008.

J.C. MOURIÑO, A. GOMEZ, L. LANDESA, J. M. TABOADA, F. OBELLEIRO, J. L. RODRIGUEZ. High Performance Computing Electromagnetics Challenge: solving tens of millions of unknowns.

VI ENCUESTRO IBERICO DE ELECTROMAGNETISMO COMPUTACIONAL.

Chiclana de la Frontera, Cádiz, (Spain). 21st October 2008.

L. LANDESA, J.M. TABOADA, F. OBELLEIRO, J.L. RODRIGUEZ, J.C. MOURIÑO, A. GÓMEZ. Fast Multipole Method in Supercomputers.

XIX IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain), 2008.

R. A. MOSQUERA, A. VILA, A.M. GRAÑA. On the Shortcomings of the Stereoelectronic Interpretation of the Anomeric Effect.

XXIII SIMPOSIUM NACIONAL DE LA UNION CIENTIFICA INTERNACIONAL DE RADIO (URSI 2008), Madrid, (Spain).

22-24th September, 2008.

L. LANDESA, J.M. TABOADA, F. OBELLEIRO, J.L. RODRIGUEZ, J.C. MOURIÑO, A. GOMEZ. FMM en problemas electromagnéticos con decenas de millones de incógnitas.

Posters at Congresses/Conferences

7th LIQUID MATTER CONFERENCE.

Lund, (Sweden) 27th June-1st July, 2008.

MANUEL M. PIÑEIRO, AMPARO GALINDO, ANDREW PARRY. Surface ordering and capillary phenomena of confined hard cut sphere particles.

- XV CONGRESO DE FISICA ESTADISTICA, FISES.
Salamanca, (Spain). 27-29th March, 2008.
MANUEL M. PIÑEIRO, G. S. DE FERRON, J. M. MIGUEZ, D. BESSIÉRES, F. PLANTIERr, J. L. LEGIDO. "Determinación de propiedades derivadas segundas de alcanos de cadena larga mediante Monte Carlo NPT".
- XV CONGRESO DE FISICA ESTADISTICA FISES.
Salamanca, (Spain). 27-29th March, 2008.
A. DOPAZO-PAZ, P. GOMEZ-ALVAREZ, L. ROMANI, D. GONZALEZ-SALGADO. Simulación de Montecarlo del sistema {Metanol + Agua}: Propiedades Termodinámicas.
- XV CONGRESO DE FISICA ESTADISTICA FISES.
Salamanca, (Spain). 27-29th March, 2008.
P. GOMEZ-ALVAREZ, A. DOPAZO-PAZ, L. ROMANI, D. GONZALEZ-SALGADO. Simulación de Montecarlo del Sistema {METANOL + AGUA}: Estructura.
- 6th CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS - ESPA 2008.
Palma de Mallorca (Spain), 2008.
A.M. GRAÑA, A. VILA, R.A. MOSQUERA. QTAIM analysis on the genesis of the anomeric effect involving sulfur and phosphorus.
- 6th CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS - ESPA 2008.
Palma de Mallorca (Spain) 2008.
L. ESTEVEZ, N. OTERO, A.M. GRAÑA, R.A. MOSQUERA. Structural Trends in Anthocyanidins.
- 6th CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS - ESPA 2008.
Palma de Mallorca (Spain) 2008.
N. OTERO, L. ESTEVEZ, M. MANDADO, R.A. MOSQUERA. An electron density study on porphin and its series of hydrogenated derivatives.
- 7th LIQUID MATTER CONFERENCE.
Lund, (Sweden) 27th June-1st July 2008.
AURIANE KNORST-FOURAN, THOMAS LAFITTE, BRUNO MENDOBOURE, CHRISTELLE MIQUEU, D. BESSIÉRES, J. M. MÍGUEZ, MANUEL M. PIÑEIRO. "Determination of on interfacial properties of confined methane: Comparison of Monte Carlo simulation and the gradient theory coupled with SAFT VR results.
- EGU.
Viena 2008.
M. N. LORENZO, J. J. TABOADA, I. IGLESIAS. Influence of the stochastic sources in climate models. ISSN 1029-7006 EUROPEAN METEOROLOGICAL SOCIETY 7th EMS. El Escorial, (Spain) 2007. M. N. LORENZO, J. J. TABOADA, I. IGLESIAS. Thermohaline circulation as an example of nonlinear-processes in the climate system. ISSN 1812-7053
- WATOC 2008.
Sydney. (Australia). 14-19th September, 2008.
CARLOS SILVA LOPEZ, ROSANA ALVAREZ RODRIGUEZ, MARTA DOMINGUEZ SEOANE, OLALLA NIETO FAZA, ANGEL R. DE LERA Thermal Isomerization of 11-cis-Retinal. An Unexpected Manifold.
- WATOC 2008.
Sydney, (Australia). September 14-19th 2008.
OLALLA NIETO FAZA, ADAN GONZALEZ PEREZ, CARLOS SILVA LOPEZ, ANGEL R. DE LERA. Complexity under Control: A Theoretical Mechanistic Study of Gold and Platinum Catalyzed Rearrangements.
- XIX IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.
Santiago de Compostela (Spain) 2008.
J.L. LÓPEZ, R. A. MOSQUERA, A.M. GRAÑA. Electron density analysis on the protonation of nitriles.
- XIX IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.
Santiago de Compostela (Spain) 2008.
L. ESTEVEZ, N. OTERO, R. A. MOSQUERA. Which is the Most Powerful Form of Anthocyanidins to Scavenge DPPH-Radical?

XIX IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 2008.

L. PITA, A.M. GRAÑA, R.A. MOSQUERA. Topological electron density analysis on activating and deactivating effects in pyridine rings.

XIX IUPAC CONFERENCE ON PHYSICAL ORGANIC CHEMISTRY.

Santiago de Compostela (Spain) 2008.

N. OTERO, L. ESTEVEZ, M. MANDADO, R. A. MOSQUERA. An Electron Density Based Study on the Chemistry of 1,3-Azoles. XV CONGRESO DE FISICA ESTADISTICA.

Universidad de Salamanca, (Spain), 2008.

A. DOPAZO-PAZ, P. GÓMEZ-ÁLVAREZ, L. ROMANÍ, D. GONZÁLEZ-SALGADO. "Simulación de Monte Carlo del sistema {metanol+agua}: Propiedades termodinámicas".

XV CONGRESO DE FISICA ESTADISTICA.

Universidad de Salamanca 2008.

P. GÓMEZ-ÁLVAREZ, A. DOPAZO-PAZ, L. ROMANÍ, D. GONZÁLEZ-SALGADO. "Simulación de Monte Carlo del sistema {metanol+agua}: Estructura".

XXIV INTERNATIONAL CONFERENCE ON POLYPHENOLS.

Salamanca (Spain), 2008.

L. ESTÉVEZ, N. OTERO, R. A. MOSQUERA. A Computational Study on the Molecular Structure of Delphinidin.

EGU GENERAL ASSEMBLY.

Vienna, (Austria). 13-18th April 2008.

M.N. LORENZO, J.J. TABOADA, I. IGLESIAS. Influence of the stochastic sources in climate models.

Graduate Thesis and Final Projects

ANA MARIA DOPAZO PAZ.

"Análisis de un Potencial Intermolecular para el sistema {agua + metanol}".

Universidad de Vigo, (Spain), 22nd December, 2008.

Director: Diego González Salgado, Universidad de Vigo.

Books and Book Chapters Published

J.R. FLORES. 2008. Further quasi-classical trajectory studies on the C++ H₂O reaction. Molecular Simulation. DOI. 10.1080/08927020802430760.

K. KANKOWSKI, R. SLUPSKI, J.R. FLORES. 2008. Asymptotic behaviour of MP2 correlation energies for closed-shell atoms. Advances in Quantum Chemistry, 53, 151-175 (Chapter 9).

SERVICIO GALEGO DE SAÚDE (SERGAS) GALICIAN HEALTH SERVICE



Scientific Articles Published

MARTINEZ, A; GUTIERREZ-DE-TERAN, H; BREA, J. 2008. Synthesis, adenosine receptor binding and 3D-QSAR of 4-substituted 2-(2-furyl)-1,2,4-triazolo[1,5-a]quinoxalines. Bioorganic & Medicinal Chemistry, 16: 2103-2113.

Presentations at Congresses and Conferences

VIII JORNADAS NACIONALES DE BIOINFORMATICA.

Valencia, (Spain) 13-15th February 2008.

GUTIERREZ-DE-TERÁN, H.; ORRLING, K.; DUNN, B.M.; AQVIST J. Investigating Promiscuous Inhibition of Proteases by Computational Methods.

Posters at Congresses and Conferences

EURO QSAR 2008.

Uppsala, 21-26 September 2008.

