technical management report 2009

CSIC
Consejo Superior de Investigaciones Científicas

XUNTA DE GALICIA

UNIÓN EUROPEA
FEDER
FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN

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2009 Highlights

Intense activity was carried out in research, technological development, and innovation projects that were awarded funding at European, national, and regional competitive calls. Activity was also intense in both user support services as well as staff and user training initiatives. Likewise, great efforts were undertaken to fulfil all necessary administrative requirements in order to manage the future construction of CESGA's new headquarters.

The most relevant activities carried out in 2009 are summarised below.

- CESGA actively participated in 44 RTD projects and in 19 thematic research networks and technological platforms.

- The amount of CPU hours consumed by the community of users on CESGA's servers increased by 57% as compared to the previous year.

- The first open call for "Computational Challenges" was successfully launched in 2009 and had an excellent reception within the user community.

- The first edition of CESGA's Computational Science Summer School took place with training sessions, speakers, and students of the highest quality standards.

- CESGA, along with users and project partners, was recognised with three different international awards in 2009.

- Preliminary work for the deployment of dark fibre in the Galician Research and Education Network, RECETGA, was undertaken.

- CESGA renewed its ISO:9001 certification under 2008 new version.

- Preliminary work was undertaken toward the implementation of Norm UNE:166002 that governs the management of research, technological development, and innovation activity.

Mission Statement

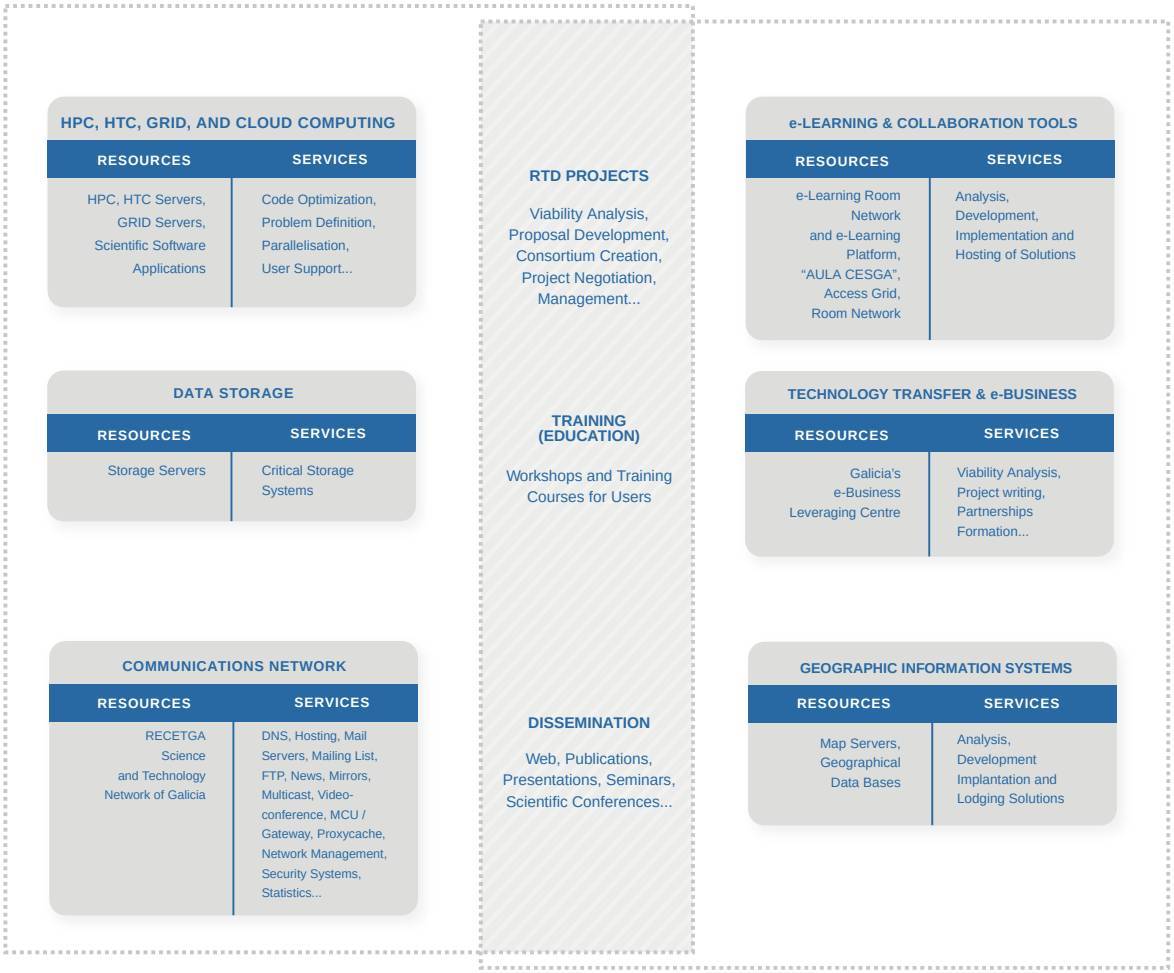
The **mission of CESGA** is:

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



Government Bodies of the Legal Entities that constitute **CESGA**

BOARD OF TRUSTEES OF **CESGA FOUNDATION**

XUNTA DE GALICIA REGIONAL GOVERMENT OF GALICIA	PRESIDENT	Ricardo Capilla Pueyo	Director General for RTD Regional Ministry for Economy and Industry
	SECRETARY	Patricia Iglesias Rey	Legal Adviser Regional Ministry for Economy and Industry
	MEMBER	Manuel Mauro Fernández Dabouza	Director General of the Computing Centre for Tax Management, Finances and Accounting Regional Ministry of Finance
	MEMBER	José Alberto Díez de Castro	Secretary General for Universities Regional Ministry for Education and University System Organisation
	MEMBER	Mar Pereira Álvarez	Secretary General for Modernisation &Technological Innovation Office of the President Galicia Regional Government
CSIC Consejo Superior de Investigaciones Científicas SPANISH NATIONAL RESEARCH COUNCIL	VICE-PRESIDENT	Carmen Peláez Martínez	Vice-president for Scientific and Technological Research Spanish National Research Council (CSIC)
	MEMBER	Uxío Labarta Fernández	Institutional Coordinator Spanish National Research Council, Galician Division

BOARD OF DIRECTORS **S.A.X. CESGA**

XUNTA DE GALICIA REGIONAL GOVERMENT OF GALICIA	PRESIDENT	Ricardo Capilla Pueyo	Director General for RTD Regional Ministry for Economy and Industry
	SECRETARY	Patricia Iglesias Rey	Legal Adviser Regional Ministry for Economy and Industry
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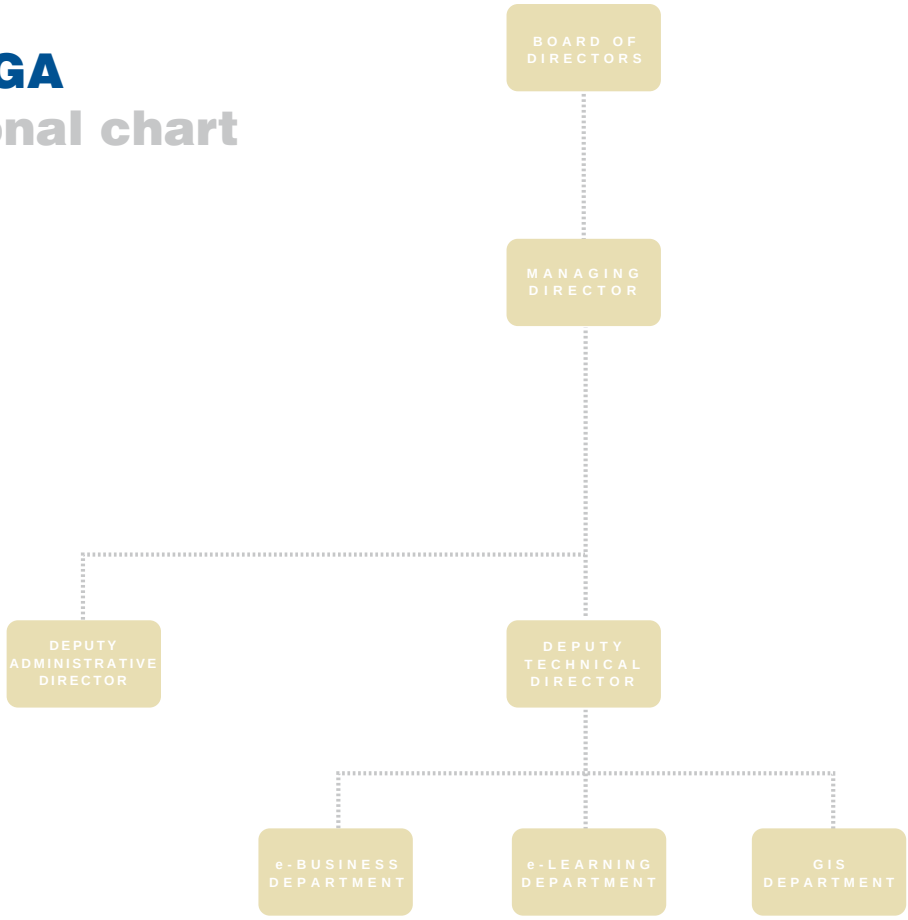
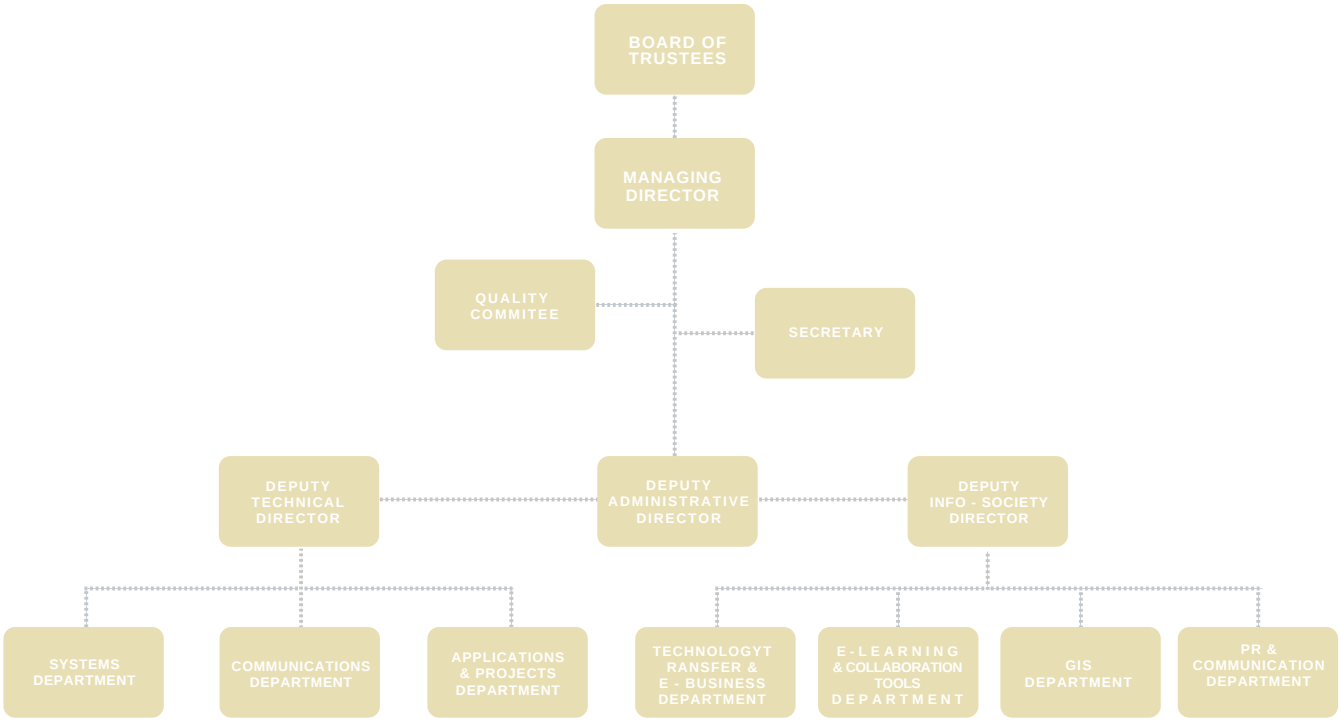
	MEMBER	José Alberto Díez de Castro	Secretary General for Universities Regional Ministry for Education and University System Organisation
	MEMBER	Alfonso Cabaleiro Durán	Secretary General for Mass Media Office of the President Galicia Regional Govenment
	MEMBER	José Carlos Riesgo Boluda	Secretary General of Regional Ministry for Economy and Industry
	MEMBER	Mar Pereira Álvarez	Secretary General for Modernisation &Technological Innovation Office of the President Galicia Regional Govenment
	MEMBER	Isabel Cadenas Pérez	Assistant Director for Business Innovation Regional Ministry for Economy and Industry
CSIC Consejo Superior de Investigaciones Científicas SPANISH NATIONAL RESEARCH COUNCIL	VICE-PRESIDENT	Carmen Peláez Martínez	Vice-President for Scientific and Technological Research Spanish National Research Council (CSIC)
	MEMBER	Carlos Manuel Abad Ruiz	Secretary General for Economic Performance Spanish National Research Council (CSIC)
	MEMBER	Uxío Labarta Fernández	Institutional Coordinator in Galicia Spanish National Research Council
	MEMBER	Antonio Álvarez Alonso	Research Associate of the Institute of Marine Research, CSIC
UNIVERSIDADE DA CORUÑA	MEMBER	María Concepción Herrero López	Vice-President for Research University of A Coruña
USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA	MEMBER	Mª José Alonso Fernández	Vice-President for Research and Innovation University of Santiago de Compostela
Universidade Vigo	MEMBER	Mª Elsa Vázquez Otero	Vice-President for Research University of Vigo

S.A.X. CESGA
organisational chart



CESGA´s work force, its most valuable asset.

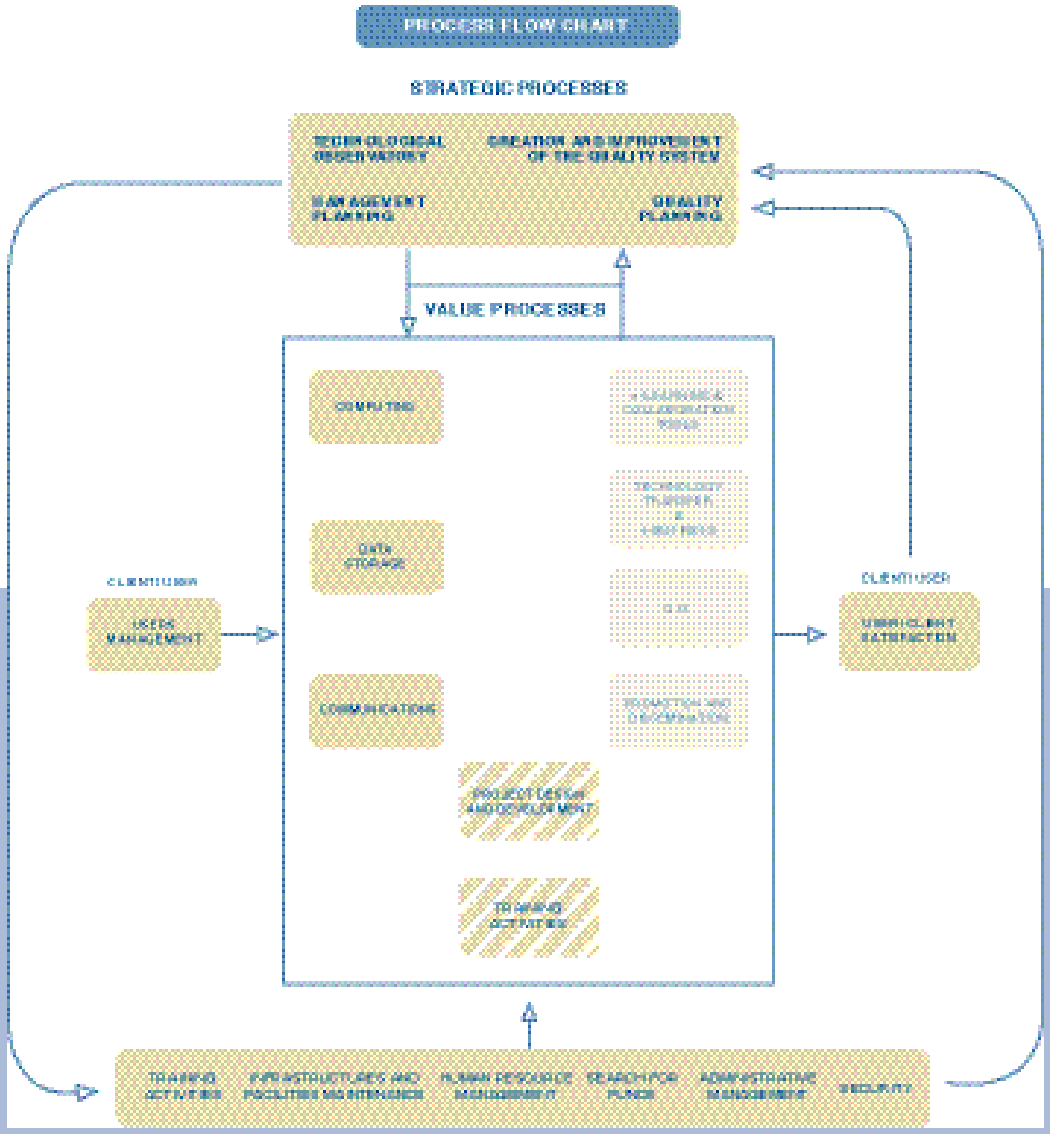
CESGA Foundation
organisational chart



CESGA'S PERSONNEL IN 2009

ACADEMIC TRAINING LEVEL	NUMBER	MALE	FEMALE	AGE AVERAGE
PhD (5 Year Higher Ed.+ Dissertation)	12	11	1	36.17
5 Year Higher Ed.Degree	28	16	12	35.07
3 Year Higher Ed.Degree	3	2	1	41.66
Secondary Ed. & Technical Schools (2 Year Degree)	16	12	4	32.32
Other	3	3	0	45.67
TOTAL	62	44	18	34.76

Quality of services



Quality, a map of processes

During 2009, the CESGA Foundation renewed the certification of quality, ISO 9001:2008, an updated version of the ISO9001:2000 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 of increasing the quality of the services provided to users.

During the specific year in which the certification was in force, 5 processes, 4 procedures, and 5 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.