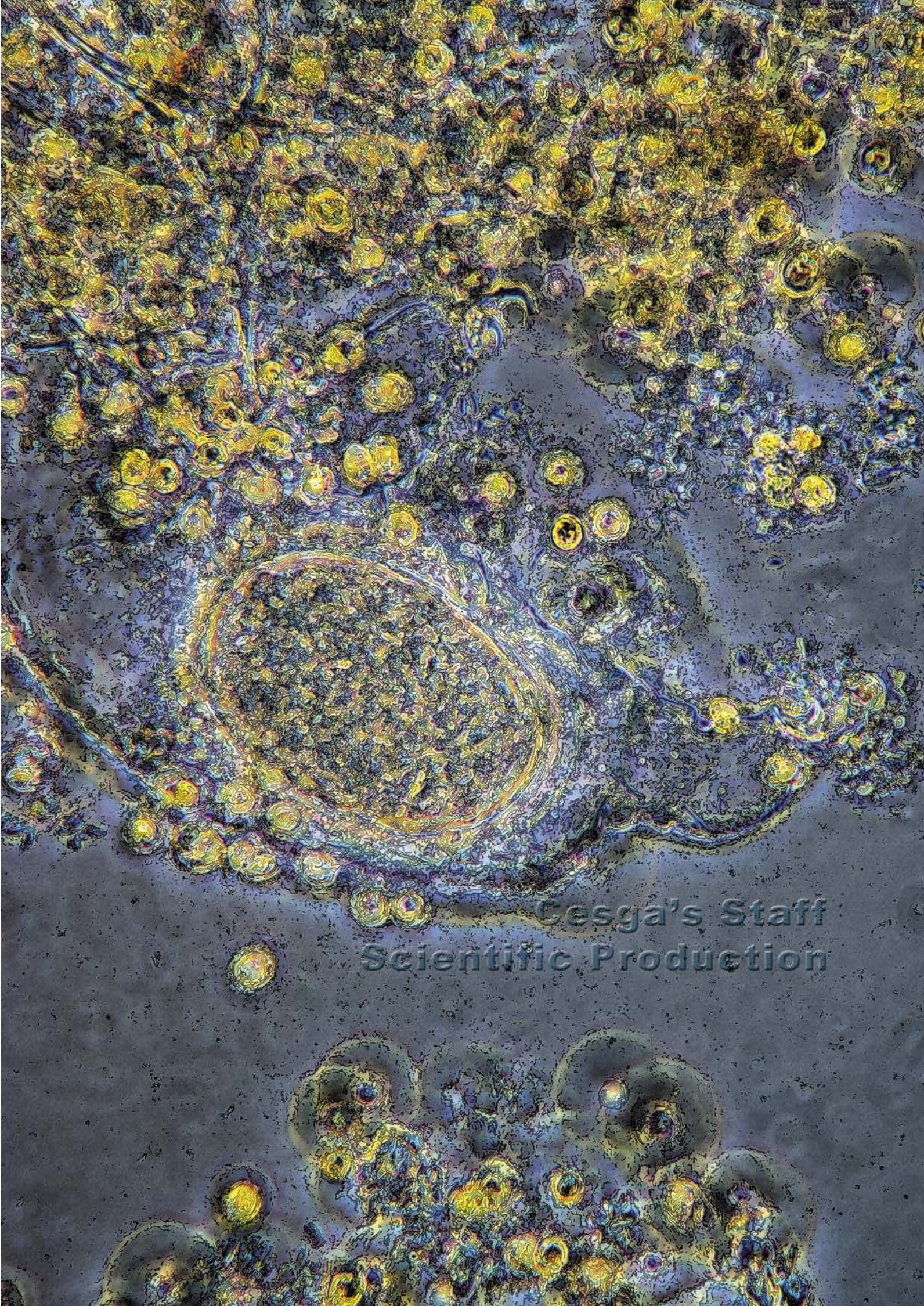
GUTIERREZ-DE-TERAN, H; AREIAS, F; RODRIGUEZ, D.; BREA, J.; PROENCA, M.F.; LOZA, M.I.: Identification of novel scaffolds from an original chemical library as potential antipsychotics.

MEMORIAL ANGEL R. ORTIZ ASSOCIATED TO JORNADAS DE BIOINFORMATICA.

To be held in Madrid, January 2009.

DAVID RODRIGUEZ, HUGO GUTIERREZ-DE-TERAN.

Adenosine Receptors: A Systematic Study of Ligand Binding Based on the Crystal Structure of Haza Receptor.



Cesga's Staff
Scientific Production

scientific production -CESGA staff- 2008

SCIENTIFIC ARTICLES IN NON SCI JOURNALS

- MARCO J, et al. 2008. The Interactive European Grid: Project objectives and achievements. *Computing and informatics*, vol.27. 2:161-171.
- GOMES J, et al. 2008. A grid infrastructure for parallel and interactive applications. *Computing and informatics*, vol.27. 2: 173-185.
- E BENDITO, A CARMONA, A.M. ENCINAS, JM GESTO, A GOMEZ, C. MOURIÑO, T. SANCHEZ. Computational cost of the Fekete problem I: the Forces Method on the 2-sphere, accepted by the *Journal of Computational Physics*.

BOOKS

- BARRA C, et al. 2008. *E-Learning for Adult Patients in Hospitals. Experiences-Challenges-Recommendations (English Edition)*, Vienna, die Berater. 48 pages.
- BARRA C, et al. *E-Learning para pacientes adultos hospitalizados. Experiencias - Retos – Recomendaciones (Spanish Edition)*, Vienna, die Berater. 48 pages.
- BARRA C, et al. *e-Hospital: Experiences with E-Learning Activities for Patients (English Edition)*, Vienna, die Berater. 152 pages.
- BARRA C, et al. *e-hospital: E-Learning para pacientes hospitalizados (Spanish Edition)*, Vienna, die Berater. 156 pages.

BOOK CHAPTERS

LÓPEZ-CABIDO, I. 2008. A computación do século XXI. In: *Dos ábacos aos computadores*. (M Bermejo Patiño, ed.), pp. 119-134. The University of Santiago de Compostela Press, Santiago de Compostela, Spain.

PARTICIPATION IN NATIONAL AND INTERNATIONAL CONFERENCES

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Porto (Portugal), May 12-14, 2008

SÁNCHEZ M T, CAO R, FERNÁNDEZ J, GARCÍA-MAGARIÑOS M, GARCÍA-TORRE F, GESTO JM, GÓMEZ A, GONZÁLEZ-MANTEIGAW, GUTIÉRREZ JM.

imath.cesga.es, the VO for European mathematicians. Oral presentation.

SECOND INTERNATIONAL CONFERENCE ON MOBILE UBIQUITOUS COMPUTING, SYSTEMS, SERVICES, AND TECHNOLOGIES

Valencia (Spain), September 29, 2008 – October 4, 2008

COTELO QUEIJO CARMEN; GÓMEZ TATO, ANDRÉS; LÓPEZ CABIDO, IGNACIO; COTOS YAÑEZ, JOSÉ MANUEL.

Adapting ROMS to Execute on GRID Using a Hybrid Parallelization Model. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Porto (Portugal), May 12-14, 2008

DAVID MERA, JOSÉ M. COTOS, PEDRO SACO, ANDRÉS GÓMEZ.

An integrated solution to the Secure User Access in the RETELAB Grid Project using a Web System based on Portlets and a RBAC Model by means of User Attribute Certificates and PKI. Oral presentation.

I JORNADA GALLEGA DE BIOINFORMÁTICA.

A Coruña (Spain), April 4, 2008

AURELIO RODRÍGUEZ.

CESGA and FINISTERRAE, a Bioinformatics Computing infrastructure. Oral presentation.

II ENCUENTRO EN COMPUTACIÓN DE ALTO RENDIMIENTO EN SIMULACIONES MOLECULARES

Madrid (Spain,) June 17, 2008

AURELIO RODRÍGUEZ.

Servicios del CESGA a la Comunidad Científica del CSIC. Oral presentation.

IBERGRID 2008 2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Porto (Portugal) May 12-14, 2008.

LINO GARCÍA TARRÉS, CÉSAR VEIGA, DAVID CORDERO PLACER, CARLOS FERNÁNDEZ SÁNCHEZ, PABLO REY MAYO, JAVIER LOPEZ CACHEIRO, IGNACIO LÓPEZ.

Accounting and Monitoring of Parallel and Interactive jobs in the Grid. Oral presentation.

XIX JORNADAS DE PARALELISMO

Castellón (Spain) May 17-19, 2008

C. TEIJEIRO, G.L. TABOADA, J. TOURIÑO, B.B. FRAGUELA, R. DOALLO, J.C. MOURIÑO, A. GÓMEZ-TATO, I. LÓPEZ-CABIDO.

Evaluación del Rendimiento de las Comunicaciones Colectivas en UPC. Oral presentation.

XIX JORNADAS DE PARALELISMO

Castellón (Spain) May 17-19, 2008

MARTA LOUREIRO, GABRIEL RODRÍGUEZ, PATRICIA GONZÁLEZ, MARÍA J. MARTÍN, J. CARLOS MOURIÑO, MARÍA TERESA SÁNCHEZ.

Tolerancia a fallos en aplicaciones reales utilizando CPPC. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Porto (Portugal) May 12-14, 2008

LUIS LANDESA PORRAS, JOSÉ MANUEL TABOADA VARELA, FERNANDO OBELLEIRO BASTEIRO, JOSÉ LUIS RODRÍGUEZ, JOSÉ CARLOS MOURIÑO, ANDRÉS GÓMEZ TATO. High Performance Computing Electromagnetic Challenge: Solving tens of millions of unknowns. Oral presentation.

XXIII SIMPOSIUM NACIONAL DE LA UNIÓN CIENTÍFICA DE RADIO

Madrid (Spain) September 22-24, 2008

L LANDESA, J M TABOADA, F OBELLEIRO, J L RODRÍGUEZ, J MOURIÑO A GÓMEZ. FMM en problemas electromagnéticos con decenas de millones de incógnitas. Oral presentation.

VI IBERIAN MEETING ON COMPUTATIONAL ELECTROMAGNETICS

Chiclana (Spain) October 22-24, 2008

L LANDESA, J M TABOADA, F OBELLEIRO, J L RODRÍGUEZ, J MOURIÑO, A GÓMEZ. Fast Multipole Methods in Supercomputers. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Oporto (Portugal) May 12, 2008

G BORGES, M DAVID, J GOMES, J P MARTINS, M MONTECELO, N DIAS, J LÓPEZ, A SIMÓN, E GARCÍA. Resource integration in gLite based grid infrastructures. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Oporto (Portugal) May 12, 2008

E FREIRE, A SIMON, J LÓPEZ, C FERNÁNDEZ, A RETICO, AND N THACKRAY.

EGEE Pre-Production service: A distributed testing cluster. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Oporto (Portugal) May 12, 2008

C VEIGA, C FERNÁNDEZ, L GARCÍA, D CORDERO, J LÓPEZ. Accounting and Monitoring of Parallel and Interactive Jobs in the Grid. Oral presentation.

EGEE '08 CONFERENCE

Istanbul (Turkey) September 24, 2008

J LÓPEZ, E FREIRE, A SIMÓN AND A RETICO. The deployment test: How it is and how it should be. Oral presentation.

EGEE'08 CONFERENCE

Estambul (Turkey) September 25, 2008

PKUNSZT, J LÓPEZ, E FREIRE, A SIMÓN, S DÍAZ, C FERNÁNDEZ, ETAL.

Production sites best practices. Oral presentation.

JORNADAS TÉCNICAS DE RedIRIS

Madrid (Spain) August 21, 2008

C F IGLESIAS. Proyecto Formiga, Reaprovechando recursos para la investigación. Oral presentation.