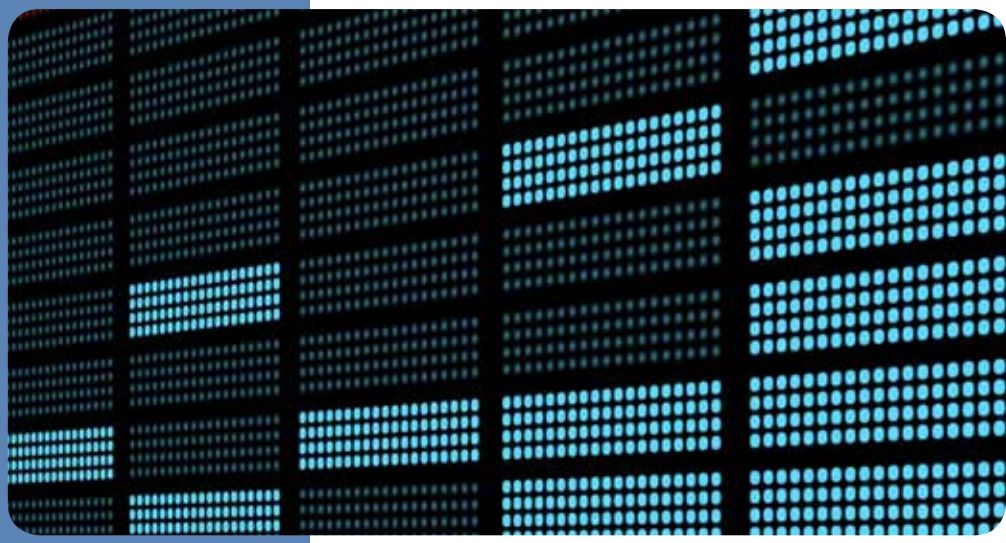
Additionally, in 2009, continued advances in the automating of all processes associated with quality control were made in addition to improvements in the monitoring systems of the centre (users, systems, applications, etc.) in accordance with the norm ISO 9001:2008.

In addition, CESGA paved the way this year for obtaining a new certification by 2010 (UNE166002), related to the management of research, development and innovation activities.

User satisfaction levels keep scoring high

Every year, CESGA attempts to measure user satisfaction levels with regard to the technical solutions and support services provided by the Centre's staff and resources. Since 2007, when we first started taking these measurements, user satisfaction levels have remained high as indicated by the data collected from the survey. Users are asked to value their perception of the quality of services on a scale ranging from 1 (terrible) to 5 (excellent). Year after year, users have marked their perceived quality of services on the high end of the scale (consistently above the 4.5 mark). We would like to express our deepest appreciation to our user community for their participation in these surveys.The comments we receive from users through such surveys are most useful in our attempt to constantly ameliorate and permanently maintain updated services, demonstrating the highest standards of quality.

Computing Users

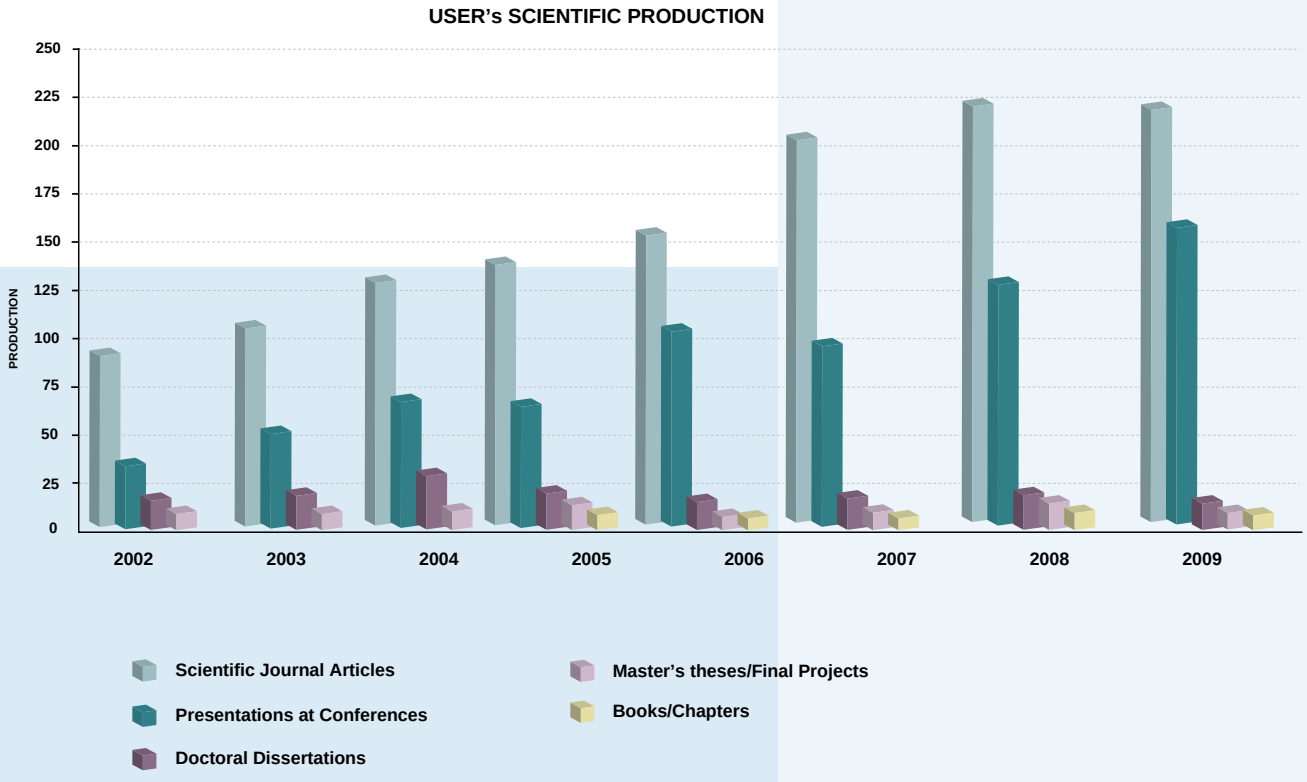


Most active users in 2009 by institution

USER	DEPT./CENTRE	HOURS USED
UNIVERSIDADE DE SANTIAGO DE COMPOSTELA (USC)		
Jaime Souto Casares	Condensed Matter Physics	807,666.6
Lucas Vázquez Besteiro	Condensed Matter Physics	376,512.3
Manuel María González Alemany	Applied Physics	226,686.7
Roberto Longo Pazos	Applied Physics	226,304.2
Manuel Pereiro Pazos	Applied Physics	225,513.6
Luis Tortajada Iavlu	Condensed Matter Physics	198,657.3
UNIVERSIDADE DA CORUÑA (UDC)		
Daniel Rivero Cebrián	Communications & Information Technologies	800,839.6
Ana Belén Porto Pazos	Communications & Information Technologies	151,209.7
Noha Veiguela Blanco	Communications & Information Technologies	115,311.6
Daniel Rodríguez Ramos	Chemistry, Physics and Chemical Engineering I	99,061.9
María Victoria García Dopico	Chemistry, Physics and Chemical Engineering I	80,484.6
Luis Rodríguez Vázquez	Chemistry, Physics and Chemical Engineering I	66,163.7
UNIVERSIDADE DE VIGO (UVIGO)		
Juan Antonio Añel Cabanelas	Applied Physics	838,147.9
Laura Estévez Guiance	Chemistry Physics	184,816.5
Otalia Nieto Faza	Organic Chemistry	130,637.8
José Manuel Hermida Ramón	Chemistry Physics	93,773.8
Rosana Álvarez Rodríguez	Organic Chemistry	92,457.3
Carlos Silva López	Organic Chemistry	54,107.7
SPANISH NATIONAL RESEARCH COUNCIL (CSIC)		
Sandra García Gil	Electronic Structure of Materials	562,560.1
Jorge Sánchez Dolado	Nanostructured Materials Unit	406,930.4
Carolina Mendoza Parra	Mathematics	398,931.8
Regla Ayala Espinar	FQM292	350,907.3
Roberta Poloni	Electronic Structure of Materials	331,602.6
Octavio Roncero Villa	Atomic & Molecular Physics Theory Dept.	314,625.6
UNIVERSITAT DE LES ILLES BALEARS (UIB)		
Sascha Husa	Physics	32,323.6
Helena Viaño Viñuales	Physics	6,384.9
Juan Frau Munar	Chemistry	2,891.5
METEOGALICIA - XUNTA DE GALICIA WEATHER SERVICE (GALICIAN REGIONAL GOVERNMENT)		
Vicente Pérez Muñuzuri	MeteoGalicia: Numerical Prediction and Research	32,552.1
TECHNOLOGY CENTRES (CTAG)		
Santiago Cabello Vieites	Technological development in the automotive industry in Galicia	12,466.2

Scientific production reported by CESGA´s users in 2009

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.



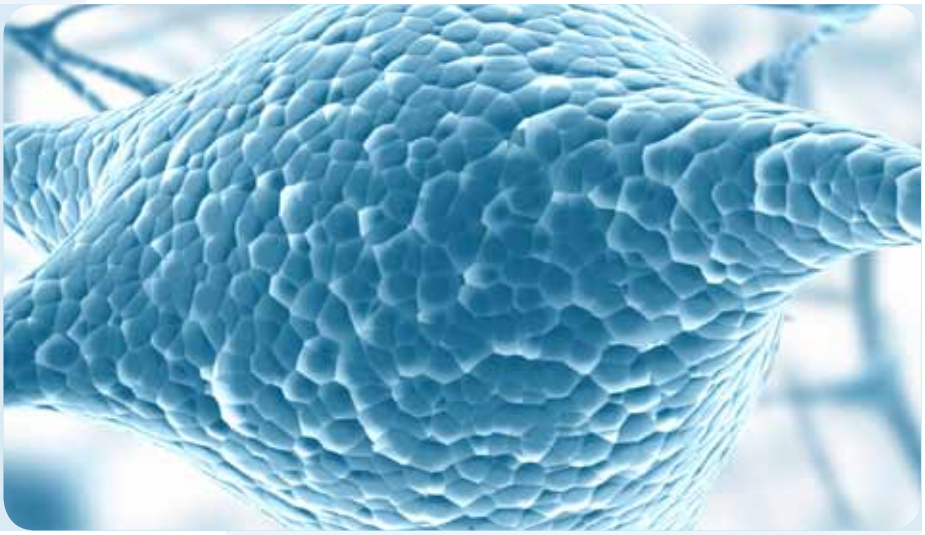
DISTRIBUTION OF ALL USER's SCIENTIFIC PRODUCTION PER YEAR

	2002	2003	2004	2005	2006	2007	2008	2009
SCIENTIFIC ARTICLES	93	107	134*	147	154	208	225	218
ACCEPTED / IN PRESS	4	8	20	16	26	19	21	24
SUBMITTED	16	29	26	27	23	24	31	14
PUBLISHED	73	70	91	104	105	165	173	180
CONFERENCE PRESENTATIONS	42	52	72*	65	105	101	148	160
POSTER PRESENTATIONS	33	40	53	37	53	46	60	101
	9	12	35	28	52	47	88	59
DOCTORAL THESES	17	21	32	24	18	18	20	14
DEFENDED	9	4	5	9	10	11	10	10
PRESENTED	–	–	–	–	3	5	1	–
IN PROCESS	8	17	27	15	5	2	9	4
MASTERS THESES GRADUATE PROJECTS	12	9	12	14	5	10	14	12
DEFENDED	6	4	5	13	3	8	10	12
IN PROCESS	6	5	7	1	2	2	4	–
BOOKS / CHAPTERS	NA**	NA**	NA**	5	4	3	9	13
ACCEPTED / IN PRESS	NA**	NA**	NA**	4	1	1	1	2
SUBMITTED	NA**	NA**	NA**	1	–	2	–	–
PUBLISHED	NA**	NA**	NA**	–	3	–	8	11
TOTAL	169	194	256	260	301	351	416	417

* 8 PUBLICATIONS & 16 CONFERENCES WITH AUTHORS FROM MORE THAN ONE INSTITUTION
** NA: Non Available

DISTRIBUTION OF SCIENTIFIC PRODUCTION DECLARED BY USERS FROM CSIC AND GALICIAN UNIVERSITIES

	CSIC	UDC	USC	UVIGO	TOTAL
SCIENTIFIC ARTICLES	90	25	44	42	201
ACCEPTED/ IN PRESS	11	1	7	5	24
SUBMITTED	9	-	3	2	14
PUBLISHED	70	24	34	35	163
CONFERENCE PRESENTATIONS	63	19	37	15	134
POSTER PRESENTATIONS	33	16	24	8	81
	30	3	13	7	53
DOCTORAL THESES	2	5	2	4	13
DEFENDED	1	3	2	4	10
PRESENTED	-	1	-	-	-
IN PROCESS	1	2	-	-	3
MASTERS THESES / GRADUATE PROJECTS	-	4	5	3	12
DEFENDED	-	4	5	3	12
BOOKS / CHAPTERS	1	2	3	2	8
ACCEPTED/ IN PRESS	-	-	1	1	2
PUBLISHED	1	2	2	1	6
TOTAL	156	55	91	66	368

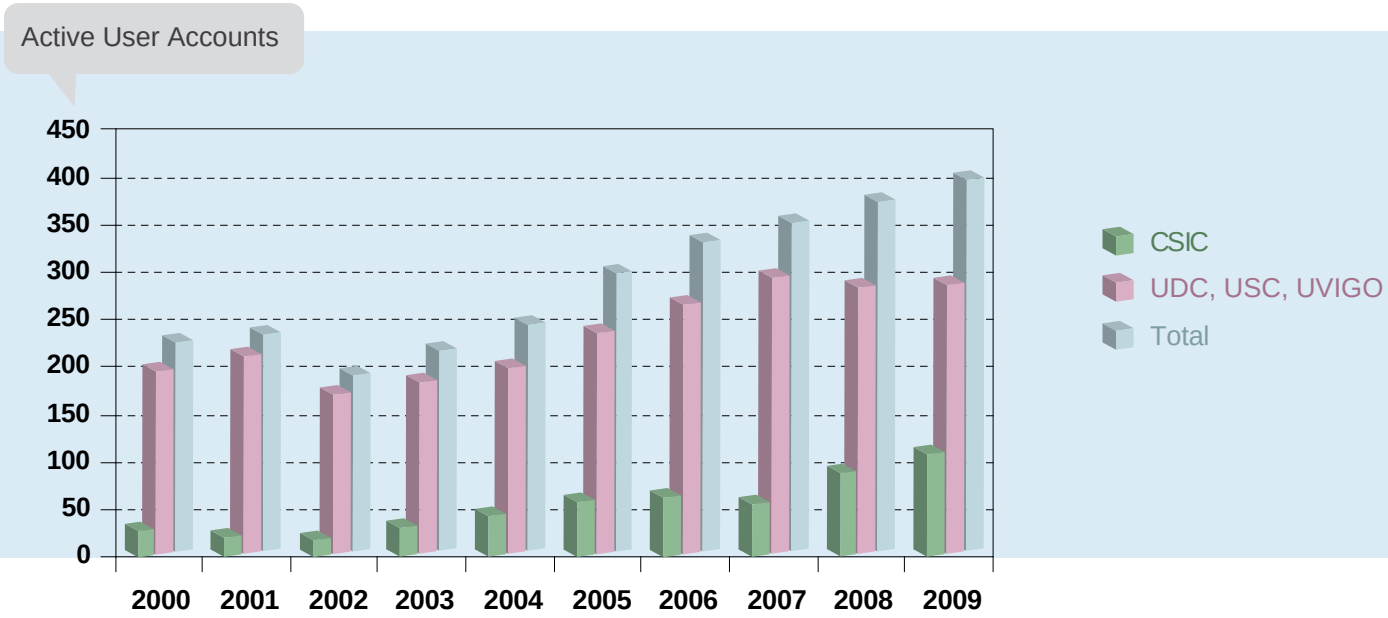


Number of Active User Accounts

Finis Terrae is the system with the greatest number of active accounts (that is, users with significant CPU time consumption throughout the year) with 363 users during its first year of operation (50 more users than the previous year).

The SVG system had 317 active user accounts, increasing by 104 that of the previous year, in addition to Grid project users that this year grew to 72 user accounts which belong 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 the National Grid Initiative, RETELAB and CYTEDGRID, and regional projects such as FORMIGA and G-FLUXO). In total, the number of active accounts decreased from 986 in 2008 to 809 in 2009 because the number of production systems were reduced from 5 to only 2 (Superdome integration into FinisTerrae and HPC320 decommissioned), which simplifies the usage of the supercomputer by the users.

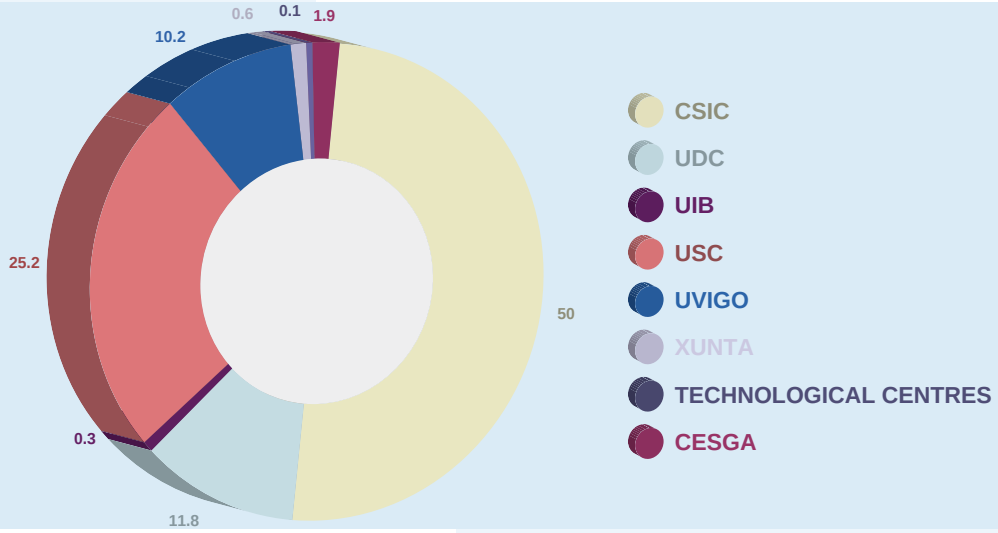
active user account evolution per institution per year 2000 - 2009



Distribution by Institutions of the CPU Hours Consumed in all Systems

All user institutions increased the CPU hours with respect to the previous year. There was a 57% increase in the number of hours used. The Universidade de Santiago de Compostela (USC) and CSIC registered the greatest number of computing hours used. The USC consumed 25.2% of the total hours (10.6% less than in 2008) but increased the number of CPU hours from 3.6 million to 3.9 million this year. CSIC grew from 35.8% in 2008 to 50% in 2009. As a whole, the three Galician universities represent 47% of the total consumption (decreasing from 53% during the previous year, increasing to more than 2 million CPU hours in the current year). The projects in which CESGA participated were responsible for only 2.4% of the hours consumed (down from 11.2% for the previous year, mainly because challenges of this year are registered to their respective institution).