ARM 11

Lyon (France) February 5-6, 2008

PABLO REY, JOHN GORDON. Accounting & Accounting Portal developments. Oral presentation.

GDB MEETING

Geneva (Switzerland) February 6, 2008

PABLO REY. Accounting in EGEE/WLCG. Oral presentation.

COD-15

Lyon (France) February 6-8, 2008

PABLO REY. Accounting Portal. Oral presentation.

HP-CAST 10

Singapur. May 19-22, 2008

CARLOS FERNÁNDEZ. "Finis Terrae" (End of the Earth) Experiences with a Very Large Itanium Site in Production. Oral presentation.

CESGA-FINIS TERRAE COMPUTATIONAL SCIENCE CONFERENCE 2008

Santiago de Compostela (Spain) June 12, 2008

CARLOS FERNÁNDEZ. Using Finis Terrae. Oral presentation.

GRID OPEN DAY

Poznan (Poland) April 25, 2008

LINO GARCÍA. e-IMRT. Oral presentation.

EELA2 KoM

Trujillo (Spain) April 23, 2008

JAVIER LÓPEZ. CESGA. Oral presentation.

EGEE'08 SA3 ALL HANDS MEETING

Prague (Czech Republic) March 11, 2008

E FREIRE, A SIMON, J LÓPEZ. CESGA-SA3 Status Report. Oral presentation.

EGEE'08 USER FORUM 3

Clermont Ferrand (France) February 11, 2008

E FREIRE, A SIMON, J LÓPEZ, C FERNÁNDEZ, A RETICO, N THACKRAY. Advantages of Pre-Production WLCG/EGEE services for VOs and Users. Oral presentation.

EGEE'08 SA3 ALL HANDS MEETING

Cern (Switzerland) May 12, 2008

E FREIRE, A SIMON, J LÓPEZ. CESGA-SA3 Status Report. Oral presentation.

2ND IBERIAN GRID INFRASTRUCTURE CONFERENCE

Oporto (Portugal) May 12, 2008

S DIAZ, S REYES, A NIÑO AND C MUÑOZ-CARO. A General Approach to the Analysis and Design of Grid Portals for Scientific Virtual Organizations. Oral presentation.

EGEE'08 CONFERENCE

Istanbul (Turkey) September 22-26, 2008

S.DIAZ, P.REY, J.LOPEZ, C.FERNÁNDEZ, J. GORDON, C. DEL-CANO. Intra-VO and individual user accounting in EGEE. Demonstration.

VECPAR'08

Toulouse (France) June 24-27, 2008

L. GARCÍA, E. GUARDIA, J. CASURELLAS. The Impact of Virtualization on Grid Parallel Molecular Dynamics Simulations. Oral presentation.

EDUTEC 08

Santiago de Compostela (Spain) September 1-5, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS. T-Learning: e-learning al alcance de todos. Oral presentation.

EDUTEC 08

Santiago de Compostela (Spain) September 1-5, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS. Formación, adultos hospitalizados y tecnologías: el e-learning necesario. Oral presentation.

EDUTEC 08

Santiago de Compostela (Spain) September 1-5, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS.

Proyecto EFELCREN: Ejemplos de buenas prácticas de materiales de e-learning. Oral presentation.

EDUTEC 08

Santiago de Compostela (Spain) September 1-5, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS.

Proyecto e-Hospital: formación de pacientes adultos hospitalizados. Oral presentation.

EDUTEC 08

Santiago de Compostela (Spain) September 1-5, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS.

Las TIC como apoyo para la intervención indirecta en la calidad de vida familiar de las personas con diversidad funcional. Oral presentation.

V CONGRESO INTERNACIONAL DE PSICOLOGÍA Y EDUCACIÓN: LOS RETOS DEL FUTURO

Oviedo (Spain) April 23-25, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS.

La atención familiar en la búsqueda de apoyos y calidad de vida a través de las TIC en las personas con diversidad funcional. Oral presentation.

V CONGRESO INTERNACIONAL DE PSICOLOGÍA Y EDUCACIÓN: LOS RETOS DEL FUTURO

Oviedo (Spain) April 23-25, 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS. Software libre al servicio de las personas con diversidad funcional. Oral presentation.

CONGRESO NACIONAL INTERNET EN EL AULA. LA IMPORTANCIA DE LAS TIC EN LAS AULAS.

Virtual Conference January 2004-October 2008

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS. Diversidad Funcional y Tecnologías de la Información y Comunicación. Oral presentation.

REPORTS

AURELIO RODRÍGUEZ, MARIO VALLE, UGO VARETTO

Quantum Chemistry common data format Q5COST and OpenBabel: A first answer to interoperability in Quantum Chemistry. 31 pages. Technical report, CESGA.

SERGIO BERNARDI (CINECA), CLAUDIO CACCIARI (CINECA), FRANCESCO D'ANDRIA (ATOS), ROBERTO D'IPPOLITO (LMS), HENNING EICKENBUSCH (ANSYS), NAJI EL MASRI (LMS), ANDRÉS GÓMEZ (CESGA), BJÖRN HAGEMEIERS (FZJ), JIADAO LI (FZJ), DANIEL MALLMANN (FZJ), JOSEP MATRAT SOTIL (ATOS), JOSE CARLOS MOURIÑO GALLEGU (CESGA), ANGELA RUMPL (SCAI), EBERHARD SEKLER (INTES), CHRISTIAN SIMMENDINGER (T-SYSTEMS), DEVARAJAN SUBRAMANIAN

(GRIDCORE), WOLFGANG ZIEGLER (SCAI), CSILLA ZSIGRI (451 GROUP)

SmartLM Deliverable D1.1: Functional requirements of the new licensing architecture for Grids. 102 pages. Deliverable (technical document).

THESES and SIMILAR DOCUMENTS:

MASTER DEGREE TRAINING

JOSÉ ANTONIO LÓPEZ LÓPEZ

Aspectos Médico-Biológicos y Físicos de la Radioterapia como Tratamiento del Cáncer. Modelo Determinista para el Cálculo de la Dosis Absorbida.

University of Santiago de Compostela, July 17, 2008

Directors: Óscar López Pouso (USC), Andrés Gómez Tato (CESGA), María González Taboada (UDC)

DAMIÁN ÁLAVAREZ MALLÓN

Análisis Técnica de Rendimiento de Sistemas HPC

Universidad da Coruña, September 15, 2008.

Director: Andrés Gómez Tato

MASTER/DEA

SERGIO DÍAZ MONTES

Official Masters: Tecnologías Informáticas Avanzadas

UCLM, July 9, 2008.

Director: Camelia Muñoz Caro and Alfonso Niño Ramos

TEACHING

MASTER DEGREE PROFESSOR

CARLOS FERNÁNDEZ SÁNCHEZ

Master in Mathematical Engineering

USC, UDC, UVigo. February, 2008.

MANUEL GROMAZ CAMPOS

Master in e-learning,

UOC, 2008.

OTHER COURSES

AURELIO RODRÍGUEZ

Introduction to computational chemistry codes at CESGA (Gaussian, GAMESS, NWCHEM)
CESGA, Santiago de Compostela, December 15, 2008

JAVIER LÓPEZ CACHEIRO

GRID and e-Science
IFIC, July 17, 2008.

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS, BRUNO RUBIO GAYO, MIGUEL BERMEJO
An OpenOffice suite in Galician. Teaching and didactic uses.
Galician Regional Ministry of Education, 2008.

MARÍA JOSÉ RODRÍGUEZ MALMIERCA

MATHDI: Didactic Mathematics Database
Galician Regional Ministry of Education, 2008.

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS

Experto en eLearning: Tecnologías y Métodos de Formación en Red.
University of Salamanca, 2008.

MANUEL GROMAZ CAMPOS

Recursos multimedia para la enseñanza de idiomas
Centro de Formación y Recursos de Lugo, 2008.

MARÍA JOSÉ RODRÍGUEZ MALMIERCA Y MANUEL GROMAZ CAMPOS

Diseño de contenidos didácticos para sistemas de gestión del aprendizaje acorde a estándares internacionales a través de la utilización de herramientas de autor de software libre o gratuitas.
Centro de Formación y Recursos de Santiago, 2008.

SCIENTIFIC DISSEMINATION

Conference participation: COMPUTACIÓN GRID EN LA EMPRESA

ANDRÉS GÓMEZ TATO

The improvement of IMRT radiotherapy treatment planning using on demand GRID services. Parque Tecnológico de Álava-Miñano. September 2008.

Conference participation: CESGA-FINIS TERRAE COMPUTATIONAL SCIENCE CONFERENCE 2008

ANDRÉS GÓMEZ TATO

Finis Terrae: Tools and Applications
Santiago de Compostela (Spain), June 12, 2008.

Conference participation: CESGA-FINIS TERRAE COMPUTATIONAL SCIENCE CONFERENCE 2008

AURELIO RODRÍGUEZ

Finis Terrae Computing Challenges
Santiago de Compostela (Spain), June 12, 2008.

Conference participation: COMPUTACIÓN GRID EN LA EMPRESA

COMPUTACIÓN GRID EN LA EMPRESA

CARLOS FERNÁNDEZ SÁNCHEZ

CESGA: 10 years of Grid Services
Centro de Supercomputación de Galicia: 10 años de servicios Grid
Álava (Spain), September 16, 2008.

Conference participation: CESGA-FINIS TERRAE COMPUTATIONAL SCIENCE CONFERENCE 2008

JOSÉ IGNACIO LÓPEZ CABIDO

Finis Terrae Architecture
Santiago de Compostela (Spain), June 12, 2008.

Conference participation: IIR – TELEPRESENCE

NATALIA COSTAS LAGO

BEST PRACTICE-The practical experience of CESGA.
Collaboration tools for research and teaching environments.
Madrid (Spain). September 30, 2008.

Conference participation: IIR - DATACENTER 2008

JOSÉ IGNACIO LÓPEZ CABIDO

Adjusting CESGA's Data Centre for the housing of the Finis Terrae Supercomputer.

Madrid (Spain). November 18, 2008.

Conference organisation: EDUTEC 08

MARÍA JOSÉ RODRÍGUEZ MALMIERCA

MANUEL GROMAZ CAMPOS

EDUTEC 08

Santiago de Compostela (Spain), May 1, 2008.

Conference participation: INFORENSINO 2008

MANUEL GROMAZ CAMPOS

CESGA e-learning research and innovation projects.

Proyectos de investigación e innovación en el área de e-learning del CESGA.

Lugo (Spain), September 12-14, 2008.

Conference organisation: SPEDECE '08

V PLURIDISCIPLINARY SYMPOSIUM ON DESIGN AND EVALUATION OF REUSABLE EDUCATIONAL CONTENTS (SPEDECE '08)

MANUEL GROMAZ CAMPOS

Alcalá de Henares (Spain), October 20-21, 2008.

DISSEMINATION ARTICLES

AURELIO RODRÍGUEZ. 2008. MODULES: Configuración rápida do contorno dunha aplicación. Díxitos, Nov-08:12.

ANDRES GÓMEZ. 2008. Finis Terrae: Tools and Applications. Díxitos, Jul-08: 7.

ANDRÉS GÓMEZ, MARÍA TERESA SÁNCHEZ RÚA. 2008. Achegando as Matemáticas ao Grid. Díxitos, Feb-08:7.

JAVIER LÓPEZ CAHEIRO, AURELIO RODRÍGUEZ LÓPEZ. 2008. G-Fluxo: Un proxecto que simplificará o uso do Finis Terrae. Díxitos, Feb-08: 11.

MANUEL GROMAZ CAMPOS, MARÍA JOSÉ RODRÍGUEZ

MALMIERCA, MANOEL BAÑA CASTRO, BEATRIZ LÓPEZ GONZÁLEZ, JAVIER GARCÍA TOBÍO. 2008. Software libre y Diversidad Funcional. Quaderns Digitals, Feb-00:1-12.

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, MANUEL GROMAZ CAMPOS, CARMEN FERNÁNDEZ MORANTE, BEATRIZ CEBREIRO LÓPEZ, JAVIER GARCÍA TOBÍO. 2008.

E-learning para e-inclusión: el proyecto e-hospital. Quaderns Digitals, Feb-00:1-12.

AAVV. 2008. Observatorio gallego de e-learning: El estado del e-learning en la universidad gallega. Revista Galega de Educación, 41.

MANUEL GROMAZ CAMPOS, MARÍA JOSÉ RODRÍGUEZ MALMIERCA, JOSÉ MANUEL ABUÍN MOSQUERA, JAVIER GARCÍA TOBÍO. 2008. Formación continua mediante b-learning a profesionales de recursos humanos de las PYMES en Europa: El Proyecto YES. Quaderns Digitals, Feb-00: 1-13.

MANUEL GROMAZ CAMPOS, MARÍA JOSÉ RODRÍGUEZ MALMIERCA, JAVIER GARCÍA TOBÍO. 2008. Experiencias exitosas de e-learning en la universidad gallega. Pixel-Bit, 33: 173-182.

RESEARCH VISITS

MARTA GONZÁLEZ BUGUEIRO.

SLA Negotiation and GridWay Integration
Universidad Complutense de Madrid (Spain), 17 November 17-28, 2008.

AWARDS

Centro de Supercomputación de Galicia, CESGA Foundation
APPLUS+ Prize for Excellence in Quality Management.
APPLUS+
Santiago de Compostela (Spain), 2008.





GIS

geographic information systems (GIS)

The objective of the Department of Geographic Information Systems include conducting analysis and calculus projects in the area of GIS, working with and processing raster and vector geo-referenced information, alphanumeric data bases, conducting studies in the field that include analysis, programming, visualization, and diverse outputs (print, applications, intranet, Internet). In addition, this department is responsible for the promotion and support of the use of GIS technology in the research community.

Noteworthy Activity in 2008

Projects

GIS Tool for Environmental Risk Assessment in Agricultural and Industrial Sectors. During 2008 the development of the tool for the analysis of atmospheric contamination in the industrial sector was accomplished, integrating the models of atmospheric pollution and its geoprocessing in order to represent the elements affected by a given incident thereby providing the ability to perform simulations for the design of emergency plans.

Forest Industry Information System- SIFI Galicia. The programming of an application for data base management in the industrial lumber sector of Galicia was concluded and a map server was published on Internet.

Archaeological Patrimony 2008 – Government of Galicia. The information exploitation tasks that correspond to the inventory of archaeological goods from the province of A Coruña were performed as well as an analysis of the information collected from the document system of the government's archaeological service. Information derived by means of the analysis of existing data was produced.

TERRA. A map server of Galicia for the educational project TERRA that is to be a tool and a teaching resource in primary and secondary Galician educational centres was developed.

Participation in the Network of Geographic Information for Research in Galicia - REDIX. A survey was elaborated that concerned the utilisation of GIS by the local administration. Various proposals were developed regarding participation in different calls for research projects, national as well as European.

Dissemination Activities

Map Server of Surnames of Galicia. The map of Surnames that was developed by the University of Santiago Galician Language Institute (ILGA) on Internet was maintained operative.

Sueloempresarial.com. The web of industrial parks developed for the Consorcio Zona Franca of Vigo was maintained operative.

GIS Technology Days. Collaboration in the production of Technology Days for the dissemination of GIS technology.

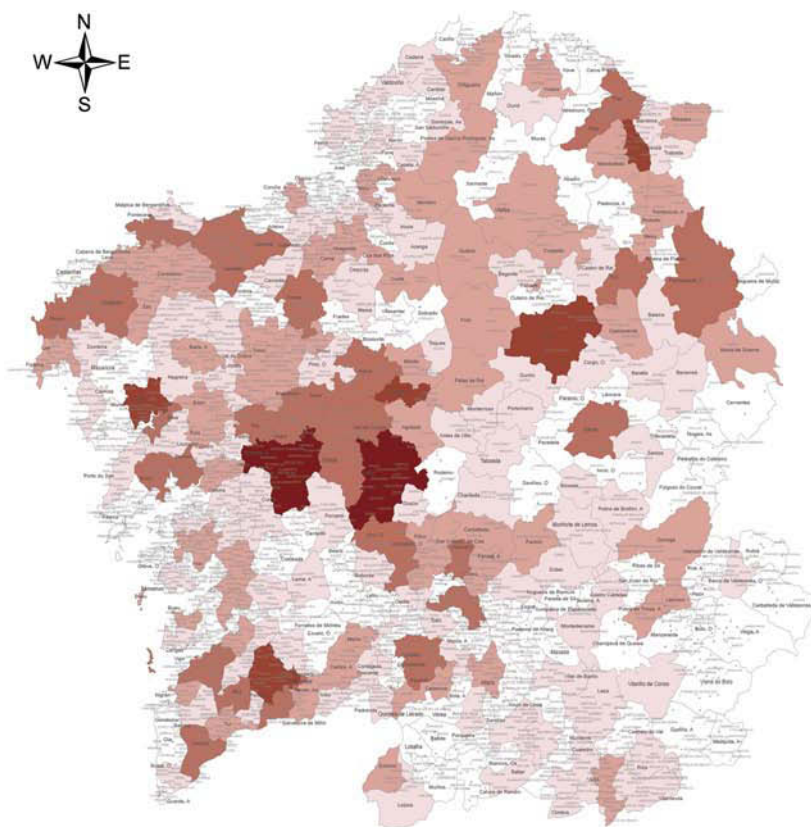
Training

Teacher Training course of the Regional Ministry of Education, "Opportunities posed by Networked Geographic Information Systems as a Learning Tool", 2008.

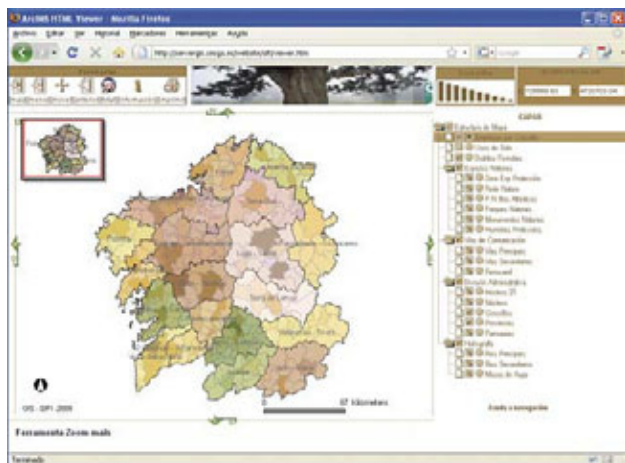
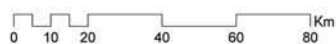
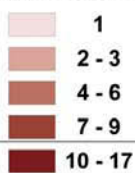
"I Course in Geographic Information Systems", celebrated from July 7 – 11, for the Galician Delegation of the Professional Association of Geographers.

"II Course in Geographic Information Systems", celebrated September 22-26, for the Galicia Delegation of the Professional Association of Geographers.

Empresas por Sector - Act. Serrado e Cepillado da Madeira



Nº de empresas por sector





A microscopic image of plant tissue, likely a cross-section of a stem or root, showing various cellular structures. The image is overlaid with the text "e-Learning & Collaboration Tools".

**e-Learning
& Collaboration Tools**

e-learning & collaboration tools

Objectives

- To conduct research in the area of e-learning in different environments.
- To promote and disseminate the use of ICT applied to learning processes.
- To promote of the integration of educational institutions in the Information Society.

e-Learning Technological Resources

- e-Learning on-line suite, asynchronous and collaborative (Aula CESGA).
- Audio and video streaming for training sessions.
- Professional videoconferencing equipment for training sessions and meetings in real time.
- e-Learning mailing list.
- On-line seminar tool (Webinar).
- Hardware for mobile learning and T-learning.
- Dynamic portal for e-learning information and management.