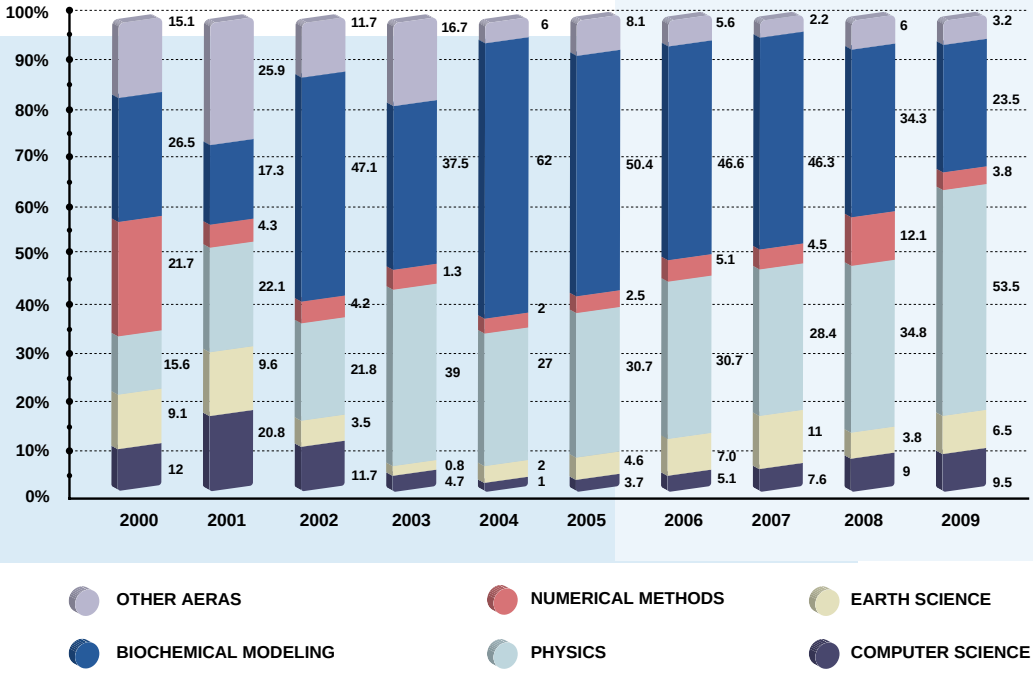
cpu use distribution by institution in 2009



CPU Distribution by Research Area

The computing time related to Computational Physics research represents 53.5% of the consumption (up from previous year figures of 34.8%), surpassing Biochemical Modelling for the second time which represents 23.5% (14.3% less than in 2008). These two areas account for 77% of the total hours consumed. It is also important to highlight the steady increase in the area of Computing Science since 2004.

cpu use distribution by research area 2000 - 2009

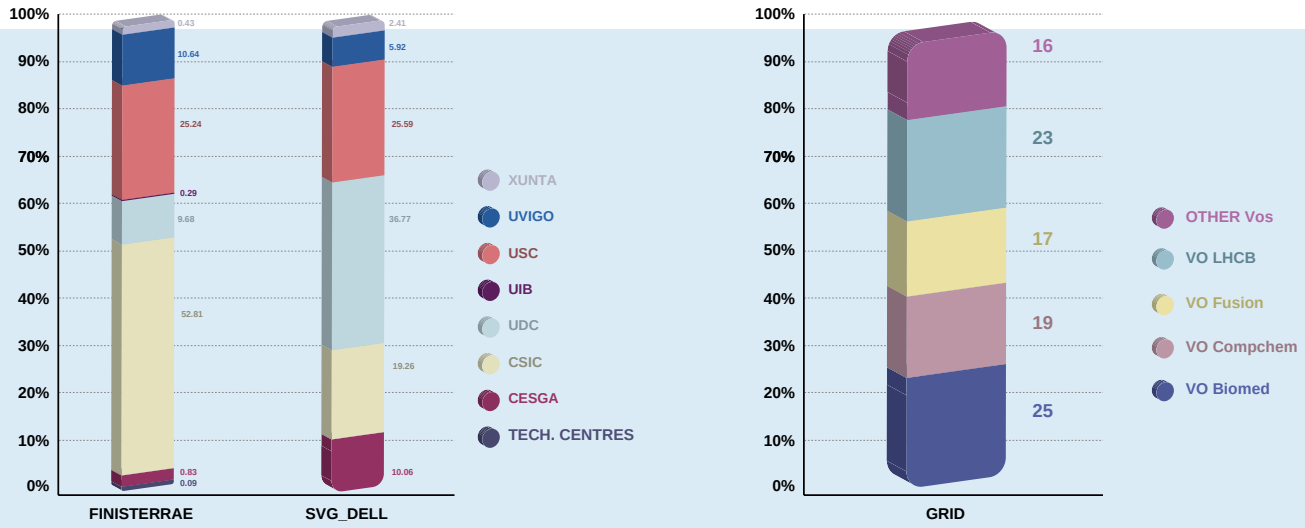


CPU Usage Distribution by Institution and Machine

In this graphic, we can see which of the systems are most demanded by each of the institutions that use the computing servers at CESGA. It can be easily appreciated that CSIC researchers mainly utilise the FinisTerrae server registering more than 50%, while the SVG is shared mainly by the researchers of the Universities of Santiago de Compostela and A Coruña, allthough there is an increase of CSIC active user accounts in SVG from 12.1% to 19.3%.

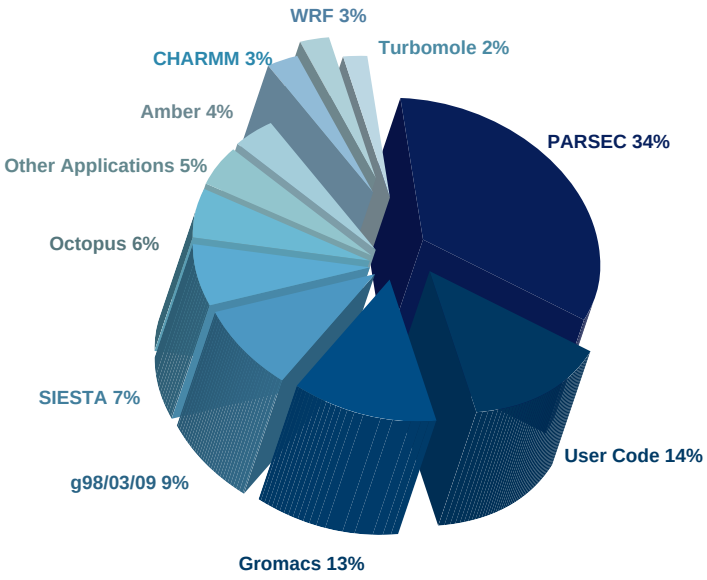
Grid systems are fundamentally used by Biomed, LHCb, Compchem, and Fusion international Virtual Organizations.

cpu usage distribution by institution and machine in 2009

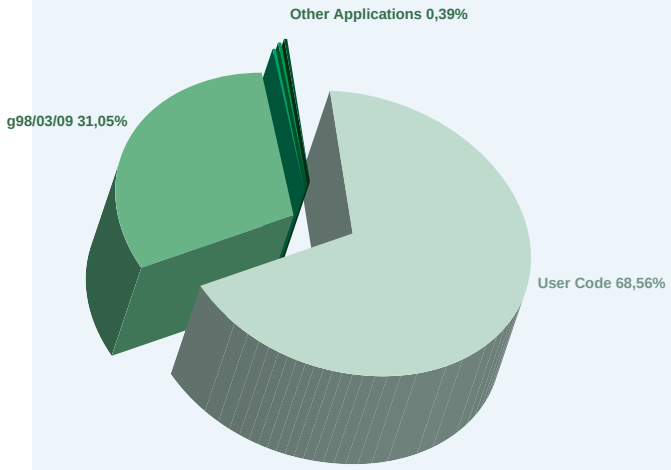


Application Use per Institution

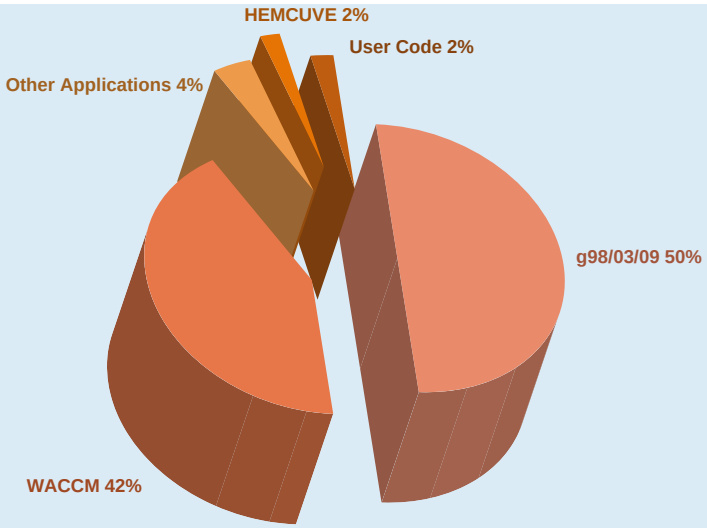
Applications use by USC users in 2009



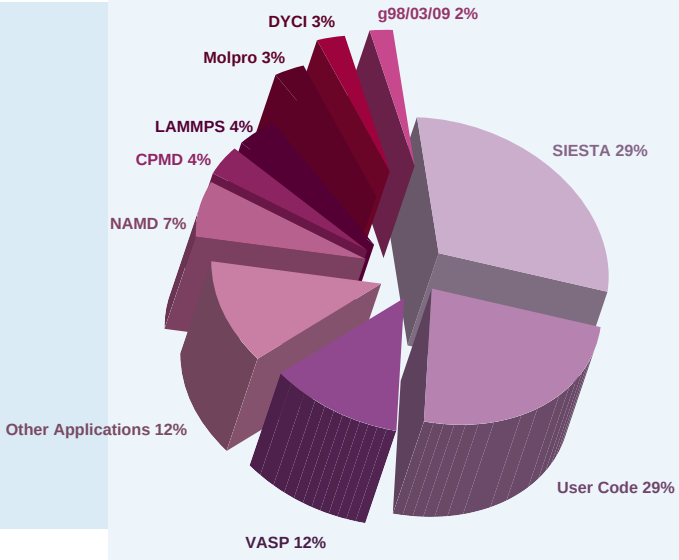
Applications use by UDC users in 2009



Applications use by UVIGO users in 2009

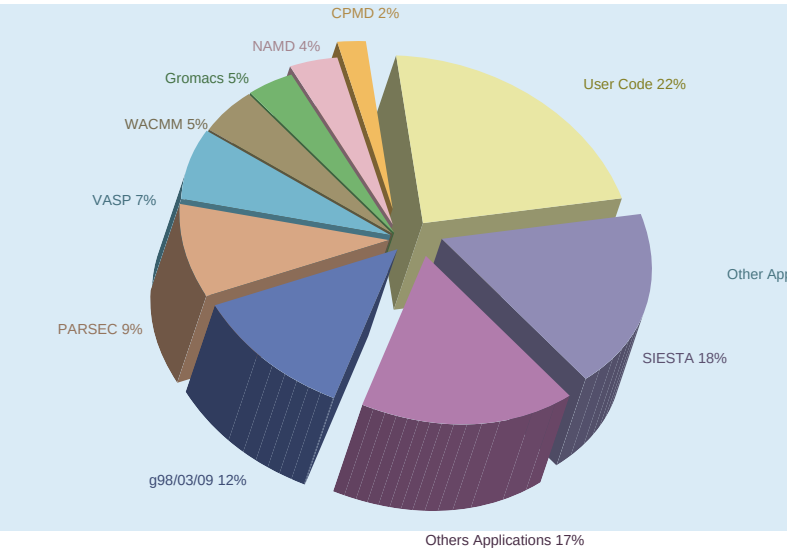


Applications use by CSIC users in 2009

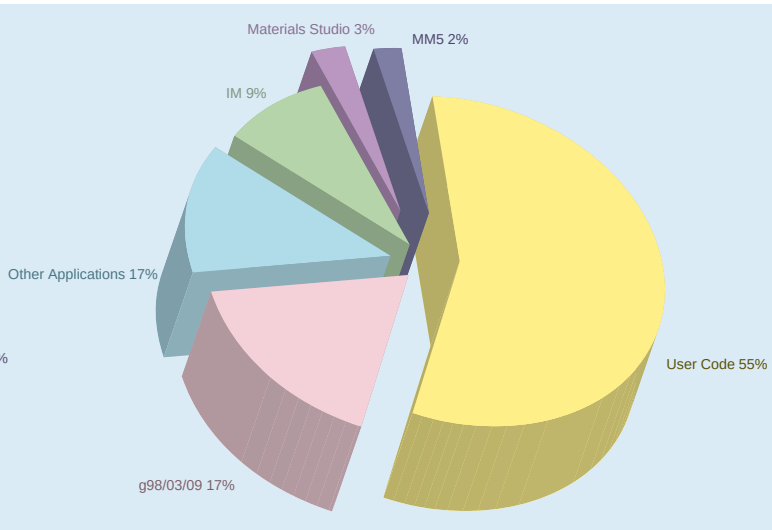


Application Use per System

Applications use in FinisTerrae Server in 2009



Applications use in SVG Server in 2009



CSIC USERS 2007-2009

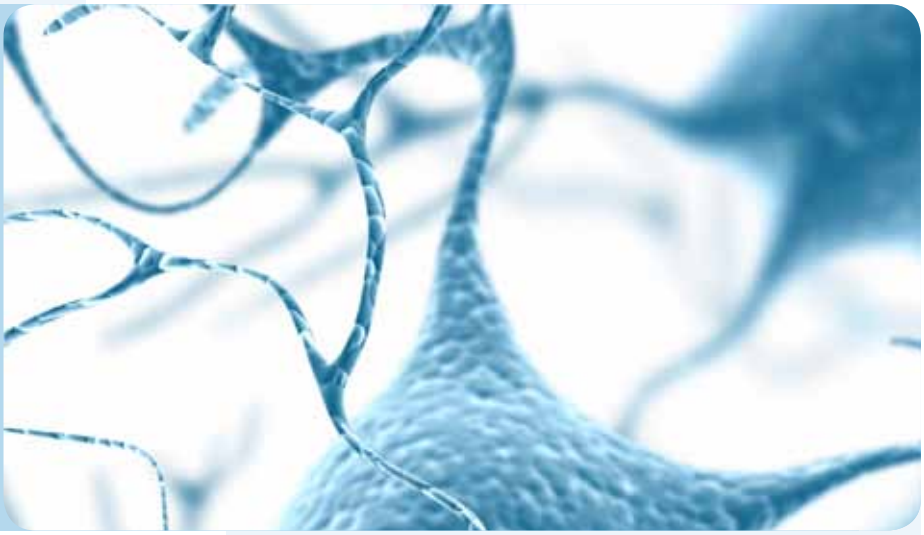
CSIC CENTRES	Dept. / Research Group	# active user accounts			CPU hours used		
		2007	2008	2009	2007	2008	2009
NATURAL RESOURCES AREA							
Estación Biológica de Doñana (EBD)	Ecología de Humedales, Genética de la Conservación en Peces Litorales	0	1	0	0	75	0
	Biología Evolutiva; Integrative Ecology Group	1	4	5	447	26,420	44,638
	Genética de la Conservación	2	4	7	12,182	29,125	94,653
Institut Mediterrani d'Estudis Avançats (IMEDEA)	PANDORA	0	1	1	0	67	11,324
Centre d'Estudis Avançats de Blanes (CEAB)	Oceanografía Operacional	0	1	2	0	1,392	52,695
MATERIALS SCIENCE AND TECHNOLOGY AREA							
Instituto de Ciencia de Materiales de Barcelona (ICMAB)	Estructura Electrónica de Materiales	0	11	11	0	635,177	2,016,049
	Departamento Teoría y Simulación de Materiales	0	2	4	0	12,783	668,296
	Nanociencia Molecular y Materiales Orgánicos	0	0	1	0	0	404
Instituto de Ciencia de Materiales de Aragón (ICMA)	Química Orgánica	1	1	1	48	5,804	42,299
	Química de los Compuestos Organometálicos	1	0	1	283	0	285
	Química/Grupo Síntesis Orgánica Estereoselectiva	1	1	1	19,088	48,016	70,839
	Grupo de Síntesis Química de la Rioja1	0	0	2	0	0	15,393
Instituto de Ciencias de Materiales de Sevilla (ICMS)	FQM282	0	1	1	0	20,850	350,807
	Superficies, Intercapas y Capas Finas	0	1	2	0	48,512	180,246
Unidad Asociada CSIC-LABEIN	Unidad de Materiales Nanoestructurados y Ecoeficientes para Construcción	1	1	1	13,193	253,738	406,930
Instituto de Ciencia y Tecnología de Polímeros (ICTP)	Química Macromolecular	1	1	1	8,242	22,362	41,830
Centre d'Investigació en Nanociència i Nanotecnologia (CIN2) Barcelona	CIN Theorie and Simulation	0	0	2	0	0	321,913
	Nanophononics and Nanophotonics	0	0	1	0	0	1
Instituto de Ciencia de Materiales de Madrid ICMM	Teoría Intercaras y Crecimiento	0	0	4	0	0	655,548
SOCIAL SCIENCE AND HUMANITIES AREA							
Instituto de Análisis Económico (IAE)	Instituto de Análisis Económico	0	1	1	0	1,924	4,408

CSIC USERS 2007-2009

CSIC CENTRES	Dept. / Research Group	# active user accounts			CPU hours used		
		2007	2008	2009	2007	2008	2009
CHEMICAL SCIENCE AND TECHNOLOGY AREA							
Instituto de Investigaciones Químicas (IIQ)	Grupo de Carbohidratos	0	1	1	0	2,453	1,256
	Departamento de Química Inorgánica y Catálisis	0	0	1	0	0	10,075
	Grupo de Síntesis Orgánica y Reconocimiento Molecular	0	1	0	0	17	0
Centro de Investigación y Desarrollo (CID)	Centro de Investigación y Desarrollo	1	0	0	5,072	0	0
Instituto de Catálisis y Petroleoquímica (ICP)	Grupo de Catálisis Fundamental y Aplicada	2	1	1	11,130	541,366	129,020
Instituto de Investigaciones Químicas y Ambientales de Barcelona (IQAB)	Química Teórica y Computacional	0	5	5	0	122,446	123,412
Instituto de Química Médica (IQM)	Quimioterapia	2	2	2	14,911	1,506	814
Instituto de Química Orgánica General (IQOG)	Química Orgánica Biológica	4	2	2	18,018	3,906	30,643
	Laboratorio de Radicales Libres y Química Computacional	0	2	4	0	2,489	53,850
	Productos Naturales	1	1	2	11,438	703	2,755
Instituto Nacional del Carbón (INCAR)	Texture of Materials for Energetic Applications	0	2	2	0	4,161	24,483
PHYSICS SCIENCE AND TECHNOLOGY AREA							
Instituto de Física de Cantabria (IFCA)	Departamento de Estructura de la Materia; Grupo de Física Estadística y No Lineal	1	1	1	41	19,376	18996
	Departamento de Astrofísica, Grupo CMB	1	0	0	90	0	0
	Computación Distribuida	0	0	1	0	0	0
Instituto de Física Fundamental (IMAFF)	Departamento de Física Atómica y Molecular Teórica	7	10	9	18,263	534,929	1,033,042
Instituto de Matemáticas (ICMAT)	Matemáticas	3	3	5	4,486	76,545	458,035
Instituto de Física Teórica (IFTE)	Instituto de Física Teórica	0	0	1	0	0	187,702
Instituto de Investigación en Inteligencia Artificial (IIIA)	Multi-Agent Systems	0	0	3	0	0	24,130
Instituto de Ciencias del Cosmos (ICE-ICC)	Grupo formación de Galaxias	0	0	1	0	0	971
Instituto de Estructura de la Materia (IEM)	Departamento de Física Molecular	3	3	2	4,282	743,093	196,878
	Instituto de Estructura de la Materia	4	3	2	3,979	159,260	27,510
	Departamento de Astrofísica Molecular e Infrarroja	5	5	3	74,003	102,699	269,116

CSIC USERS 2007-2009

CSIC CENTRES	Dept. / Research Group	# active user accounts			CPU hours used		
		2007	2008	2009	2007	2008	2009
BIOLOGY AND BIOMEDICINE AREA							
Centro Andaluz de Biología Molecular y Medicina Regenerativa (CABIMER)	Terapia Celular y Medicina Regenerativa	0	0	1	0	0	147
Centro de Investigaciones Biológicas (CIB)	Estructura y Función de Proteínas	3	1	1	13,888	41,977	18,619
	Microscopía Electrónica de Macromoléculas	1	1	0	1,066	1,223	0
	Grupo de Resonancia Magnética Nuclear	3	3	1	4,649	1,099	189
Centro Nacional de Biotecnología (CNB)	Evolución de Relaciones Planta Animal	0	2	1	0	17,356	46
	Estructura de Adenovirus	0	1	2	0	86,395	108,129
	Departamento de Estructura Macromolecular	0	4	3	0	8,484	7,596
Instituto Cajal (IC)	Neurobiología del Desarrollo	1	1	2	16,681	550	60,594
Centro de Biología Molecular Severo Ochoa (CBM)	Diseño Racional de Enzimas - BioWeb	0	1	1	0	20,043	511
AGRICULTURAL SCIENCE AREA							
Estación Experimental del Zaidín (EEZ)	Ciencias de la Tierra y Química Ambiental/Química Teórica y Modelización Molecular	7	3	2	80,929	6,941	50,107



UNIVERSITY USERS 2007-2009

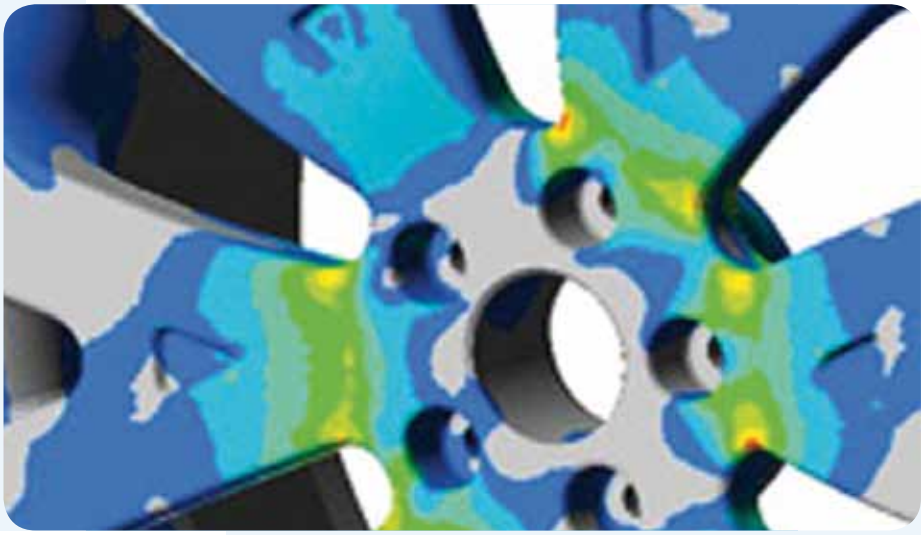
CENTERS	Department- Group	# of Active User Accounts			Hours used		
		2007	2008	2009	2007	2008	2009
UDC - Universidade da Coruña							
Escuela Politécnica Superior	Enxeñería Naval e Oceánica	0	1	2	0	2	444
	Ingeniería Industrial II	1	0	0	0	0	0
Escuela Técnica Superior de Arquitectura	Tecnología de la Construcción	3	1	1	477	0	27
Escuela Técnica Superior de Ingenieros de Caminos, Canales y Puertos	Métodos Matemáticos	3	1	0	4,666	2,184	0
Facultad de Ciencias	Biología Animal	1	0	0	141	0	0
	Química, Física e Ingeniería Química I	12	9	8	183,711	272,020	314,682
	Química Fundamental	29	17	24	169,950	368,518	247,399
Facultad de Informática	Computación	2	1	0	2,519	261	0
	Electrónica y Sistemas	4	15	16	600	93,023	83,461
	Tecnoloxías das Informacións e as Comunicacións	2	5	7	77,804	357,049	1,207,811
UDC Genérico	UDC Genérico	38	36	53	25,919	14,392	1,676
USC - Universidade de Santiago de Compostela							
Escuela Técnica Superior de Ingeniería	Ingeniería Química	4	3	0	58	27	0
Facultad de Farmacia	Bioquímica y Biología Molecular	0	0	1	0	0	0
	Farmacología	1	2	2	1,251	87,799	211,247
Facultad de Física	Electrónica e Computación	14	18	13	17,379	63,022	103,372
	Física Aplicada	28	27	18	366,451	1,935,482	1,040,604
	Fisica de la Materia Condensada	8	14	15	3,606	936,626	1,484,693
	Física de Partículas	10	9	10	180,546	87,728	122,819

UNIVERSITY USERS 2007-2009

CENTERS	Department- Group	# of Active User Accounts			Hours used		
		2007	2008	2009	2007	2008	2009
USC - Universidade de Santiago de Compostela							
Facultad de Matemáticas	Alxebra	0	1	1	0	191	522
	Estadística e Investigación Operativa	1	1	0	829	1,370	0
	Matemáticas aplicadas	4	2	1	175	1	73
Facultad de Química	Química Física	24	20	19	110,275	334,916	376,811
	Química Inorgánica	3	1	1	4,029	61	0
	Química Orgánica	30	28	30	97,855	152,731	436,064
Escuela Universitaria de Ingeniería Técnica Industrial	Instituto de Acuicultura	0	1	0	0	0	0
Instituto de Medicina Legal	Instituto de Medicina Legal	5	3	3	145	890	178,953
USC Genérico	USC Genérico	33	31	21	83	193	357
UVIGO - Universidade de Vigo							
E.T.S. de Ingenieros de Telecomunicación	Ingeniería Telemática	2	1	1	11,714	0	825
	Matemática Aplicada	1	1	0	0	433	0
	Teoría de la Señal y Comunicaciones	4	3	3	124	167,433	30,469
E.T.S. de Ingenieros Industriales	Ingeniería Eléctrica	0	1	1	0	0	0
E.U. de Ingeniería Técnica Industrial	Departamento Informática y Diseño en Ingeniería	0	1	1	0	3	3
Facultad de Biología	Bioquímica, Genética e Inmunología	0	1	2	0	71	355
Facultad de Ciencias del Mar	Física Aplicada	8	12	9	31,180	54,687	676,197
Facultad de Química	Química Analítica y Alimentaria	12	12	10	57,083	83,356	308,561
	Química Física	4	1	6	3,868	13,642	111,794
	Química Inorgánica	0	1	1	0	1,342	3,015
	Química Orgánica	11	11	13	66,122	302,443	475,159
UVI Genérico	UVI Genérico	0	0	1	0	0	0

UNIVERSITY USERS 2007-2009

CENTERS	Department- Group	# of Active User Accounts			Hours used		
		2007	2008	2009	2007	2008	2009
METEOGALICIA - Xunta de Galicia							
METEOGALICIA	MeteoGalicia: Predicción e Investigación Numérica	1	3	1	50,006	130,657	92,552
CTAG - Centro Tecnolóxico de Automoción de Galicia							
Centro Tecnolóxico de Automoción de Galicia	Desarrollo Tecnológico en la Industria de la Automoción de Galicia	0	2	1	0	2,658	12,466
CESGA - Centro de Supercomputación de Galicia							
CESGA	CESGA Genérico	66	289	233	76,506	996,729	291,342
UIB - Universitat de les Illes Balears							
Física	Física	0	0	2	0	0	38,709
Química	Química	0	0	1	0	0	2,892



Computational Challenges

In 2009, three computational challenges were tackled using FinisTerrae. A “computational challenge” is a large computational problem never before solved or executed, that now can be approached thanks to the computational power of supercomputers.

Tropopause’s Climate Change Atmospheric Modelling with High Resolution

Researchers from the University of Vigo, Department of Applied Physics, Faculty of Sciences of Ourense, directed by Juan Antonio Añel Cabanelas with the help of CESGA staff, addressed the tropopause simulation using the high resolution WACCM model, taking into account different radiation balances as well as variations in water vapour.

This challenge is designed to simulate climate changes that will occur in the tropopause due to changes in the radiation balance. To do this, different radiation balance schemes will be introduced. The study of variations in the water vapour concentrations (one of the most significant greenhouse gases) may be contemplated as well.

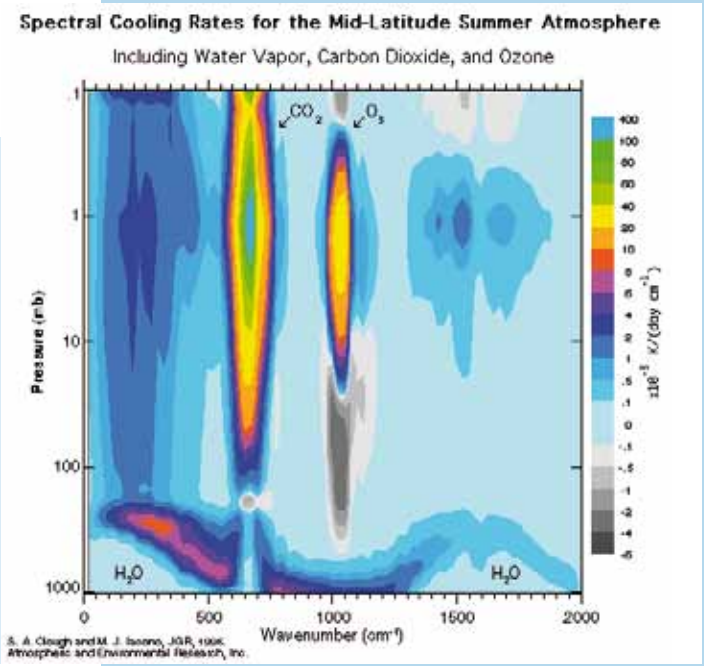


Illustration: Spectral longwave cooling rates as computed by the Line-By-Line Radiative Transfer Model (LBLRTM) for the mid-latitude summer atmosphere at a resolution of 25 cm-1 [1]

WACCM has been executed using pure MPI while harnessing the hybrid possibilities present in FinisTerrae (Infiniband / shared memory). Due to the non-local nature of transport calculations and fluid dynamics, WACCM3 demands very high performance when carrying out the communication between tasks. For the version with a horizontal resolution of 2° x 2.5°, it is roughly estimated that ~60MB of data is transferred for each "time step" associated with each MPI task. Most of this communication takes place during the advection of chemical species which, by nature, is a non-local program.
FinisTerrae's hybrid MPI computing power (Infiniband /Shared Memory) was demonstrated to be essential for those calculations.

The obtained results have permitted the study of the changes in the field of potential vorticity of the Earth for the upper troposphere/lower stratosphere (UTLS) with a very fine structure. [2]

Moreover, this version of WACCM with high vertical resolution in the UTLS has obtained one of the best results with respect to reproducing the UTLS. It will be published by the World Meteorological Organization in the upcoming CCMVal report of the evaluation of Chemistry-Climate Models.

[1] Clough, S. A., and M. J. Iacono (1995), Line-by-line calculation of atmospheric fluxes and cooling rates 2. Application to carbon dioxide, ozone, methane, nitrous oxide, and the halocarbons, J. Geophys. Res., 100(D8), 16,519–16,535.

[2] A. Gettelman, M. Hegglin, S.-W. Son, M. Fujiwara, S. Tilmes, L. Pan, P. Hoor, H. Lee, G. Manney, T. Birner, G. Stiller, M. Rex, S. Kremser, D. Wuebbles, K. Walker, J. A. Añel, Upper Troposphere and Lower Stratosphere (UTLS) in SPARC CCMVal, SPARC CCMVal Report on the Evaluation of Chemistry-Climate Models, V. Eyring, T. G. Shepherd, D. W. Waugh (Eds.), SPARC Report No. 5, (in press).

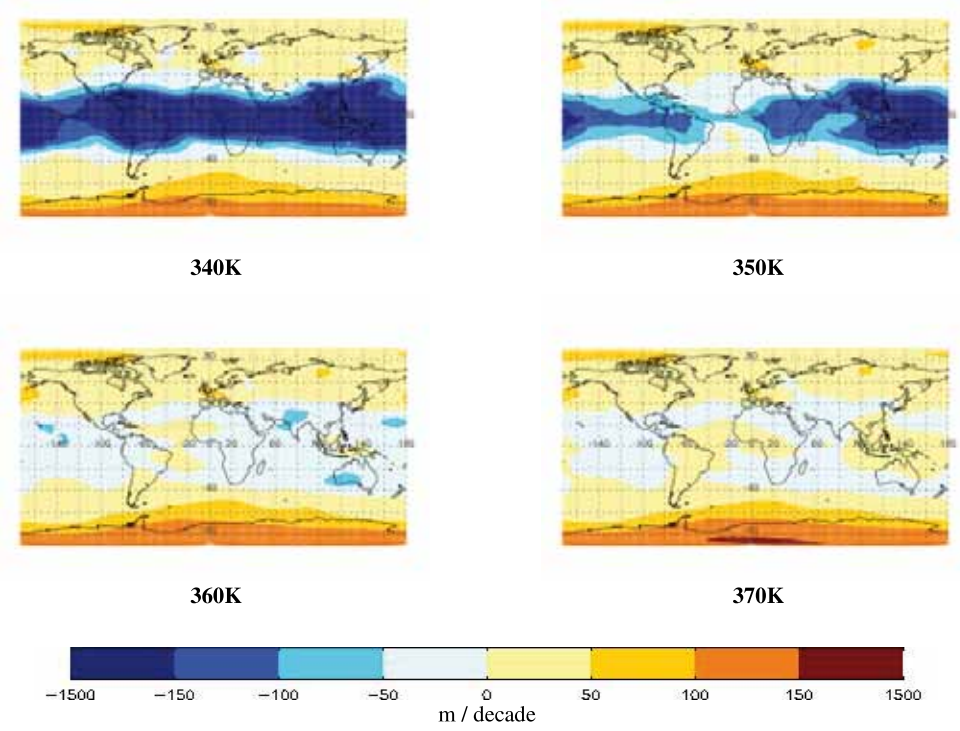


Illustration: Trend of the geopotential height (m/decade) for the period 1979-2006 for different isentropic levels obtained with the high vertical resolution version of WACCM run on FinisTerrae

Dynamic Enzyme Response against Temperature.

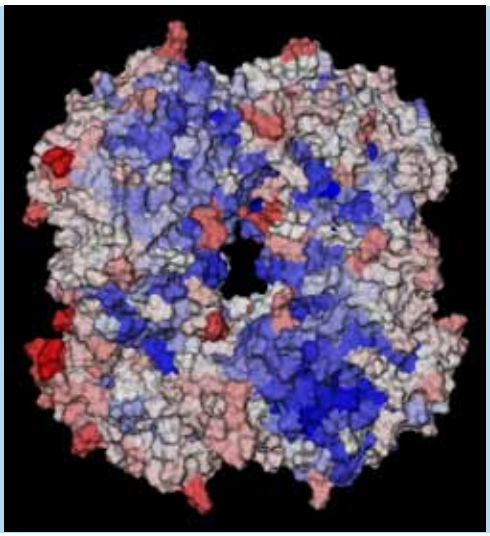
Researchers at the Institut de Química Avançada de Catalunya led by Ramon Crehuet Simon, with the help of CESGA staff, are making computer simulations of molecular dynamics. These simulations help to better understand the relationship between the structure/dynamic/enzyme activity. The enzymes have been simulated at different temperatures in order to study the response of the protein dynamics to temperature. Understanding the structural cause of the different behavior is a fundamental scientific question at the interface of chemistry and biology. Future applications will be relevant for drug design and biotechnology. The simulation of these enzymes of very high molecular weight is made with molecular dynamics calculations of hundreds of nanoseconds in order to obtain results on scales comparable with those of other experiments in the same field.

The software used for the execution is GROMACS 4.0 which offers improved scaling and maintains the high efficiency which characterizes this code.

The vast amount of CPU time required to carry out these simulations demanded an initial effort to establish proper scaling of this application in FinisTerrae. It was necessary to find the correct topology of processes that allowed for proper load balancing.

The simulations aim of this challenge has been achieved thanks to a scaling of 72 processes with a topology of 8 processes per FinisTerrae node used. It produced a computational capacity greater than 10 nanoseconds per day.

Figure 1 shows the mobility of different parts of the enzyme, color coded from blue (static) to red (dynamic). The non-homogeneous distribution is caused by the internal structure of the protein and is, presumably, related to its function. Enzymes from different organisms demonstrate different mobility distributions



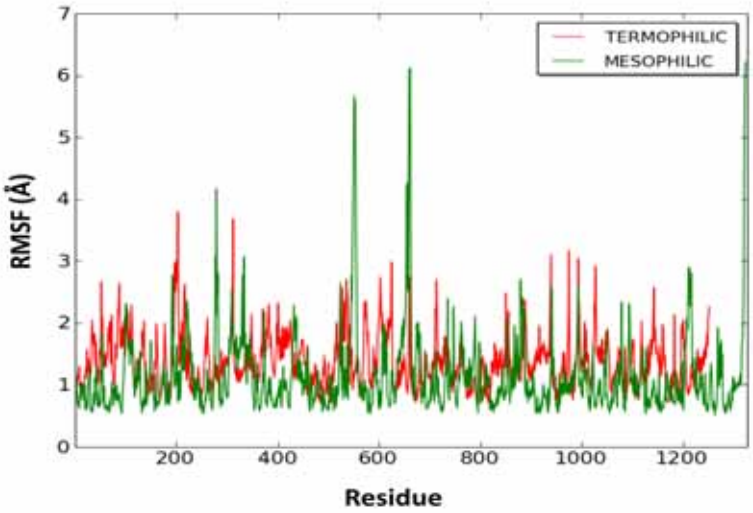


Figure 2 shows the Root Mean Square Fluctuation (which measures flexibility) of a mesophilic-thermophilic pair of enzymes. Mesophilic enzymes are unstable at high temperatures, whereas thermophilic enzymes have highest activity at these elevated temperatures. One can see that, although the thermophilic enzyme is more flexible, its flexibility is more homogeneous. On the contrary, the mesophilic organism has some regions of extremely high mobility which can potentially lead to denaturation of the enzyme and, consequently, loss of function.

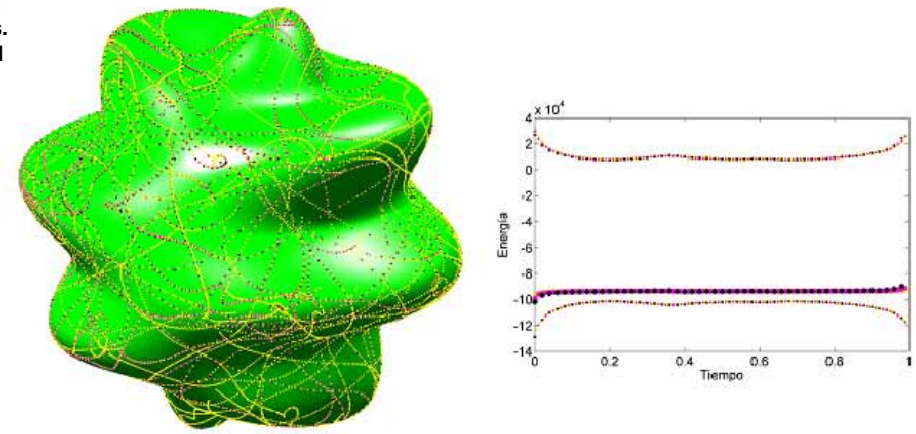
Application of the Method of Forces to the protein folding problem.