2008 Activity Highlights

- Collaboration in the planning, development, and evaluation of training activities for CESGA personnel and HPC users.
- Participation in the e-learning work group of the INES platform (Spanish Software and Services Technological Platform).
- Collaboration on the web page of the European Union: elearningeuropa.info

- Participation in the regional e-learning work group, PTAG (Galician Technological Platform of the Audiovisual Sector).
- Participation in the high-level work group concerning ethics and ICT, organised by the European Commission.
- Members of the Thematic Network of Learning Objects (REDAOPA) along with 18 other national institutions and universities.
- Collaboration with the Regional Ministry of Education on training activities for teachers such as the production of various e-learning courses concerning data bases for Didactic Mathematics (MATHDI-, MathEdu) and Open Office and its didactic use. Consulting activities in the field of new technologies applied to teaching and learning for teacher training in training centres, Galician universities, and primary and secondary education centres.
- Publication of 2 books and 7 articles in scientific journals. Participation in the organising committee of the EDUTEC'08 conference. Members of the scientific committee of the V Interdisciplinary Symposium on Design and Evaluation of Reusable Educational Contents (SPEDECE 08). Presentations at 10 conferences in the ICT and Education sectors.
- Analysis and implementation of an open source, on-line tool that permits virtual meetings and virtual seminars and is offered as a service to researchers.
- Design and development of a new Intranet for the area of e-learning.
- Participation in 9 e-learning projects during 2008, listed below.



E-Intervención: Analysis and impact of ICT utilisation in the attention to disabled persons and their families including quality of life and self-management. This is a project financed by the Director General for RTD&I of the Government of Galicia.

SUMA: The integration of e-learning services by means of standards. This concerns a national project financed by the Plan Avanza in collaboration with other private and public institutions.

E-Hospital: The evaluation of the use of e-learning with adult hospitalised patients is a project financed by the European Commission within the frame of the Socrates/Grundtvig I Program.

Efelcren: Flexible and Creative Educational Environments, EFELCREN, is a project financed by the European Commission within the frame of the Socrates / Comenius 2.1 Program.

Parents: e-learning training for parents as professional and vocational advisors of their children. Parents is a program financed by the European Commission.

Yes: e-learning training to support youth employment in SME. YES is a project financed by the European Commission.

ICTeacher: ICT skills for teachers. ICTeacher is a project financed by the European Commission within the frame of the Lifelong Learning program.

T-Maestro: An intelligent tutor that provides personalised training contents for television learning experiences (T-learning). This is a project financed by the Director General for RTD&I of the Government of Galicia.

E-Procura:

e-Procura is a system that permits searches for personalised courses using semantic technologies and is financed by the Director General for RTD&I of the Government of Galicia.



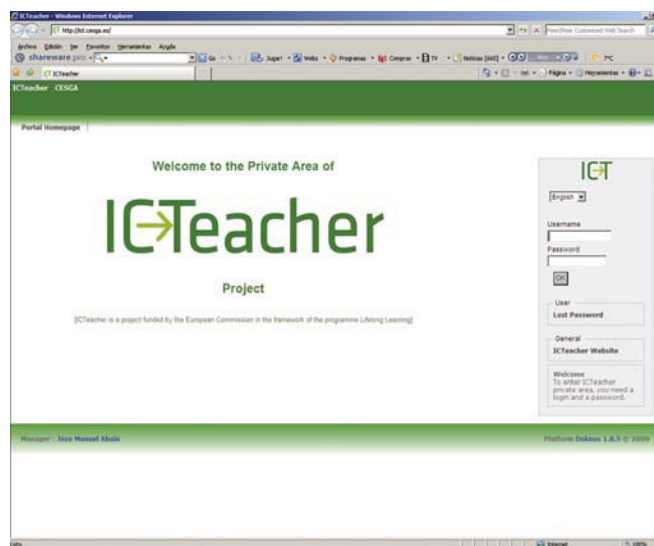
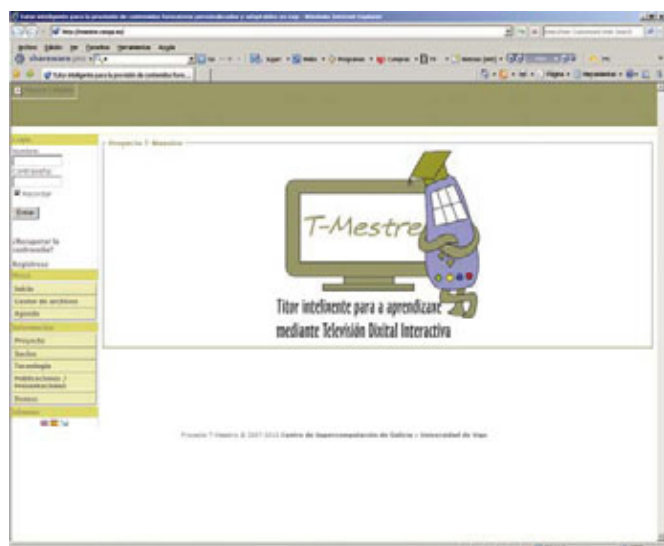
Aula CESGA Courses - 2008

Aula CESGA is a course management system based on the free/libre software platform, Dokeos. Aula CESGA addresses the needs of researchers and teachers in the Galician education system. It is a key tool for the promotion of innovation and research in the field of e-learning and ICT.

Summarised below is the activity in the Aula CESGA platform in the period 2004-2008.

TRAINING COURSES AND COLLABORATIVE PLATFORMS IN AULA-CESGA

	2004	2005	2006	2008
Number of Courses	108	162	235	461
Number of Users	1583	2533	4378	6748





Technology Transfer
& e-Business

technology transfer & e-business

The area of Technology Transfer and e-Business has the objective to raise the awareness of information and communication technologies (ICT) in Galician businesses, promoting their adoption and use, and leveraging research and innovation activity around ICT in enterprises. To that end, they take charge of the design and implementation of innovative projects concerning ITC in business environments, identifying the lines of work and research that pertain to this material. This area pursues cooperation with other organisations in order to conduct activities and projects that promote regional development by means of the use of ITC in enterprises.

HIGHLIGHTED e-BUSINESS ACTIVITIES OF 2008

During 2008 the area of e-Business continued to develop innovation and technology projects centered in the business world. It also continued its support work for projects and continued its activities regarding ICT, innovation, and business by means of access to information sources, participation in events, etc.

With regard to the CAPITA Programme (Support Centre for Technologically Advanced Innovative Projects) of INCITE, the department completed the following activities.

- The design and setting in operation of the CAPITA system in order to support innovation in Galician businesses.
- The development of the web applications of CAPITA Operations Network: Registry of Private Agents of Innovation www.redecapita.eu
- The design and development of internal management applications of the CAPITA system Operations Network (LDAP, electronic mail, groupware, CMS, CRM).
- The creation of a Network of Private Agents of Innovation. The identification, assessment, and verification of the innovation services of 84 consulting and engineering companies, intermediate organisms, and 9 interested businesses. Within the area of support activities, more than 220 consultations were attended during 2008.

Contracted projects were carried out for Vindeira CMMi&SPICE, CoopTIC, XesveTIC, and new projects were presented and con-

tracted such as IPlus and EVITA. Moreover, specific support meetings were held with Galician organisations and businesses in order to evaluate possible projects proposals of an innovative nature, and diverse consultations were attended.

The department participated in various international and national meetings and technical panels which are listed below.

- EVITA Kick-Off presentation, December, Athens.
- IPlus Project Kick-Off presentation, September 18-19, Cagliari.
- Opening Conference ICHNOS+, December 11-12, Cagliari.
- Seminar "How to implement the model of Regional Centre of Competence for OSS", December 11, Cagliari.
- Participation in events within the frame of the Vindeira CMMi&SPICE project.
 - CMMi Planning Workshops, February 27, Santiago de Compostela.
 - SEPG Conference 2008, June 10-13, Munich.
 - Living CMMi, May 23, 2008, Madrid.

The department collaborated with other organisations for operation, support, assessment, and dissemination: the Foundation for the Promotion of Industrial Quality and Technological Development of Galicia, the Galicia Technology Park - Tecnópole, Unite units, Neurona, IMAN, SEGAPI, OPIDI, and Entrepreneurship of Director General for RTD&I, the Women and Science Unit, Business Concept, CITT USC, Departments of the Regional Ministry of Agriculture, the Township of de Santiago de Compostela, EGANET, AGASOL, DXIPI SI. Additionally, assessment and support services were provided to proposals from businesses and business associations.

It is noteworthy to point out that activities earlier developed by the Department of e-Business have been selected as "best practice" and as a model for other regions in the field of capitalisation projects under Interreg IVC due to its contributions to regional development in innovation and entrepreneurship, as well as the development of e-Business in companies.

Rexistro API Busca Glosario Alta Modificación Contacto

Mapa de Axentes Privados de Innovación

No seguinte mapa pode localizar os Axentes Privados de Innovación inscritos no Rexistro. Os indicadores de situación en vermello representan a situación das sedes sociais e os indicadores brancos representan a localización das delegacións de empresas. Se preme nas iconas poderá obter máis detalles da empresa.



Volver a "Busca de Axentes Privados de Innovación"

capita
Unidade de Novos Proxectos Empresariais Innovadores

Rexistro de Axentes Privados de Innovación Busca Glosario Alta Modificación Contacto

EU para crear e fomentar os negocios.

Os profesionais do sector público.

A Consellería de Innovación e Industria, a través do Plan Galego de Investigación, Desenvolvemento e Innovación (INTEI), con en marcha o Rexistro de Axentes Privados de Innovación, unha rede de empresas especializadas en servizo de innovación capaces de levar a cabo o asesoramento e a implantación de proxectos empresariais innovadores.

A función destes Axentes Privados de Innovación será de seguimento e de asesoramento a empresas locais. O seu traballo consistirá no desenvolvemento de proxectos aptos para optar aos programas de axudas en materia de innovación subvencionados, estatais e internacionais.

Para formar parte do rexistro, as empresas interesadas deben formalizar a súa vontade mediante o seguinte formulario. A súa candidatura será revisada e, no caso de ser aceptada, a empresa entrará a formar parte dos recursos externos de CAPITA (Centro de Apoio a Proxectos Innovadores Tecnolóxicos e de Asesoramento), unha nova unidade que, a través do Plan Galego de I+D+i estimulará a innovación empresarial en Galicia e a colaboración entre empresas do sistema de I+D+i.