VARIDIS Group researchers from the Department of Applied Mathematics III at the Universitat Politécnica de Catalunya led by Enrique Bendito, along with staff from CESGA, began the implementation of this computational challenge at the end of 2009. The results will have a wide application in the Molecular Dynamics field.

The main goal of this challenge is to move forward in the development of numerical methods for integration of Newton's motion equations of complex mechanical systems, with particular emphasis in the problem of protein folding.
The Forces Method was initially designed for the numerical solution of the Fekete problem, namely the minimization of potential energy functionals dependent on the relative distances between an N particles system.
Fekete's problem is static. However, the problem of solving Newton's equations can be reduced to a Fekete problem using the principle of least action.

The goal in this challenge is to study the applicability of the Forces Method in solving problems of least action with potential energy functionals, which simulates the dynamic behaviour of molecular systems.
The Force Method main routine is well known by the CESGA technical team. Its good scalability properties have already been tested previously in FinisTerrae; its shared memory architecture facilitates the parallel execution of such problems.
For the application to Molecular Dynamics, it is necessary to distinguish between real particles (N) and virtual (actual positions of the particles in M +1 time steps). Under these conditions, each iteration of the Force Method has an MN^2 order cost. The N^2 factor corresponds to the previously parallelised part. The M factor parallelisation, corresponding to the different time steps, is trivial.

Illustration 1: Action minimization using different sets of parameters. On the right, kinetic, potential and total energy time evolution.



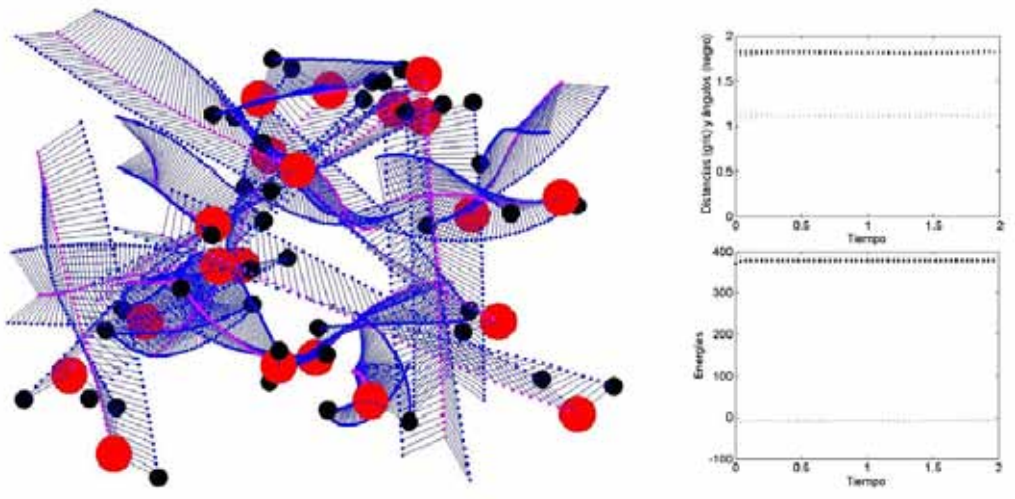


Illustration 2: Action minimization. Final trajectories

Computing Infrastructure

Different architectures of high-performance computing systems are available for the 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 2009 regarding computing servers were:

- the operation of FinisTerrae, and
- users employed more than 15 million CPU hours.

In 2009, CESGA focused its efforts on improving FinisTerrae's service and on user support.

This system ranked number 100 on the TOP500 list of November 2007 and began operation in February 2008 in order to start working on relevant computational challenges. Finis Terrae was made available to all users on April 1st, 2008.
In 2009, the following computing servers were available to users:

COMPUTING SERVERS IN 2009

HIGH PERFORMANCE COMPUTING SERVERS

SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
FINIS TERRAE	2008	SMP (NUMA) CLUSTER	2,580 CORES, 20 TB, 16 TFLOPS

HTC 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

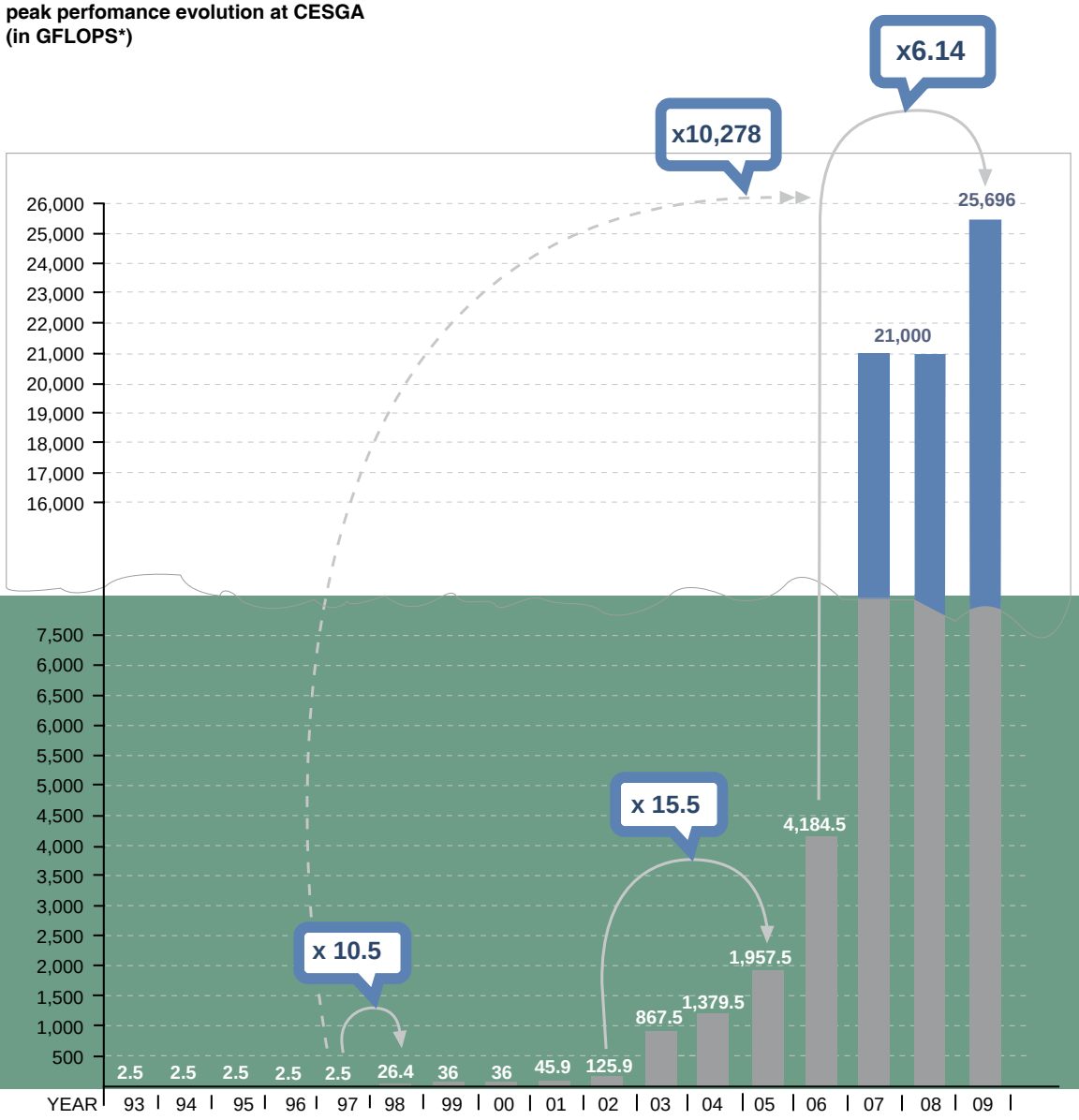
SERVERS FOR PROJECTS

SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
CLOUD PLATFORM	2009	PC CLUSTER	324 CORES, 576 GB MEMORY, 16 TB DISK
eIMRT	2009	2 NODES	4 CORES, 8 GB MEMORY, 770 GB DISK
SmartLM	2009	1 NODE	1 CPU, 1 GB MEMORY, 160 GB DISK
SIFI-GALICIA	2008	1 NODE	2 CPU, 2 GB MEMORY
RETELAB	2008	PC CLUSTER	32 CORES, 32 GB MEMORY, 288 GB DISK
Rede Galega de Bioinformática	2009	1 NODE	8 CORES + 1 GPU Tesla, 12 GB MEMORY, 146 GB DISK

SERVERS HOUSED AT CESGA

SERVERS	YEAR INSTALLED	ARCHITECTURE	PROCESSORS, MEMORY, PEAK PERFORMANCE
LHCb-USC	2002-2008	PC CLUSTER	339 CORES, 312 GB MEMORY, 1,600 GFLOPS
RGB	2009	PC CLUSTER	2 QUAD-CORE P.U. INTEL X5,520 NEHALEM 12 GB MEMORY, 146 GB DISK, 1 GPU TESLA C 1,060

peak perfomance evolution at CESGA
(in GFLOPS*)

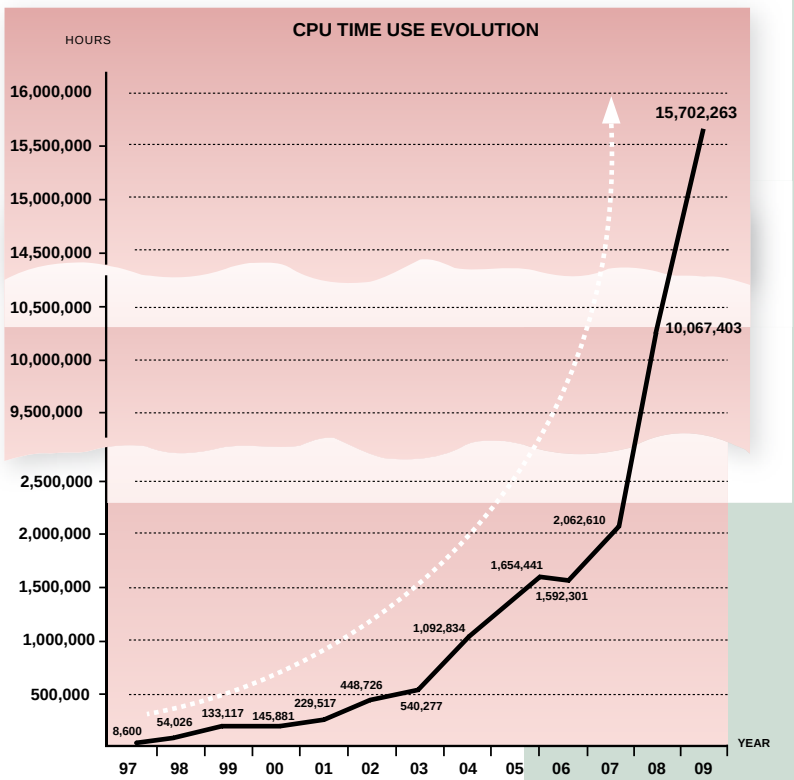


*** 1GFLOPS= 1,073,741,824 (floating point operations per second)**

Evolution of CPU Consumption

During 2009, the FinisTerrae system and the SVG cluster were the available servers at CESGA. In this year, a full integration of the Superdomes into FinisTerrae was completed and users had only 2 architectures to choose from, which simplifies usage. The number of hours consumed increased significantly, incrementing the total by 57%, from 10,067,403 hours in 2008 to 15,702,263 hours in 2009.

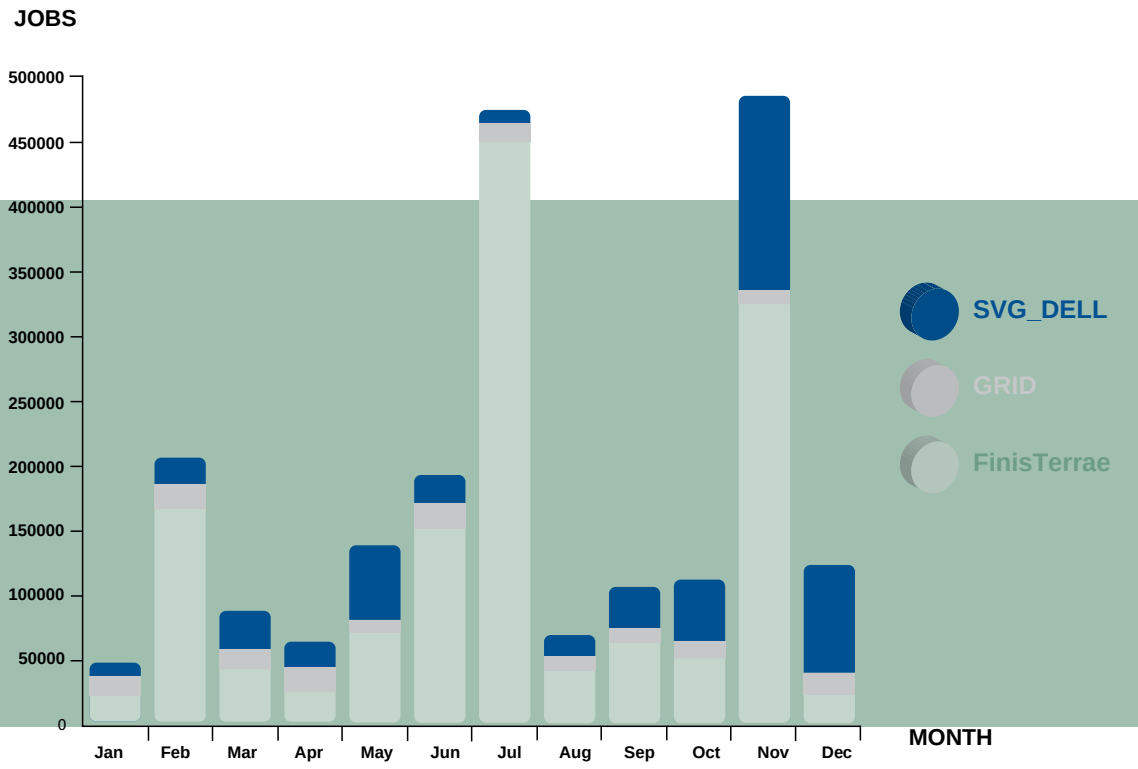
CPU time usage evolution in hours 1997 - 2009



Number of Jobs Executed

The number of jobs executed represents the quantity of simulations that users performed on each computing server. This value does not depend only on the available computing capacity but also on the resources necessary for the execution of the simulations.

Simulation jobs executed per system per month in 2009



Average in-queue time

The average in-queue time represents 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.

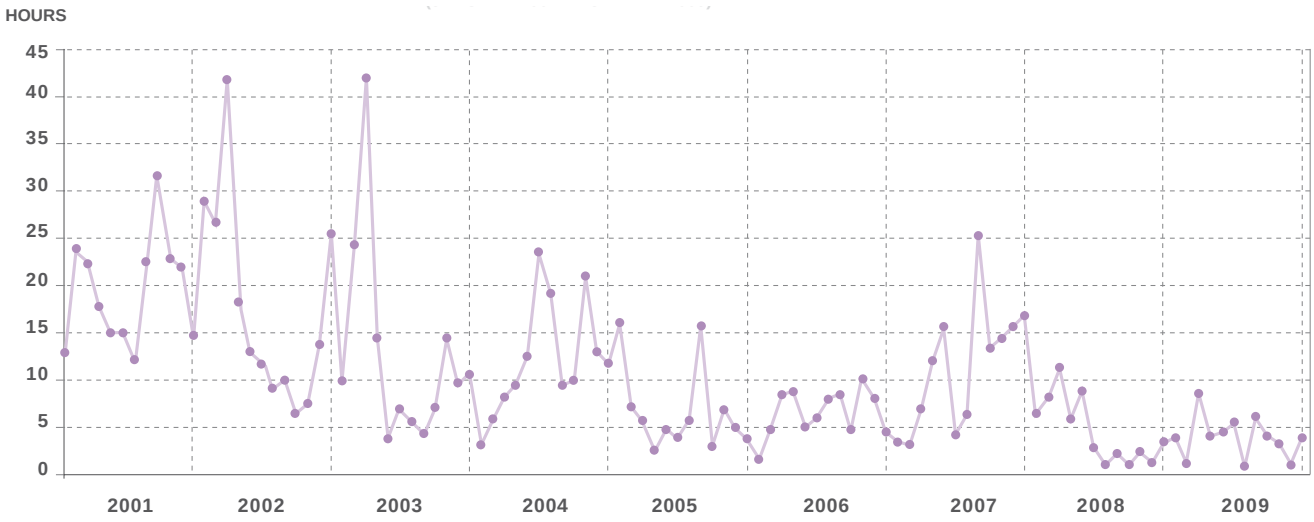
This time varies as a function of the quantity of simulations that are being performed and, desirably, it should be the closest possible to zero in order that users do not have to wait much time until they receive the results of their simulations.

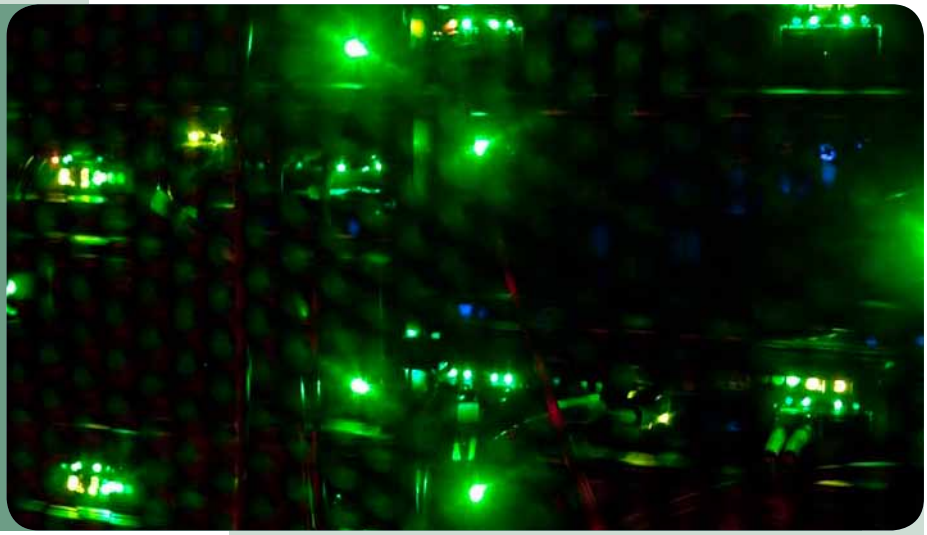
Logically, the higher the computing systems occupation level, the longer the waiting time necessary until the required resources are available. This average is a good indicator of the level of saturation that exists in the computational resources.

Usually, the waiting time decreases in summer and during the winter holidays, and increases significantly as new users are incorporated.

In summary, the waiting time has decreased significantly thanks to the incorporation of the FinisTerrae server. From an average of more than 7 hours in 2007, it decreased to an average of only 2 hours for all computing servers in 2008. However, in 2009 the FinisTerrae system was used more which increased demand on the system and raised the waiting time to an average of 3 hours.

Average in-queue time for all processes in all systems
(January 2001 - December 2009)





HPC: High performance computing servers

High performance computing systems involve machines designed to solve a reduced number of problems 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 2009, the users had access to one high performance system, FinisTerrae, a SMP NUMA Cluster.

FINISTERRAE	SMP NUMA CLUSTER TECHNICAL SPECIFICATIONS
COMPUTER	Integrity r x 7640/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
INTERCONNECT NODE	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

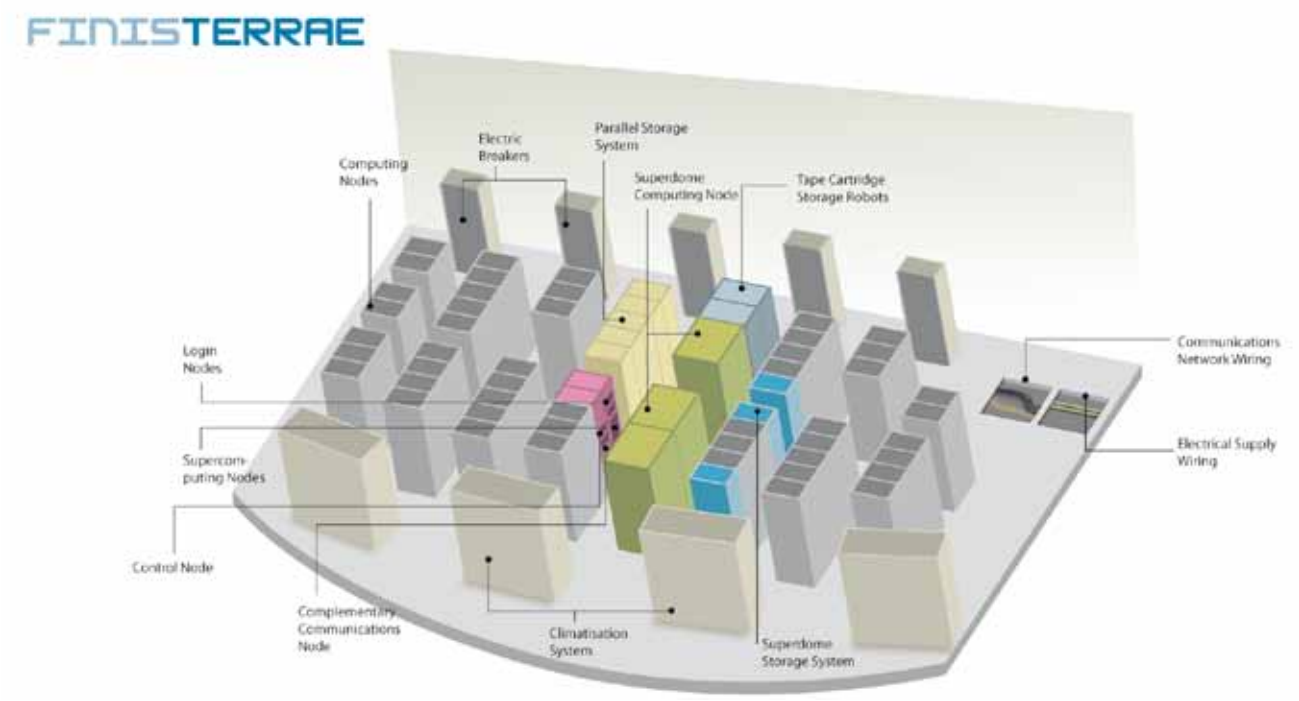
FinisTerrae

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



Cloud and HTC: Cloud computing to provide high throughput computing, grid servers, and specific project servers

CESGA offers different architectures designed to solve a large number of problems with diverse 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.

In 2006, CESGA acquired a DELL Blade Cluster with 292 processing cores, 148 GB of memory, and peak performance of 2,227 GFLOPS. This cluster was integrated into the Galician Virtual Supercomputer (SVG). In 2007, 32 processors and 32 GB of memory were added.

SVG reflects the wager that the Centre made in 1999 to provide low cost cluster systems as an ideal solution to the increased demand 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.

Due to their characteristics, the HTC servers installed at CESGA are used in GRID experiences and projects. Last year, CESGA deployed cloud computing services with the acquisition of a cloud platform.

housing of computing equipment

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 at 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.

Galician Bioinformatics Network (RGB)

Galician Bioinformatics Network (RGB) is an initiative that aims to structure and integrate research and teaching activities in Bioinformatics performed in Galicia, fostering cooperation and competitiveness in this research area of maximum interest for Biology and Biomedicine. Since September 2007, for a minimum of 2 years (extendable for another year), the RGB has been funded by the Galician Regional Ministry of Education and Universities (Xunta de Galicia), within the program "Network Research's Structure". RGB houses a server at CESGA with 2 quad-core Nehalem Intel X5520, 12GB memory, 146GB disk, and 1 Tesla C1060 GPU.

Servers for projects:

In addition to the HPC, HTC, and grid servers available, CESGA also houses equipment to provide service to the projects in which it participates that are related to its different departments such as Geographic Information Systems (GIS), e-Learning, Grid computing, and Cloud.

Cloud Platform

Configuration summary:
-32-node HP ProLiant SL2x170zG6, each with a dual quad-core Intel e5520 (Nehalem), and 16 GB of Advanced Calculus,
- 1 node HP ProLiant DL160G6 with dual quad-core Intel X5570 (Nehalem) and 32GB of memory,
- 1 HP ProLiant DL165G6 node with two six-core processors AMD Opteron 2435 and 32 GB of memory, and
- 6 HP ProLiant DL180G6 nodes with dual quad-core Intel e5520 (Nehalem) with 16 TB of total storage.

eIMRT II

(Last year known as BEinGRID and, since December, eIMRT II)
2 servers:
A virtualized server
- Project: BEinGRID and eIMRT II
- Processors: 2 Intel Xeon E5440 virtual cores with 2.83GHz
- Memory: 4 GB,
- Disk: 135 GB (plus a USB external disk 500 GB)
- Operating System: x86_64 GNU / Linux CentOS 4.6.

A physical server
- Project: BEinGRID and eIMRT II
- Processor: 2 Intel dual core processors CPU Xeon 3.60GHz
- Memory: 4 GB
- Disk: 135 GB
- Operating System: x86_64 GNU / Linux CentOS 4.6

significant computing initiatives in which CESGA participates

SmartLM

Project: SmartLM
Processors: 1x AMD Athlon (tm) 64 Processor 3500 +
Memory: 1 GB RAM
Hard Drive: 160 GB
Operating System: openSUSE 11.0 (64bit) (has a small partition with the original XP computer, but it is not used)
Servers: SmartLM License Server 0.9

SIFI-GALICIA

Project: Industry Analysis of the Transformation of Wood and Forestry in Galicia - the Potential Value of Using an Information System Industrial (Forest)
Number and type of processors, total memory: 2 Intel Xeon 3 GHz, 2 GB RAM
Number of servers: 1 Operating System: Microsoft Windows Server 2003

RETELAB

Project: RETELAB - A Virtual Laboratory for the National Network for thr Oceanographic Remote Sensing
Cluster formed by 4 HP ProLiant BL460c servers:
2 Intel Xeon QuadCore X5355 (8 cores per team)
Frequency: 2.66 GHz, 8 GB of RAM, and 4 x 2 MB cache (L2).
Original records: 4 x 36 GB with subsequent enlargement of 2 72 GB discs
Operating System: Scientific Linux 4.5 on the nodes and Fedora Core 6

RGB

Project: Galician Bioinformatics Network
RGB houses a server in CESGA with 2 quad-core Nehalem Intel X5520
Memory: 12 GB
Disk: 146 GB and 1 Tesla C1060 GPU

Data Storage

In 2009, capacity for massive data storage on tape was increased after the acquisition of 740 new LTO-4 tapes for the robotic cartridge libraries, reaching a total of 1360 TB. In total, available storage by the end of 2009 reached 1739 Terabytes which represented an increase of 76% with respect to the previous year.

The data storage service now uses a type of hierarchy for the stored data in order to assure the best quality of service as a function of the information (criticality of data and speed of access). There were 37 requests for storage service of which 20 had an increase in their usage quota on the computing servers, 9 concerned massive data storage and 8 concerned security copies to disk and backups to tape (some users subscribe to more than one service).

Storage service criteria for the classification of information

In 2009 the Centre maintained the criteria regarding the classification of the types of data in the storage service.

This system permitted the accommodation of the distinctive services to the specific necessities of each group of information, responding in this manner to the growing demand for quantity and quality of service such as the 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 operation of the computing services of the Centre depends on their availability. As such, they should have maximum availability and the best balance between capacity and performance. 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 typically are of the WORM type) and the access velocity is not critical, although they require a high bandwidth to access the servers. Back-ups can be made on demand.

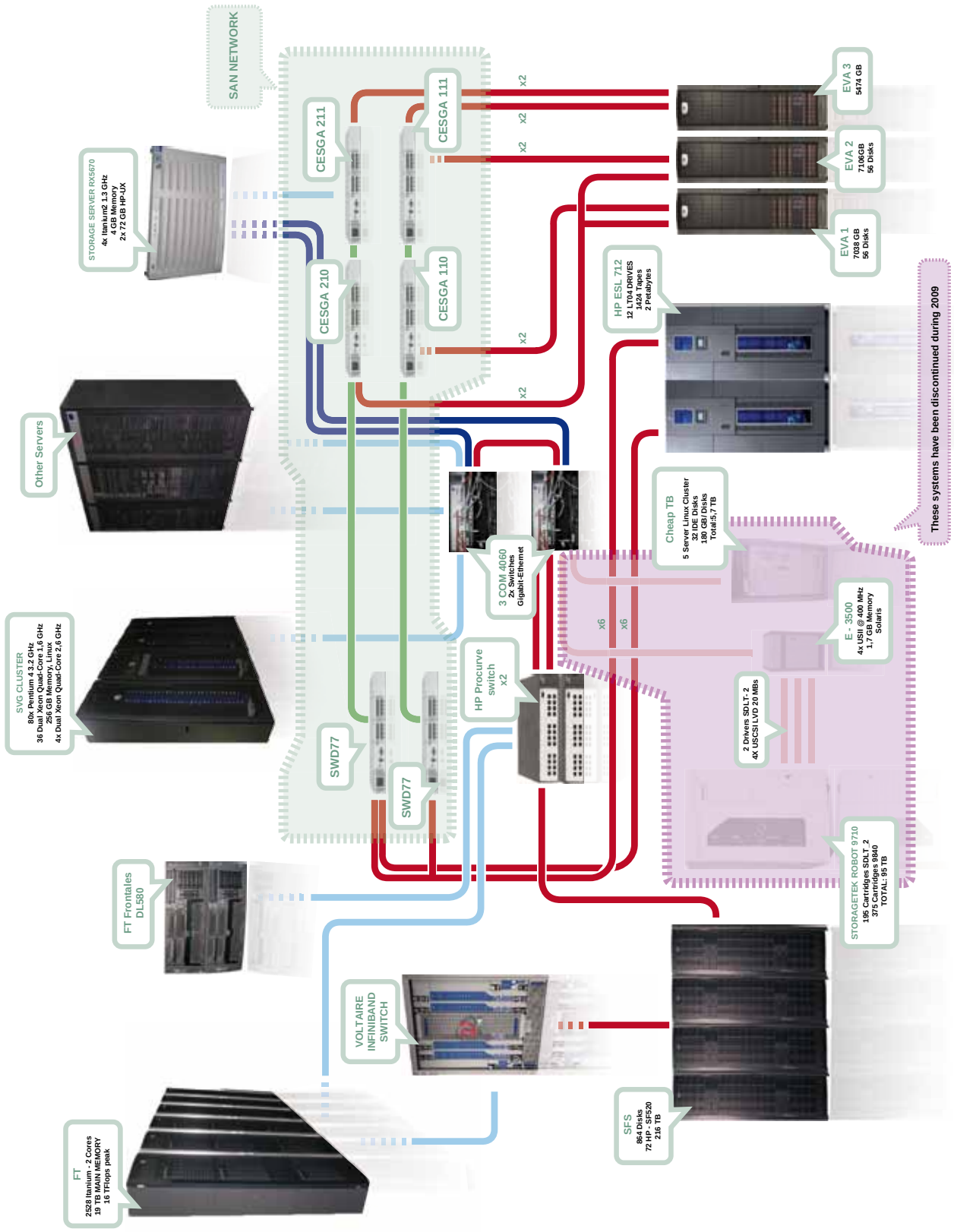
Back-ups to disk are the copies of the data that users have in their own servers or PCs that are stored in CESGA's systems in order to have a secure copy of their data. The availability of the service may be low.

Parallel Scratch has the best performance (maximum bandwidth). 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 disk 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 in 2009

TYPE OF STORAGE	CAPACITY (TB)
Temporary or Scratch	130
Temporary Parallel	223
Permanent Disk	25
Tape	1,360
TOTAL	1,739

data storage resources 2009



Scientific Applications

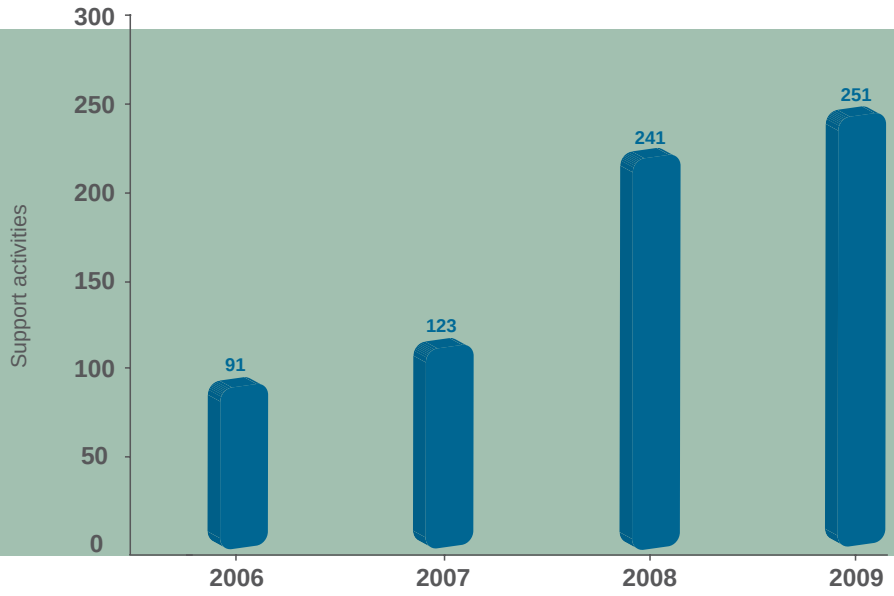
The predominant activity in the applications area during 2009 is listed below.

- The execution of 3 scientific computational challenges throughout the year.
- The completion of a large number of user support activities (251)
- The installation of all applications demanded by
- The development environment for X86/X86_64 architectures available at CESGA was completed including the completion of the installation of Portland Group development tools in the SVG server together with Intel development tools.
- A development node with a GPU Tesla C1060 was installed in collaboration with the Galician Bioinformatics Network. CUDA development tools and the latest related version of Portland Group compilers were installed as well.

Application activity is summarized below.

- 74 applications or scientific computing libraries were put into production.
- 94 new versions of applications were installed or updated.
- Support was provided to 3 computational challenges that led to the adaptation and modification of various applications.
- 251 requests for assistance were addressed.

user support activities 2006-2009



The installation of all applications demanded by CESGA users along the year. A total of 94 new application versions, libraries, compilers, and development tools were installed. A list of all ported elements follows.

Application	Version
4ti2	1.3.2
abinit	5.7.3
Aires	2.8.4a
Amber	10.0
AutoDock	4.2
batwing	2004-06-09
BEAST	1.4.8
CDO	1.3.2
CHARMM	c34b2
Dalton	2.0
Desmond Schrodinger	2009u02
dftb-plus	Snapshot-081217
EMAN	1.9
Gamess	12 Jan 2009 (R3)
Gaussian 09	A.02
Genehunter	parallel-v2.1_r2
Grace	5.1.22
Gromacs	4.0.3
Haddock	9.0
HyperWorks	5/6/2009 & 2009.09.01
IM	IM
IMa2	2.0
Mathematica	7.0
Migrate	3.0.3
modulef	99
MOLCAS	7.4
molpro	2008.1 & 2009.1
MSC - Nastran	2008r1
MSVAR	0.4.1b, 0.4.2 & 1.3
octave	3.0.3
Octopus	3.0.1, 3.0.1-mpi, 3.2.0 & 3.2.0-mpi
phylobayes	phylobayes2.3c & phylobayes-2.3c-gsl
qhull	2003.1
RAxML	7.2.1, 7.2.2 & 7.2.5
ROOT	5.22.00
Schrodinger Suite	2008 & 2009u02
SIESTA	2.0.2
Structure	2.3.1
Turbomole	5.10
VASP	5.1.40
VMD	1.8.6 & 1.8.6-python

Library	Version
ARPACK	2.1 & 2.1-parallel-extension
Blitz++	0.9
boost	1.34.1 & 1.38.0
cernlib	2006
FFTW	3.2
etsf_io	1.0.2
gperf	3.0.3
gsl	1.12
Intel MPI Library	3.1.038 & 3.2.1.009
Desmond Schrodinger	1.6.8, 1.8.1-szip & 1.8.1-api-1.6
HDF5	2.3.0.0
HP MPI	10.1.1 & 10.1.2
MKL	3.9.9
NCO	Gaussian 09
NetCDF	4.0.1 & parallel-1.0.3
NumPy	1.2.1
pyMPI	2.5b0
SPARSKIT	2
szip	2.1