CAPITA establecerá desde agora unha rede de empresas especializadas en servizo de innovación capaces de levar a cabo o asesoramento e a implantación de proxectos empresariais innovadores cos fondos de garantía e coa colaboración e a súa colaboración. Estes expertos asesorarán a empresas locais no desenvolvemento de proxectos en distintos ámbitos afíns do relacionado co I+D+i, ciencia e servizo ao e desenvolvemento I+D+i, por exemplo, servizos relacionados coa propiedade industrial.

Se a súa organización non cumpre os requisitos para a súa inclusión no Rexistro de Axentes Privados de Innovación pero está interesada noutras modalidades de participación en CAPITA, pode cubrir o formulario de expresión de interese.

XUNTA DE GALICIA
CONSELLERÍA DE INNOVACIÓN E INDUSTRIA
Dirección Xeral de Investigación, Desenvolvemento e Innovación

in.ci.te
Innovación, Ciencia e Tecnoloxía

Fundación para o Fomento da Calidade Industrial e o Desenvolvemento Tecnolóxico de Galicia

CESGA

tecnopole

cybertrust

INFORMACIÓN DE INTERESE PARA CONSULTORIAS E ENXEÑERÍAS CON ACTIVIDADE EN INNOVACIÓN

XUNTA DE GALICIA
CONSELLERÍA DE INNOVACIÓN E INDUSTRIA
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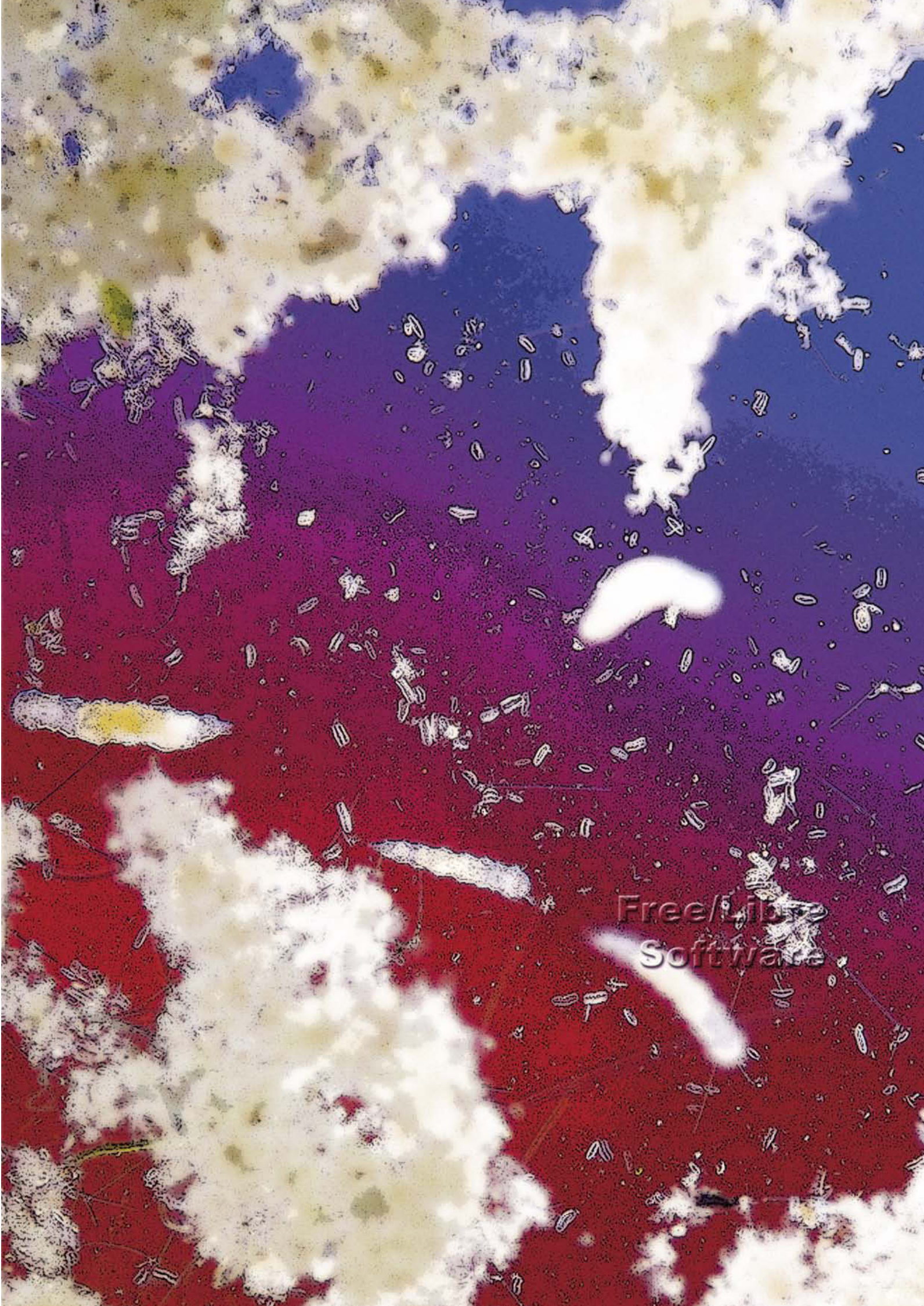
Fundación para o Fomento da Calidade Industrial e o Desenvolvemento Tecnolóxico de Galicia

CESGA

tecnopole

Rexistro de Axentes Privados de Innovación





Free/Libre
Software

area of free/libre software

Activities associated with free/libre software are managed according to the agreement of collaboration signed with the Director General for Industrial Promotion and Information Society by way of Project Mancomún – a Reference and Services Centre for Free/Libre Software in Galicia. This Centre has three strategic objectives.

1.To stimulate the consolidation of an endogenous ICT fabric able to respond to the technological demands of the citizenry, the institutions, and the different sectors of production in Galicia.

2.To move forward with the effective implementation of Information and Knowledge Society resources and services with special attention given to the Galician language.

3.To strengthen the free/libre software community by means of dissemination, sponsorship, and participation in the most relevant initiatives, events, and organisations.

2008 Activity Highlights

Activities for Software Localization into Galician

- Maintenance of the Galician translation of desktop applications: OpenOffice.org, Firefox, Thunderbird, pidgin, sunbird, gimp, and Gnome.
- Maintenance of the Galician orthographic corrector for OOo: correction of errors, update and integration in the official version of OOo 3.0.
- Important milestone: Integration into the Mozilla community, achieving an official version of Firefox 3.0.5 in Galician.
- Maintenance and update of the on-line translation tool, Entrans.
- Improvements in the “Linguistic Corpus Search Engine” application.
- Maintenance of the DVD - Software tools for the SME - and translation of the programs included. Distribution of approximately 6000 DVDs among the SME and the Galician society.
- Development of a GNU/Linux distribution in Galician in order to facilitate the introduction of ICT in society by means of the distribution of free/libre installable software in Galician.
- Development of a metapackage that modifies the graphic look of the Ubuntu based distribution and configures the Galician language for multimedia desktop applications.
- Creation of two GNU/Linux distributions using the metapac-

kage: araOS and Galinux.

- Presentation of Galinux to the media.

Activities for Software Development

- Promotion of the use of Mancomun’s source forge, “Forxa”.
- Publication under free license of Mancomun developed Projects in Forxa:
 - Linguistic Corpus Search Engine.
 - Modifications performed by Mancomún to the Entrans project.

Implementation Activities

- Maintenance and improvement of the Free/Libre SME directory that includes 73 businesses.
 - Maintenance of different services in order to facilitate collaborative work in the network: wiki, mailing lists, forum, etc.
- #### Training Activities
- Elaboration of the ICT Skill Development Plan directed to Galician ICT companies to enable them to take on implementation projects and support services in Free/Libre Software. This arises as a complement to the DVD – Free/Libre Software Tools for the SME and as a response to the demand of Galician ICT businesses.
 - First pilot edition of the skill development plan and elaboration of the ICT Skill Development Guide as documentation for training.
 - Planning of the second edition of the ICT Skill Development Plan.
 - Collaboration with the e-Learning Dept. regarding the development of contents and the delivery of an OpenOffice.org Course for Secondary teachers under the Aula CESGA Platform. This course was organised by the Director General Innovation in Education of the Galician Regional Government.
 - Organisation of the course: Introduction to GIS through gvSIG.
 - Organisation of an Advanced Course in eBOX oriented to the training of installers and developers of this platform.
 - Elaboration of the documentation and Cds of support for the installation of Free/Libre Software in Galician on Ubuntu for the SME that distribute hardware.
- #### Observatory Activities
- Elaboration of reports of the study of Free/Libre Software use

in Galician entities during 2007.

- Coordination with the Galician Observatory of the Information Society for the publication of results.
- Collaboration with OGSi concerning the preparation of the 2008 study.

Dissemination Activities

Publication of daily news on the webpage www.mancomun.org

Publication of weekly news bulletins regarding Mancomun.

Publication of Free/Libre Software success stories in Galicia.

Coverage of relevant events such as SEMIC and OSOR presentation event.

Maintenance of an agenda of events related with Free/Libre Software at the regional and state levels

Participation in Events Related to Free/Libre Software

- Xuventude Galicia Net 2008
- Participation in FESTIGAL 2008 in coordination with local Linux User Groups.
- Planning and coordination of Galician participation in the

International Conference on Free/Libre Software celebrated in Malaga.

- Organisation of the participation and broadcast of the III Encounter of BrOffice. <http://encuentro.broffice.org/2008/gl>

Events Organised to Promote Mancomun's Activities

• The "I G11n Day: I translate your software" was organised with the objective of elaborating a translation method to integrate different agents from the development communities. The translation community of free/libre software to Galician was invited. Persons of recognised prestige in the field of free/libre software translation to Galician were also invited as were experts from elsewhere in Spain in order to share their experiences. In addition, these work days coincided with the second anniversary of Mancomun. For that reason, the Director General presented the new corporate image of Mancomun, making special mention of the new nomination as Free/Libre Software Reference and Services Centre of Galicia.

- In the last quarter of the year, the II meeting of the G11n took place. This was an internal meeting celebrated with the



Galician translation community where the first version of the Localization Manual was presented. This manual compiles the linguistic criteria applied to translations coordinated by Mancomun as a response to the request from the community.

- Coordination and organisation of the event, "Free/Libre Software of interest to the SME" with the objective of guaranteeing that the DVD – Free/Libre Software Tools for the SME will be a truly useful and efficient tool.
- Coordination and organisation of the act of presentation of GALINUX.