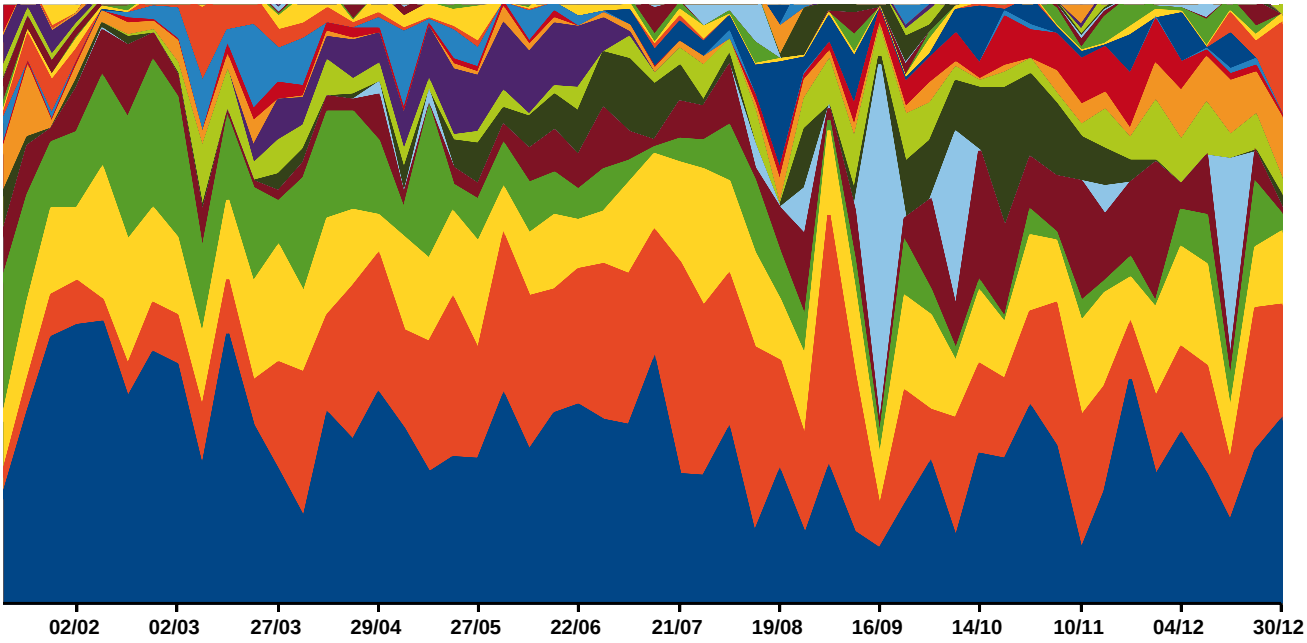
Compilers and Development Tools	Version
Cmake	2.4.6
CUDA	2.3
Intel C++ Compiler	11.0.074 & 11.0.083
Intel Fortran Compiler	11.0.074 & 11.0.083
jdk	1.5.0_14, 1.6.0_12 & 1.6.0_13
pcre	7.9
PGI Compilers	9.0.4 & 10.0
Python	2.4.6
Intel Thread Checker	3.1.012
Intel Trace Analyzer and Collector	7.2.1.008
Total View	8.7.0

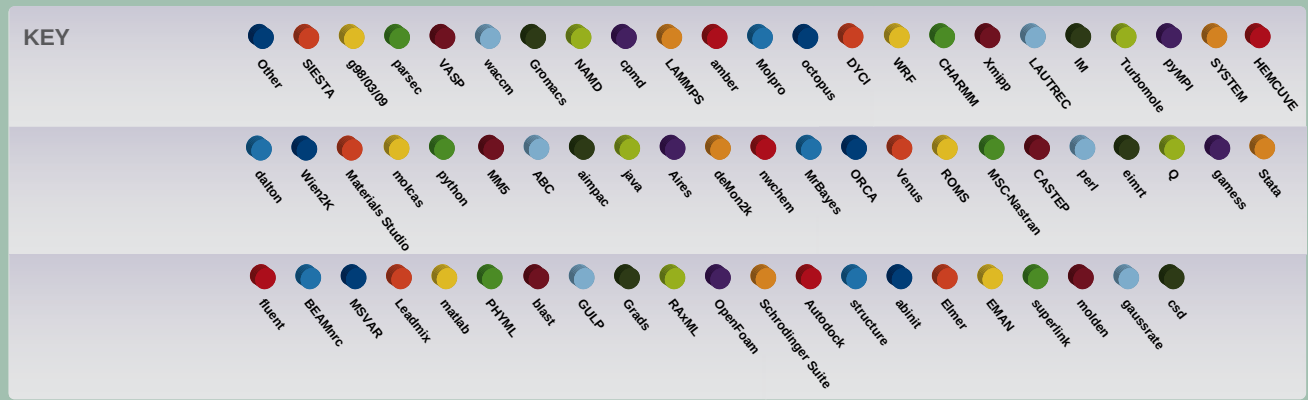
Statistics of applications use during 2009

These statistics extracted from the accounting records summarise the use of applications from January 1, 2009 until December 31, 2009. Data collected for accounting purposes include only those entries with execution times greater than 30 seconds (including both system and user time) in order to avoid saturating the system, except for CSD or other explicitly marked applications in which the threshold is lower, since the time used on this sort of application is much less.

The 35 most used applications are presented in this Table (“others” means non-classified applications, fundamentally, those that are installed or developed by the users themselves, “system” means system management executables).

distribution of CPU time consumed by aplications 2009





The catalogue of applications and utilities libraries installed in January 2010 in CESGA computational servers, with access for all users, is presented below.

Area	Application	FINISTERRAE	SVGD	Others
Scientific Analysis	4ti2	×	—	—
	R	×	—	—
	Singular	×	—	—
Scientific Databases	CSD	—	×	—
	ZENTRALBLATT	—	—	zmath.cesga.es
Bioinformatics	batwing	—	×	—
	BEAMnrc	—	×	—
	BEAST	—	×	—
	Blast	—	×	—
	Genehunter	×	×	—
	IM	—	×	—
	IMa2	—	×	—
	JAGS	×	—	—
	Lamarc	—	×	—
	Leadmix	×	×	—
	Migrate	×	×	—
	MrBayes	×	×	—
	MSVAR	—	×	—
	phylobayes	—	×	—
	PHYML	—	×	—
	RAxML	—	×	—
	Structure	—	×	—
Structural Modeling, Fluids, and Magnetism	Elmer	×	—	—

Area	Application	FINISTERRAE	SVGD	Others
Molecular Simulation	abinit	—	×	—
	Amber	×	×	—
	AutoDock	×	—	—
	CPMD	×	—	—
	Dalton	×	×	—
	Desmod Schrodinger	—	×	—
	Gamess	×	×	—
	Gaussian 03	×	×	—
	Gaussian 09	×	—	—
	Gaussian 98	—	×	—
	Gromacs	×	×	—
	LAMMPS	×	—	—
	Molden	×	×	—
	NAMD	×	×	—
	NWChem	×	×	—
	Octopus	×	—	—
	Schrodinger Suite	×	×	—
	SIESTA	×	×	—
Compilers	Cmake	×	—	—
	Intel C++ Compiler	×	×	—
	Intel Fortran Compiler	×	×	—
	pcre	—	×	—
	PGI Compilers	—	×	—
	Python	—	×	—
	Sun JDK	—	×	—
Profiling Tools	Intel Thread Checker	×	—	—
	Intel Thread Profiler	×	—	—
	Intel Trace Analyzer and Collector	×	—	—
	TotalView	×	×	—
MPI	HP MPI	×	—	—
	Intel MPI Library	×	—	—
	pyMPI	×	×	—

Area	Application	FINISTERRAE	SVGD	Others
Mathematical Libraries	ACML	—	×	—
	ARPACK	×	—	—
	ATLAS	—	×	—
	Blitz++	×	—	—
	boost	×	—	—
	cernlib	—	×	—
	CGAL	×	—	—
	CLHEP	—	×	—
	FFTW	×	×	—
	gperf	—	×	—
	gsl	×	×	—
	MKL	×	×	—
	Numeric Python	—	×	—
	NumPy	×	×	—
	octave	×	×	—
	ghull	—	×	—
	SPARSKIT	×	—	—
Simulation	EMAN	×	×	—
	F2PY	—	×	—
	Geant	—	×	—
	Xmipp	—	×	—
Scientific Visualization and Animation	CDO	×	—	—
	Grace	—	×	—
	Grads	×	×	—
	HDF	×	—	—
	HDF5	×	×	—
	JasPer	—	×	—
	Ncarg	×	×	—
	NCO	×	—	—
	NetCDF	×	×	—
	szip	×	—	—
	udunits	×	—	—
	VMD	×	×	—
Software Management	Modules	×	×	—

Many new applications or libraries of utilities were incorporated during 2009 at the request of users or for the installation of new versions. They are listed below.

Molecular Simulation

ABINIT (new version 5.7.3, in the SVG)

ABINIT is a package whose main program allows the user to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT), using pseudopotentials and a plane wave basis.

Amber (new version 10.0, in the FinisTerrae)

Amber is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. The term “amber” is also sometimes used to refer to the empirical forcefields that are implemented here. It should be recognized, however, that the code and forcefield are separate; several other computer packages have implemented the amber forcefields, and other forcefields can be implemented with the amber programs.

Autodock (new installation, version 4.2, in the FinisTerrae)

AutoDock is a suite of automated docking tools. It is designed to predict how small molecules, such as substrates or drug candidates, bind to a receptor of known 3D structure.

Dalton (new installation, version 2.0, in the FinisTerrae)

Dalton quantum chemistry is a program for computing SCF, MCSCF, MP2, and Coupled Cluster wave functions as wll as for calculating molecular properties and potential energy surfaces. The program represents an experimental code that is under constant development.

Desmond Schrödinger Suite (new installation, version 2009u02, in the SVG)

Desmond is a software package developed at D. E. Shaw Research to perform high-speed molecular dynamics simulations of biological systems on conventional commodity clusters. The code uses novel parallel algorithms and numerical techniques to achieve high performance and accuracy on platforms containing a large number of processors but it may also be executed on a single computer.

GAMESS (new version 12 Jan 2009 (R3), in the FinisTerrae)

Gamess is a program for ab initio molecular quantum chemistry. Briefly, GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include Configuration Interaction, second order perturbation Theory, and Coupled-Cluster approaches, as well as the Density Functional Theory approximation.

Gaussian 09 (new installation, version A.02, in the FinisTerrae)

Gaussian 09 is the latest in the Gaussian series of programs. It provides state-of-the-art capabilities for electronic structure modelling. Starting from the fundamental laws of quantum mechanics, Gaussian 09 predicts the energies, molecular structures, vibrational frequencies, and molecular properties of molecules and reactions in a wide variety of chemical environments.

GROMACS (new version, 4.0.3, in the FinisTerrae)

Gromacs is a versatile package to perform molecular dynamics, i.e., to simulate the Newtonian equations of motion for systems with hundreds to millions of particles. It is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have many complicated bonded interactions but since GROMACS is extremely fast at calculating the non bonded interactions (that usually dominate simulations), many groups are also using it for research on non-biological systems, e.g., polymers.

OCTOPUS (new installation, versions 3.0.1, 3.0.1-mpi, 3.2.0 and 3.2.0-mpi, in the FinisTerrae)

Octopus is a pseudopotential real-space package aimed at the simulation of the electron-ion dynamics of one-, two-, and three-dimensional finite systems subject to time-dependent electromagnetic fields. The program is based on time-dependent, density-functional theory (TDDFT) in the Kohn-Sham scheme. All quantities are expanded in a regular mesh in real space, and the simulations are performed in real time. The program has been successfully used to calculate linear and non-linear absorption spectra, harmonic spectra, laser induced fragmentation, etc. for a variety of systems.

Schrödinger Suite (new installation, versions 2008 and 2009u02, in the SVG and FinisTerrae)

Schrödinger provides a complete suite of software that addresses the challenges in pharmaceutical research. For structure-based drug design, Prime is an accurate protein structure prediction package. Glide performs accurate, rapid ligand-receptor docking. Liaison predicts binding affinity. QSite can be used to study reaction mechanisms within a protein active site. Phase is used for ligand-based pharmacophore modelling. QikProp for ADME properties prediction of drug candidates. LigPrep is a rapid 2D to 3D conversion program that can prepare ligand libraries for further computational analyses. CombiGlide provides focused library design. Epik offers accurate enumeration of ligand protonation states in biological conditions. Jaguar is the high-performance ab initio quantum mechanics application. MacroModel, the most trusted name in molecular modelling, have been widely applied to address the full range of chemical research from materials to life sciences. Strike is a chemically aware statistical package for examining structure-property relationships. Maestro is the graphical user interface for all of Schrödinger's computational programs and provides a powerful, fully-integrated molecular visualization and analysis environment.

SIESTA (new version 2.0.2, in the FinisTerrae)

Siesta (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method as well as a computer program implementation that is used to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.

Applications with limited licensing (User or specific institution/s) RESTRICTED TO SPECIFIC USERS

CHARMM (new installation, version c34b2, in the SVG)

CHARMM (Chemistry at HARvard Macromolecular Mechanics): is a versatile and widely used molecular simulation program with broad application to many-particle systems. It has been developed with a primary focus on the study of molecules of biological interest including peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates (as they occur in solution), crystals, and membrane environments.

DFTB+ (new installation, version Snapshot-081217, in the FinisTerrae)

The aim of the DFTB+ (DFTB Plus) project is to create a highly modularised, but nevertheless fast and efficient stand alone Density Functional based Tight Binding (DFTB) implementation, containing all useful extensions, which had been implemented in several separate programs before now, and adding new useful features.

HADDOCK (new installation, version 2.0, in the SVG)

HADDOCK (High Ambiguity Driven biomolecular DOCKing) is an approach that makes use of biochemical and/or biophysical interaction data such as chemical shift perturbation data resulting from NMR titration experiments, mutagenesis data, or bioinformatic predictions. This information is introduced as Ambiguous Interaction Restraints (AIRs) to drive the docking process.

MOLCAS (new version 7.4, in the FinisTerrae)

MOLCAS is quantum chemistry software developed by scientists to be used by scientists. The authors of MOLCAS have tried to assemble their collected experience and knowledge in computational quantum chemistry. The basic philosophy behind MOLCAS is to develop methods that will allow an accurate ab initio treatment of very general electronic structure problems for molecular systems in both ground and excited states. MOLCAS contains a number of codes that can perform such calculations (MP2, CC, CPF, DFT, etc.).

MOLPRO (new versions 2008.1 and 2009.1, in the FinisTerrae)

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. Using recently developed, integral-direct, local electron correlation methods which significantly reduce the increase of the computational cost with molecular size, accurate ab initio calculations can be performed for much larger molecules than with most other programs.

Turbomole (new version 5.10, in the SVG)

TURBOMOLE is a powerful Quantum Chemistry (QC) program package for ab initio Electronic Structure Calculations covering a wide range of research areas from both academia and industry. Presently, TURBOMOLE is one of the fastest and most stable codes available for standard quantum chemical applications (HF, DFT, MP2). 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 with reasonable time and memory requirements.

VASP (new version 5.1.40, in the SVG and FinisTerrae)

VASP is a complex package for performing ab initio quantum-mechanical molecular dynamics (MD) simulations using pseudopotentials or the projector-augmented wave method and a plane wave basis set. The approach implemented in VASP is based on the (finite-temperature) local-density approximation with free energy as a variational quantity, providing an exact evaluation of the instantaneous electronic ground state at each MD time step.

Bioinformatics

BATWING (new installation, version 2004-06-09, in the SVG)

Batwing is a program written in C for the analysis of population genetic data. BATWING reads in multilocus haplotype data, and model and prior distribution specification, uses a Markov chain Monte Carlo (MCMC) method based on coalescent theory to generate approximate random samples from the posterior distributions of parameters such as mutation rates, effective population sizes and growth rates, and times of population-splitting events.

BEAST (new installation, version 1.4.8, in the SVG)

BEAST is a cross-platform program for Bayesian MCMC analysis of molecular sequences. It is entirely oriented towards rooted, time-measured phylogenies inferred using strict or relaxed molecular clock models. It can be used as a method of reconstructing phylogenies but it is also a framework for testing evolutionary hypotheses without conditioning on a single tree topology. BEAST uses MCMC to average over tree space, so that each tree is weighted proportional to its posterior probability.

Genehunter (new installation, version parallel-v2.1_r2, in the SVG and FinisTerrae)

Genehunter is a software package for locating human genetic diseases using linkage analysis. Linkage analysis attempts to locate genes responsible for a disease using genetic data from a family affected by that disease. The package allows efficient multipoint analysis of pedigree data to be performed rapidly in a single user-friendly environment.

IM/IMa (new versions 5/6/2009 and 2009.09.01, 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.
IMa implements the same Isolation with Migration model, but does so using a new method that provides estimates of the joint posterior probability density of the model parameters. IMa also allows log likelihood ratio tests of nested demographic models.

IMa2 (new installation, version 2.0, in the SVG)

IMa2 implements a method for generating posterior probabilities for complex demographic population genetic models. IMa2 can handle data and implement a model for multiple populations (for numbers of sampled populations between one and ten) - not just two populations (as was the case with the original IM and IMa programs).

Migrate (new version 3.0.3, in the SVG and FinisTerrae)

Migrate estimates effective population sizes and past migration rates between n population assuming a migration matrix model with asymmetric migration rates and different subpopulation sizes. Migrate uses maximum likelihood or Bayesian inference to jointly estimate all parameters.

MSVAR (new installation, versions 0.4.1b, 0.4.2 and 1.3, in the SVG)

A program to detect past population growth or decline using autosomal microsatellite frequencies. This program is designed to help the user explore the most probable demographic and genealogical histories consistent with a sample of chromosomes typed at one or more loci. It relies on Markov Chain Monte Carlo (MCMC) simulation.

PhyloBayes (new installation, versions 2.3c and 2.3c-gsl, in the SVG)

PhyloBayes is a Bayesian Monte Carlo Markov Chain (MCMC) sampler for phylogenetic reconstruction using protein alignments. Compared to other phylogenetic MCMC samplers (e.g. MrBayes), the main distinguishing feature of PhyloBayes is the underlying probabilistic model, CAT. CAT is a mixture model especially devised to account for site-specific features of protein evolution. It is particularly well suited for large multigene alignments such as those used in phylogenomics.

RAxML (new installation, versions 7.2.1, 7.2.2 and 7.2.5, in the SVG)

RAxML (Randomized Axelerated Maximum Likelihood) is a program for sequential and parallel Maximum Likelihood-based inference of large phylogenetic trees. It was originally been derived from fastDNAml which in turn was derived from Joe Felsentein's dnaml which is part of the PHYLIP package.

Structure (new version 2.3.1, 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. It can be applied to most of the commonly-used genetic markers including SNPs, microsatellites, RFLPs, and AFLPs.

Structural modelling, Fluids, and Magnetism

MODULEF (new installation, version 99, in the SVGD)

MODULEF is a general purpose finite element library developed with the aim of bringing together universities and industry in order to design and implement an extensive library of finite element modules which cater to problems in fields such as: steady state or time-dependent, linear or non-linear, two- or three-dimensional heat conduction problems, static and dynamic elasticity problems, and fluid mechanical problems.

Applications with limited licensing (User or specific institution/s) RESTRICTED TO SPECIFIC USERS

HyperWorks (new installation, version 9.0, in the FinisTerrae)

Altair Engineering's HyperWorks is a computer-aided engineering (CAE) simulation software platform made up of Modelling & Visualization, Analysis & Optimization, and Enterprise solutions.

MSC-Nastran (new installation, version 2008r1, in the FinisTerrae)

MSC Nastran is a Finite Element Analysis (FEA) solver for simulating stress, dynamics, or vibration of real-world complex systems. MSC Nastran is built on work done by NASA scientists and researchers and is trusted to design mission critical systems in every industry. Nearly every spacecraft, aircraft, and vehicle designed in the last 40 years has been analysed using MSC Nastran.

Simulation

Aires (new installation, version 2.8.4a, in the FinisTerrae)

AIRES (AIRshower Extended Simulations) identifies a set of programs and subroutines to simulate particle showers produced after the incidence of high energy cosmic rays on the Earth's atmosphere as well as to manage all of the data associated with these simulations.