Technical Support Activities

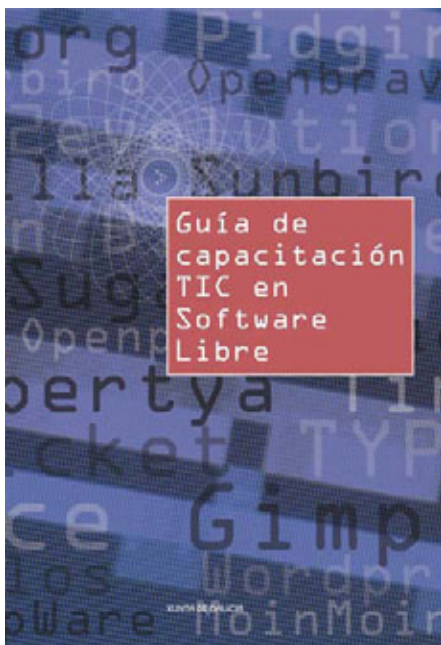
- Technical support to Mancomun users, SME, local government, administrative organs, etc.



- Technical support to free/libre software projects of the Director General of Industrial Promotion and the Information Society.
- Support of the Dynamization Network regarding the installation classrooms with free/libre software.
- Training regarding the SME DVD for the personnel of the Dynamization Network.
- Support for the migration of the

Information Society Office.

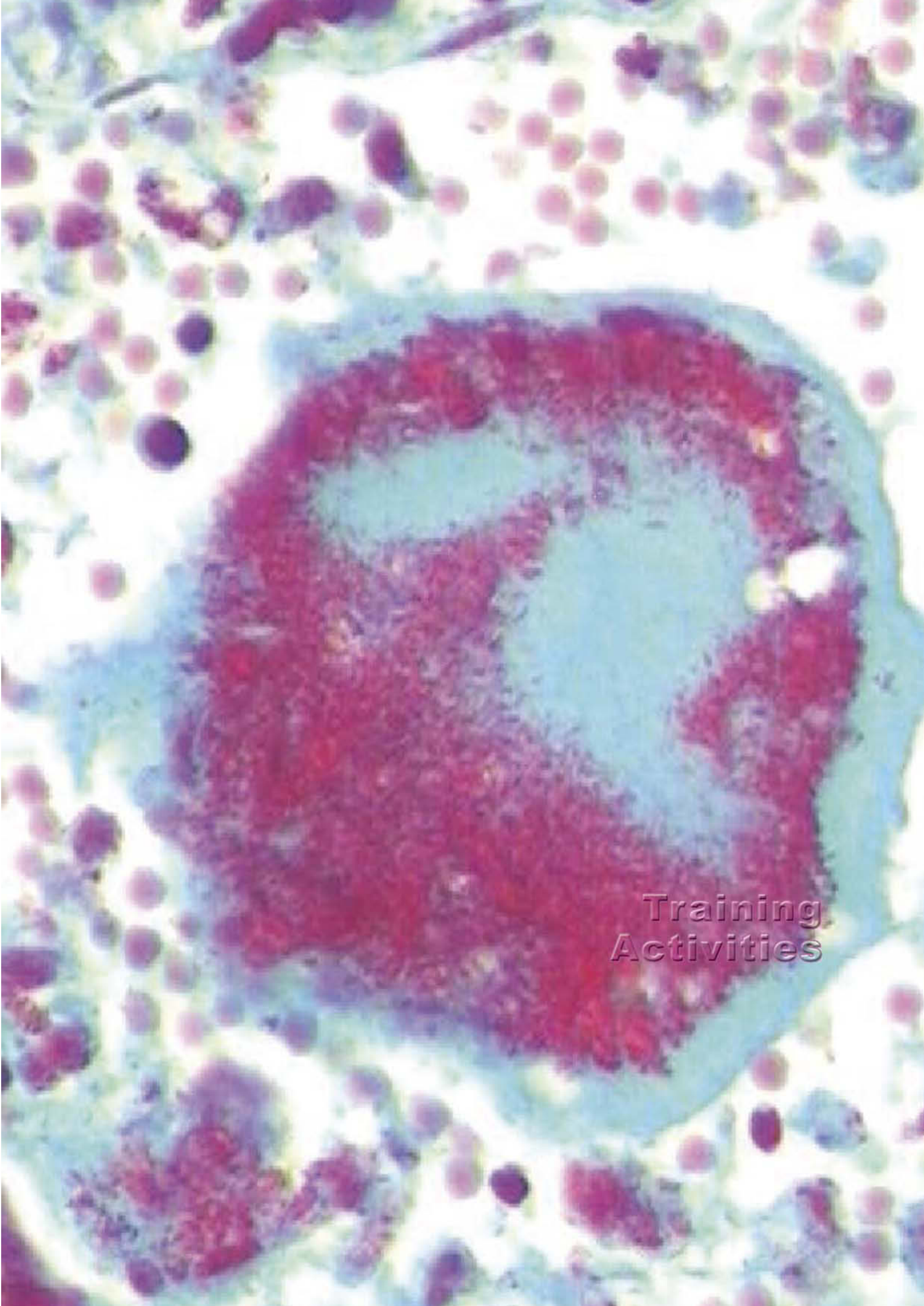
- Coordination with the Director General and the Linux User Groups in order to sign a collaboration agreement.
- Meeting to set in operation the Free/Libre Software Offices of the universities.
- Coordination with the Free/Libre Software Offices of the 3 universities.
- Coordination with the GaliciaXa.tv platform.



Collaboration agreements with Linux user groups







Training
Activities

training activities

CESGA provides Training Opportunities for Users and Personnel. During 2008, the Centre participated in the organization of a total of 58 training activities, distributed as indicated in the table below.

SUMMARY OF TRAINING EVENTS	2004	2005	2006	2007	2008
COURSES	16	21	22	16	49
SESSIONS AND SEMINARS	8	7	8	11	7
CONFERENCES	1	3	2	1	2
	25	31	32	28	58

Concretely, it is the users of the Centre, RTD personnel in industry, public administration officials, teachers, researchers, students, and the Centre's personnel who benefit from these activities. The Annual Training Plan is the key stone around which the organisation of these activities is structured.

The majority of these activities were related to the installation and optimal use of advanced technologies. Most courses focused on topics related to the best use of computing systems and included such themes as compilation, optimisation, parallelisation, programming languages, debugging, and algorithms.

2008 User & Staff Training Programme

Training Activity Title	Type	In Collaboration with	Date of Activity	Duration (h)
HPCMU + General Cluster Overview + Management Tricks	course	HP	1st Quarter	18
HP SFS	course	HP	1st Quarter	18
Intel Development Tools	course	Intel	1st Quarter	25
Finis Terrae Maintenance	course	CESGA	1st Quarter	4
Voltaire Technical Training Class	course	CESGA	1st Quarter	14
General Superdome Hardware Vision	course	HP Invent	2nd Quarter	6
Django	course	CESGA-GIS	2nd Quarter	12
Fortran	course	CESGA	2nd Quarter	12
Introduction to Computing	course	USC/UDC	3rd Quarter	20
Introduction to MPI Programming	course	USC/UDC	3rd Quarter	15
Fortran (2nd edition)	course	CESGA	4th Quarter	12
Parallel Programming using OPENMP Directives	course	CESGA	4th Quarter	15
Scientific Application Optimisation on Multicore Systems	course	CESGA	4th Quarter	15
Open Source Tools for Debugging and Application Performance Analysis	course	CESGA	4th Quarter	20
Access to and Use of Finis Terrae Supercomputer	course	CESGA	4th Quarter	5
Introduction to Chemical Codes at CESGA (Gaussian, GAMESS, NWCHEM)	course	CESGA	4th Quarter	5

Training Activity Title	Type	In Collaboration with	Date of Activity	Duration (h)
Course of English	Course	Piccadilly	Year round	Year Round Classes
CESGA's Web CMS Use	Course	CESGA	Year round	One on one Tutoring
New Law of Public Tenders: novelties and implications for businesses	Course	APD	1st Quarter	8
High Performance Interconnect Networks	Course	Voltaire	1st Quarter	8
Open Code Geographic Information Systems	Course	SIGTE	1st Quarter	24
How to Implement an in-Company RTD Management System	Course	FEUGA	1st Quarter	21
How to Deliver winning Presentations	Course	APD	1st Quarter	8
Contracting Law for the Public Sector Workshop	Workshop	Xunta de Galicia	1st Quarter	4
Voltaire Technical Training Class	Course	Voltaire HP	1st Quarter	14
FinisTerraie Maintenance	Course	HP	1st Quarter	4
Visual Basic.NET	Course	Pcarrier	2nd Quarter	60
Organisational Climate and Work Performance	Course	APD	2nd Quarter	2
The new Law 30/2007 for Public Sector Contracting	Course	Xunta de Galicia	2nd Quarter	13
Phyton & Django	Course	SCA Informática	2nd Quarter	12

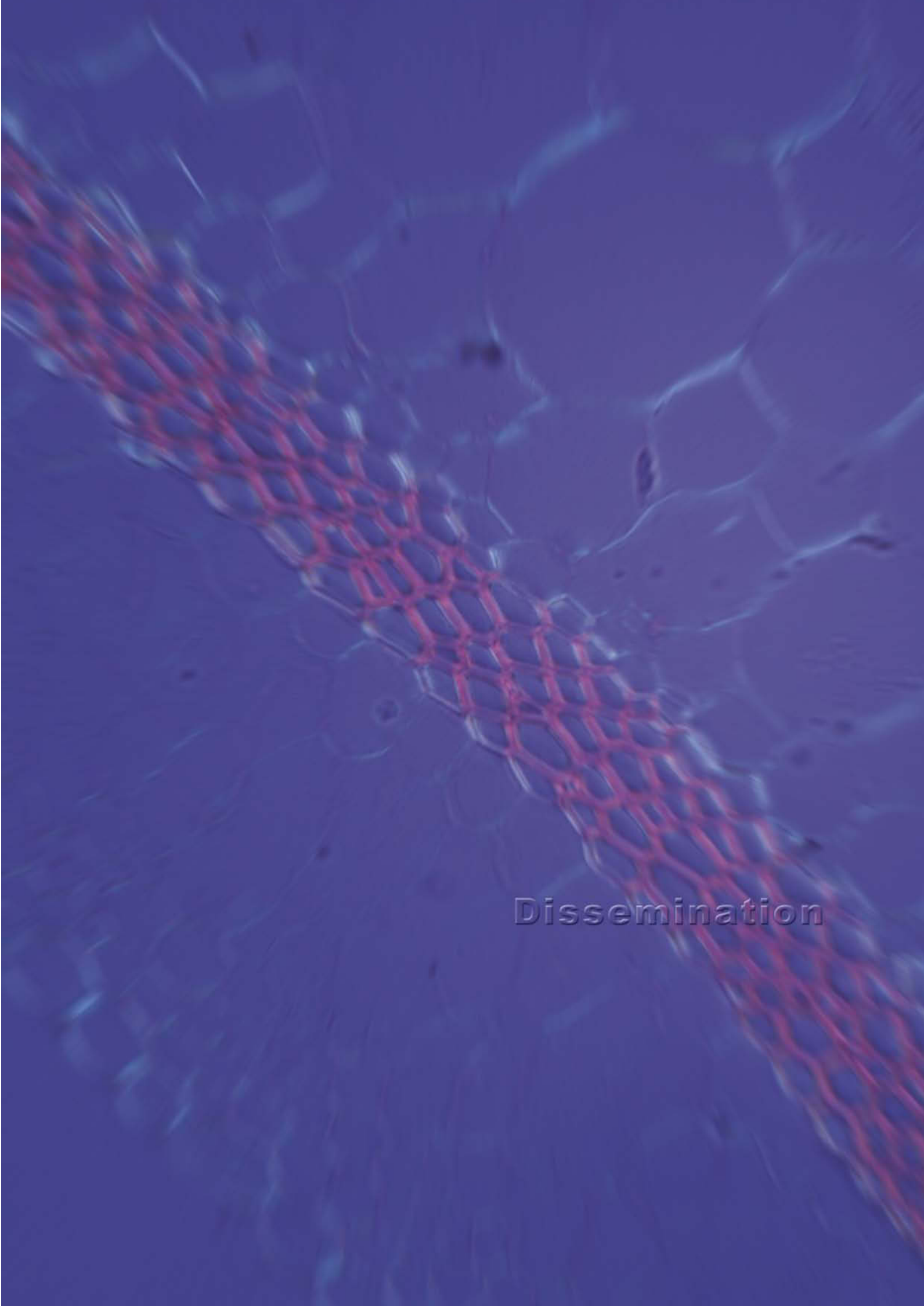
Training Activity Title	Type	In Collaboration with	Date of Activity	Duration (h)
Ontologies, SOA & WEB Services	Course	USC	2nd Quarter	9
Designing Cisco Network Service Architecture	Course	Global Knowledge Spain	2nd Quarter	40
New General Accounting Plan	Course	Xunta	2nd Quarter	15
Effective Implementation of Safety Plans in Businesses	Course	APD	2nd Quarter	5
BeinGRID Portal Training	Course	Beingrid	3rd Quarter	15
Qualitative Research Tools and Methodologies for Projects	Course	USC	3rd Quarter	15
Sixth International Summer School on Grid Computing	Course	Various	3rd Quarter	80
BEinGRID Components Training	Course	Beingrid	3rd Quarter	15
BEinGRID Business and Dissemination Training	Course	Beingrid	3rd Quarter	15
How to Communicate Science, Technology and Innovation	Course	Feuga	4th Quarter	4
LAMP Programming	Course	Professional Training	4th Quarter	20
Parallel Application Development	Course	USC/UDC	4th Quarter	25
ITIL V3 Fundamentals	Course	CNTG	4th Quarter	20
ICT Project Management	Course	CNTG	4th Quarter	36

Training and Outreach activities organised by or participated in: CESGA - 2008

Activity Title	Type	In Collaboration with	Date
CESGA FINISTERRAE Computational Science Conference	Scientific Conference	CSIC Spanish Ministry of Science & Innovation Regional Government of Galicia, Xunta de Galicia	12-06-08
Structural Bioninformatics Course: Biological Molecule Modelling and Simulation	Seminar	Rede Galega de Bioinformática USC Fundación Pública Galega de Medicina Genómica	05-11-08
FP7 Project Management Course	Seminar	OPIDI, DXIDI, Xunta de Galicia	26/28-11-08
GIS Course of the Professional Association of Geographers	Course	Professional Association of Geographers USC	11-9-08
Ten Reasons to Design an Accessible Website	Conference	Spanish Chapter of the Internet Society. ISOC	12-02-08

Mathematica.nodo.cesga.es Outreach Activities in 2008

Activity	Type	Responsible Organisation	Date
Course on Nanotechnology and Mathematics	Course	USC	05/06-08/08
i-MATH Free/Libre Software for Science and Engineering Intensive Course	Course	UDC, UCA, UC, USC, UVIGO, CESGA	06/30-09/26/08
Computational Math: Compiling, Execution and Program Optimization	Course	CESGA	06/30-07/04/08
Introduction to Programming with MPI	Course	CESGA	07/28-30/08
Statistics in Quality Control Methods	Forum	UDC	02/01/2008
Applied Math and Industry Interaction Day	Forum	UDC	04/25/08
Statistics for the Sports Industry	Forum	UVIGO	10/08/08
Math Consulting for Industry and Public Administration	Industrial Days	USC	02/11-13/08



Dissemination

dissemination

Objectives

- Planning, coordination, and execution of CESGA dissemination activities.
- Development and maintenance of diffusion tools (website, "Díxitos" magazine, annual workshop, etc.).
- Edition of CESGA's publications.
- Organization of the logistics of the Annual Training Plan for CESGA personnel and users.

2008 Highlights.

- The publication of the quarterly magazine, "Díxitos". Publication of the first monograph, "Papers on Computational Science", as a showcase of CESGA users' research projects.
- Publication of the 2007 CESGA Annual Activity Report.
- Organisation of "CESGA-Finis Terrae Computational Science Conference" that coincided with the new supercomputer inauguration events.
- Maintenance of the content management application for www.cesga.es
- Participation in 14 courses, workshops, and seminars for CESGA personnel and users.
- Implementation of CESGA's Communication Plan.
- Support to the production of HP's corporate video about Finis Terrae installation and close collaboration with HP and Intel in the production of two Case Studies related to this installation.
- Preparation of presentations, dossiers, and reports for the Management and personnel of CESGA, including:
 - The presentation of FINIS TERRAE,
 - The proposal for the creation of a node of the Spanish Institute of Mathematics in Galicia (IEMath),
 - The Annual Activity Report for CSIC's Delegation in Galicia, and
 - The proposal for the implementation of the "CESGA Computational Science Research Center" (C2SRC).
- Communication, public relations and in general dissemination support to the Centre's projects and activities including: NextCESGA, IEMath, EGEE, e-HOSPITAL, Formiga, T-MAESTRO, MANCOMUN, ISOC, eIMRT, RECETGA, i-Math, and FINIS TERRAE.

- Management of media relations. The production and distribution of press releases and the organisation of media conferences related to CESGA projects and initiatives.
- Participation in the European Science Week in close collaboration with the Director General for Research, Technological Development and Innovation of the Galician Government (Xunta de Galicia).
- Dissemination support to thematic networks and technological platforms: the Galician Bioinformatics Network (Rede Bioinfo), the Galician Network of High Performance Computing (Rede GHPC), the Network of Technological Centres of Galicia (RETGALIA) and the Galician ITC Technological Platform (VINDEIRA).
- Collaboration with CSIC officials in the creation of contents for dissemination materials regarding computing resources available for researchers.
- Planning and execution together with the consultancy firm 'Cidadania' of a thorough survey of satisfaction of users regarding computing and storage services, promoting the adoption of measures in accordance with the survey results.
- Compilation of users' scientific production data from 2007 and preparation for the collection campaign of the same type of data for 2008.
- Planning of the Bibliometric Study of Scientific Production of the Users between 2002-2007 in collaboration with the Consortium of University Libraries of Galicia, BUGALICIA.
- Support to the Spanish Royal Society of Mathematics (RSME), the International Mathematics Olympics (IMO), the Society of Statistics and Operative Research (SEIO) and the European Courses in Advanced Statistics (ECAS) concerning the hosting of their Websites on CESGA servers.
- Collaboration regarding the setup of CESGA's on-demand video repository of training and dissemination activities, tv.cesga.es
- The organisation of institutional and educational visits to CESGA.

Institutional visits:

- The Vice-President of the Government of Galicia.
- Institutional visits during the Finis Terrae Inauguration Day:
 1. The President of the Government of Galicia, the State Secretary of Research, Board members of Innovation and Industry as well as Education of the Galician Government, The Secretary General of Scientific Policy and Technology of the Ministry of Science and Innovation, the President of the Spanish National Research Council (CSIC), the President of CESGA, the General Director of Research and Technological Development of the Galician government, The General Director of Planning and Coordination from the Ministry of Science and Innovation, the President of HP-Spain, and the Director of the Public Sector Area of Intel.
 2. A guided visit for media representatives including local, national, and international publications.
 3. Visits for Users that participated in the Cesga-Finis Terrae Computational Science Conference.
 4. On June 13th, and with the motive of presenting the strategic plans of CESGA along with their technological plans concerning FT, more than 50 representatives from businesses, technological centres, universities, and administrations from all over Spain attended the meeting.

They also visited the installations of the new supercomputer, Finis Terrae.

Other visits:

- The Bioinformatics Network of Galicia
- The Ramón Maria Aller Astronomical Observatory of the University of Santiago de Compostela
- The Astronomical Institute, St.Petersburg State University, Russia
- Wind farm monitoring and control company
- I-maxin Software Company
- The Galician HPC Network, Rede GHPC
- Technicians and officials from the Galician Public Health System, SERGAS
- The Scientific Park of Murcia
- The HP Corporation BU Manager
- The Foundation Supercomputing Centre of Castilla y Leon
- The University and the regional government of Extremadura
- Technicians and officials of Galicia's Public Television (TVG)
- The Basque Government IT Company: EJIE
- The Agency for Innovation of the Canary Islands Government







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