EMAN (new version 1.9, in the FinisTerrae)

EMAN is a powerful image processing library as well as a complete software suite for single particle reconstruction. This is a process for converting randomly oriented, 2D projection images into a 3D model. It is typically used in conjunction with electron cryomicroscopy. This technique is able to determine particle structures with subnanometric resolution in a range of 10-1000nm. EMAN's fundamental part is the image processing scientific library, suitable for it use in Python. EMAN also incorporates a number of tools for the docking of crystalline structures (coming from X-ray diffraction) in low-resolution density maps.

Scientific Visualisation and Animation

Etsf_io (new installation, version 1.0.2, in the FinisTerrae)

ETSF_IO is a library built on top of NetCDF that gives easy access to files conforming to ETSF specifications. NetCDF files are binary files with key-values access, optimized to store large volumes of data. The ETSF specifications define all key-value pairs that are normalized for a file containing informations for an electronic calculation. This library is available in Fortran90.

CDO (new installation, version 1.3.2, in the FinisTerrae)

CDO is a collection of command line Operators used to manipulate and analyse climate model data. Supported data formats are GRIB, netCDF, SERVICE, EXTRA, and IEG.

Grace (new version 5.1.22, in the FinisTerrae)

Grace is a WYSIWYG tool for constructing two-dimensional plots of numerical data. Its capabilities are roughly similar to GUI-based programs such as Sigmaplot or Microcal Origin, plus script-based tools such as Gnuplot or Genplot. Its strength lies in the fact that it combines the convenience of a graphical user interface with the power of a scripting language which enables it to perform sophisticated calculations or automated tasks.

HDF5(new versions, 1.8.1-api-1.6, in the SVG and 1.8.1-api-1.6, 1.6.8, 1.8.1-szip, in the FinisTerrae)

HDF5 is a unique technology suite that makes the management of extremely large and complex data collections possible. The HDF5 technology suite includes: 1) a versatile data model that can represent very complex data objects and a wide variety of meta data; 2) a completely portable file format with no limit on the number or size of data objects in the collection; 3) a software library that runs on a range of computational platforms, from laptops to massively parallel systems, and implements a high-level API with C, C++, Fortran 90, and Java interfaces; 4) a rich set of integrated performance features that allow for access time and storage space optimizations; and 5) tools and applications for managing, manipulating, viewing, and analysing the data in the collection.

NCO (new installation, version 3.9.9, in the FinisTerrae)

The netCDF Operators, or NCO, are a suite of programs known as operators. The operators take netCDF files as input, then perform a set of operations (e.g., deriving new data, averaging, hyperslabbing, or meta-data manipulation) and produce a netCDF file as output. The operators are primarily designed to aid manipulation and analysis of gridded scientific data.

NetCDF (new versions 4.0.1 y parallel-1.03, in the FinisTerrae)

NetCDF (network Common Data Form) is an interface for array-oriented data access and a library that provides an implementation of the interface. The netCDF library also defines a machine-independent format for representing scientific data. Together, the interface, library, and format support the creation, access, and sharing of scientific data.

SZIP (new installation, version 2.1, in the FinisTerrae)
Szip is an implementation of the extended-Rice lossless compression algorithm. The Consultative Committee on Space Data Systems (CCSDS) has adopted the extended-Rice algorithm for international standards for space applications. Szip is reported to provide fast and effective compression, specifically for the EOS data generated by the NASA Earth Observatory System (EOS). It was originally developed at the University of New Mexico (UNM) and integrated with HDF4 by UNM researchers and developers.

VMD (new installation, version 1.8.6, in the SVG and new version, 1.8.6-python, in the FinisTerrae)
VMD is designed for the visualization and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies, etc. It may be used to view more general molecules as VMD can read standard Protein Data Bank (PDB) files and display the contained structure. VMD provides a wide variety of methods for rendering and colouring molecules. VMD can be used to animate and analyse the trajectory of molecular dynamics (MD) simulations and can interactively manipulate molecules being simulated on remote computers (Interactive MD).

Mathematical Libraries

ARPACK (new installation, versions 2.1 and 2.1-parallel-extension, in the FinisTerrae)
ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems. ARPACK software is capable of solving large scale symmetric, nonsymmetric, and generalized eigenproblems from significant application areas. The software is designed to compute a few (k) eigenvalues with user specified features such as those of largest real part or largest magnitude.

Blitz++ (new installation, version 0.9, in the FinisTerrae)
Blitz++ is a C++ class library for scientific computing which provides performance on a par with Fortran 77/90. It uses template techniques to achieve high performance. The current versions provide dense arrays and vectors, random number generators, and small vectors and matrices.

BOOST (new installation, versions 1.34.1 and 1.38.0, in the FinisTerrae)
Boost provides free peer-reviewed portable C++ source libraries. It includes libraries that work well with the C++ Standard Library. Boost libraries are intended to be widely useful across a broad spectrum of applications.

CERNLib (new version 2006, in the SVG)
CERNLIB (CERN Program Library) is a collection of programs of general intention and functions for FORTRAN 77 maintained by the CERN. Many of these programs were developed in the CERN and are oriented toward the necessities of research in physics. Nevertheless, it includes functions and modules that can be applied in other areas.

FFTW (new version 3.2, in the FinisTerrae)

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 even/odd data, i.e., the discrete cosine/sine transforms or DCT/DST). Benchmarks performed on 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, however, FFTW's performance is portable; the same program will perform well on most architectures without modification.

Gperf (new installation, version 3.0.3, in the SVG)

GNU gperf is a perfect hash function generator. For a given list of strings, it produces a hash function and hash table, in the form of a C or C++ code, for looking up a value depending on the input string. The hash function is perfect which means that the hash table has no collisions.

GSL (new installation, version 1.12, in the SVG , in the FinisTerrae)

The GNU Scientific Library (GSL) is a numerical library for C and C++ programmers. The library provides a wide range of mathematical routines such as random number generators, special functions, and least-squares fitting.

MKL (new versions 10.1.1 in the SVG and 10.1.1 and 10.1.2, in the FinisTerrae)

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 current and next-generation Intel processors, it includes improved integration with Microsoft Visual Studio, Eclipse, and XCode. Intel MKL allows for full integration of the Intel Compatibility OpenMP run-time library for greater Windows/Linux cross-platform compatibility.

NumPy (new installation, version 1.2.1, in the SVG and new version 1.2.1, in the FinisTerrae)

NumPy is an extension to the Python programming language, adding support for large, multi-dimensional arrays and matrices, along with a large library of high-level mathematical functions to operate on these arrays. This package contains: a N-dimensional array object, basic linear algebra functions, basic Fourier transforms, random number capabilities and tools for integrating Fortran and C/C++ codes. Numpy contains the packages, Python-Numeric and F2PY.

Octave (new installation, version 3.0.3, in the SVG and FinisTerrae)

GNU Octave is a high-level language, primarily intended for numerical computations. It provides a convenient command line interface for solving linear and nonlinear problems numerically and for performing other numerical experiments using a language that is generally compatible with Matlab. It may also be used as a batch-oriented language.

Qhull (new installation, version 2003.1, in the SVG)

Qhull computes the convex hull, Delaunay triangulation, Voronoi diagram, halfspace intersection about a point, furthest-site Delaunay triangulation, and furthest-site Voronoi diagram. The source code runs in 2-d, 3-d, 4-d, and higher dimensions. Qhull implements the Quickhull algorithm for computing the convex hull. It computes volumes, surface areas, and approximations to the convex hull.

SPARSKIT (new installation, version 2, in the FinisTerrae)

SPARSKIT is a tool package for working with sparse matrices. Its main objectives are to convert between different storage schemes in order to simplify data exchange between researchers and to performe basic linear algebra and matrix manipulation.

Scientific Analysis

4ti2 (new installation, version 1.3.2, in the FinisTerrae)

4ti2 is a software package for algebraic, geometric, and combinatorial problems on linear spaces.

ROOT (new version 5.22.00, in the SVG)

ROOT provides a set of packages oriented to objects with all the functionalities necessary to treat and to analyze great amounts of data efficiently.

Applications with limited licensing (User or specific institution/s) RESTRICTED TO SPECIFIC USERS

Mathematica (new version 7.0, in the SVG)

Mathematica provides the World's largest collection of algorithms in a single system, each able to operate across the widest applicable scope of numeric, symbolic, or graphical input. Mathematica is a computational tool for numerics of any precision, symbolics, or visualization, with system-wide technology to ensure reliability, ease-of-use, and performance.

Java

SUN JDK (new installation, version 1.6.0_12, in the SVG and versions 1.5.0_14 and 1.6.0_13, in the FinisTerrae)

Java refers to a number of computer software products and specifications from Sun Microsystems that, together, provide a system for developing application software and deploying it in a cross-platform environment. Java is used in a wide variety of computing platforms from embedded devices and mobile phones on the low end, to enterprise servers and supercomputers on the high end.

Parallel Libraries

HP MPI (new version 2.3.0.0, in the FinisTerrae)

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 shared memory for intra-node communications.

Intel MPI Library (new versions 3.1.038 and 3.2.1.009, in the FinisTerrae)

Implementing the high performance MPI-2 specification on multiple fabrics, Intel MPI Library 3.1 focuses on making applications perform better on IA-based clusters. Intel MPI Library enables the quick delivery of maximum end user performance even if there is a change or upgrade to new interconnects, without requiring major changes to the software or to the operating environment. Intel also provides a free runtime environment kit for products developed with the Intel MPI library.

PyMPI (new version 2.5b0, in the SVG)

The Python interpreted language provides a good frame for building scripts and control environments. While Python has a (co-routining) thread model, its basic design is not particularly appropriate for parallel programming. The pyMPI extension set is designed to provide parallel operations for Python on distributed, parallel machines using MPI.

Compilers

CUDA (new installation, version 2.3, in the SVG)

NVIDIA CUDA is a general purpose parallel computing architecture that leverages the parallel compute engine in NVIDIA graphics processing units (GPUs) to solve many complex computational problems in a fraction of the time required on a CPU. It includes the CUDA Instruction Set Architecture (ISA) and the parallel compute engine in the GPU.

CMAKE (new installation, version 2.4.6, in the FinisTerrae.)

CMake, the cross-platform, open-source build system, is a family of tools designed to build, test, and package software. CMake is used to control the software compilation process using simple platform and compiler independent configuration files. CMake generates native makefiles and workspaces that can be used in the compiler environment of your choice.

Intel C++ Compiler (new versions 11.0.074 and 11.0.083, in the FinisTerrae)

Intel C++ Compiler Professional Edition 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-parallelisation, OpenMP, data prefetching, and loop unrolling, along with highly optimized C++ templates for parallelism, math processing, and multimedia libraries.

Intel Fortran Compiler (new versions 9.1.052, 10.1.012 and 11.0.069, in the FinisTerrae. new version 11.0.083 in the SVG)

The Intel Fortran Compiler for Linux delivers rapid development and good 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 parallelises software to take best advantage of multi-core Intel processors, including dual-core mobile, desktop, and enterprise platforms.

PCRE (new installation, version 7.9, in the SVG)

The PCRE library is a set of functions that implement regular expression pattern matching using the same syntax and semantics as Perl 5. PCRE has its own native API, as well as a set of wrapper functions that correspond to the POSIX regular expression API.

PGI Compilers (new versions, 9.0.4 and 10.0, in the SVG)

PGI parallel compilers and tools harness the full power of x64+GPU systems for science and engineering applications. PGI's industry-leading performance, reliability, native multi-core, and OpenMP support, GPGPU programming, and parallel-capable graphical debugging and profiling tools provide a complete state-of-the art programming environment for scientists and engineers. PGI's support for legacy language and programming features ensures that existing applications will port easily and quickly to the latest-generation multicore x64+GPU processor-based systems.

Galician Science & Technology Network: RECETGA

The Galician Science & Technology Network, *Rede de Ciencia e Tecnoloxía de 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 a total of 43 technology 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 to serve as a technological environment that allows research, development, and innovation in the field of communications.

RECETGA
Rede de Ciencia e Tecnoloxía de Galicia

RECETGA is managed by CESGA who is licensed as a Class C Internet Service Provider by the Spanish Telecommunications Authority (CNMT).

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

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

Network users include:

Research Centres and Laboratories of the Galician Regional Government (Xunta de Galicia)
University System of Galicia
Spanish National Research Council (CSIC) Institutes and Laboratories in Galicia
Other Public and Private RTD 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 2009 are summarised below.

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
- EDUROAM
- NETWORK MANAGEMENT TOOLS

Network management and monitoring

The Galician Science and Technology Network offered its services with 99.844 % availability.

Main Highlights

A list of the main activities undertaken in 2009 to guarantee the evolution and improvement of the network is presented below.

Signing of a Collaboration Agreement with RED.es *to connect the Portuguese NREN with RECETGA and RedIRIS.*

Contribution to the Project RedIRIS NOVA *(Initial Phase for the deployment of RedIRIS NOVA)*

1. Evaluation of optical transmission equipment
2. Conducting an analysis of the Galician requirements for the requested RedIRIS Nova interconnection points in Galicia.

Contribution to the deployment of the dark fiber connection with Portugal

1.Attendance at regular meetings to monitor the public tender for RedIRIS NOVA including the dark fiber link with Portugal.

2.Support to the redesign and the initial phase of implementation with the ISP that was awarded the public tender (TELEFONICA).

Execution of a comparative cost study *of different network maintenance alternatives.*

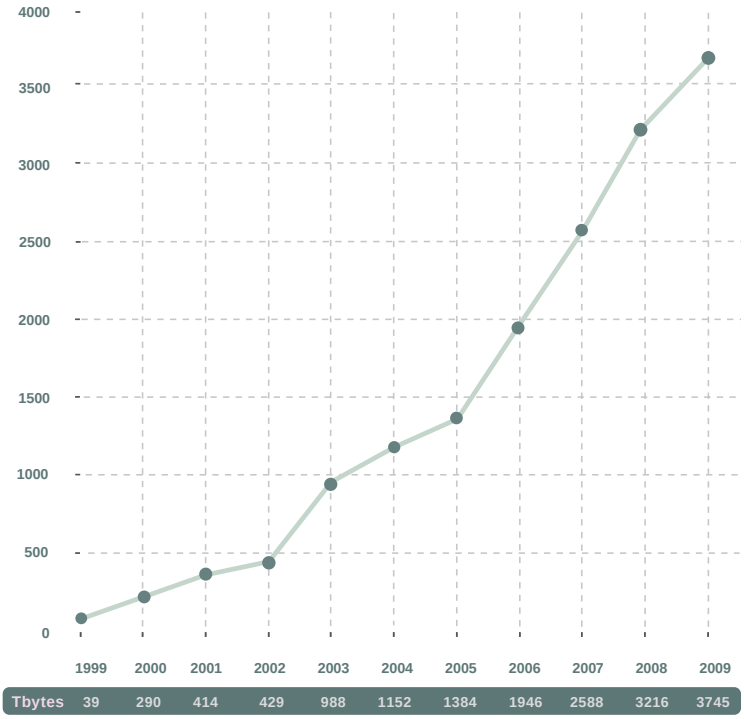
Backbone network highlights

Improvements in the link to RedIRIS with the configuration of an aggregate of 2 x 1GigabitEthernet.

CESGA's core was reshaped. Now it is constituted by 2 gigabit switches and routers, M10 and J6350. All network centres and CESGA itself benefit from the new architecture. Those centres with double access have been reconfigured dividing between the two core switches:

Universidade de Vigo
Universidade de Santiago
Universidade de A Coruña (only has one access but it was migrated to more robust equipment and intermediate equipment was removed).

Traffic exchanged in RECETGA in Terabytes
1999 - 2009



Access network Highlights

Connection of the CITI centre, *Universidade de Vigo, to the Galician Technology Park (TECNOPOLE)*

Migration of the H. Clinico connection from a *10 Mbps connection based on ATM technology to Gigabit Ethernet*

Migration of the SERGAS-RECETGA *ATM connection at 155 Mbps to Gigabit Ethernet*

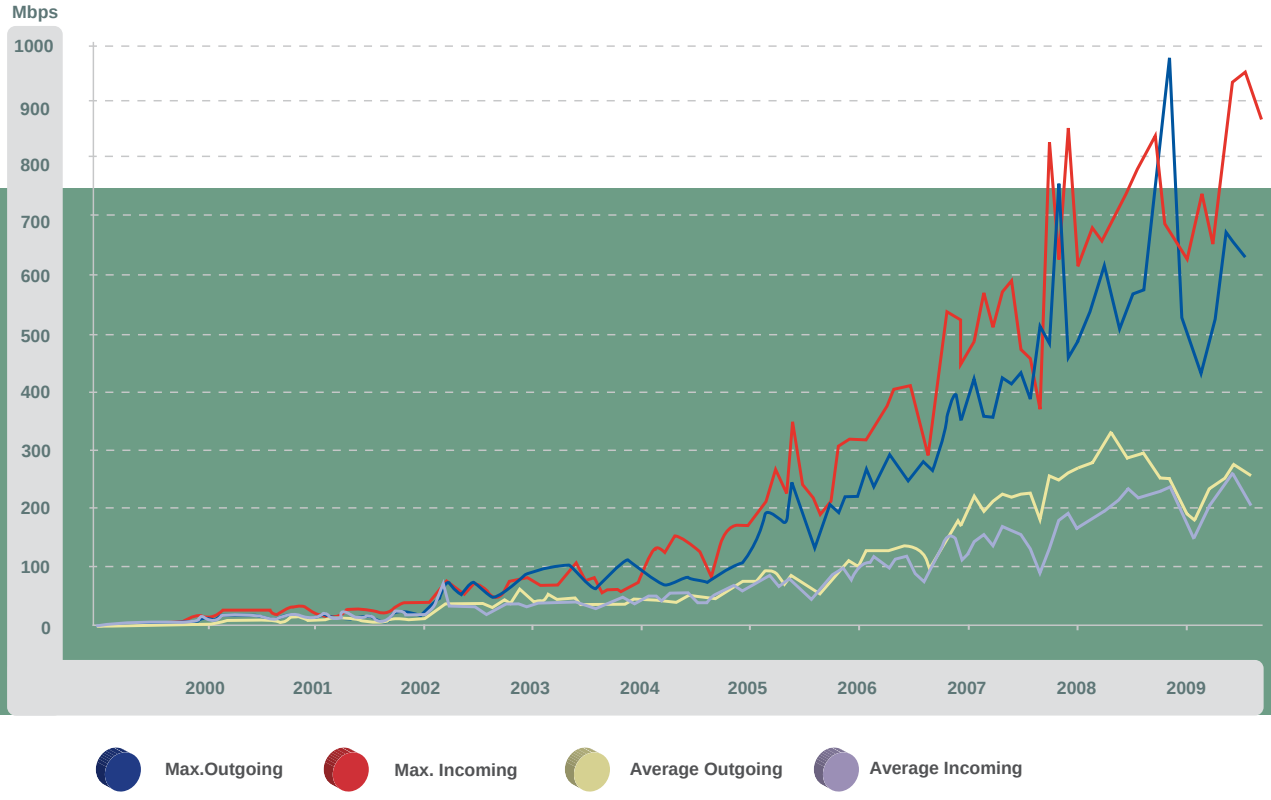
Connection to Universidade de Santiago de Compostela Classroom, *located in the Complexo Hospitalario Universitario de Santiago de Compostela, to RECETGA*

Adaptation of the internal network *to accommodate new supercomputer nodes and the Summer School Laboratory*

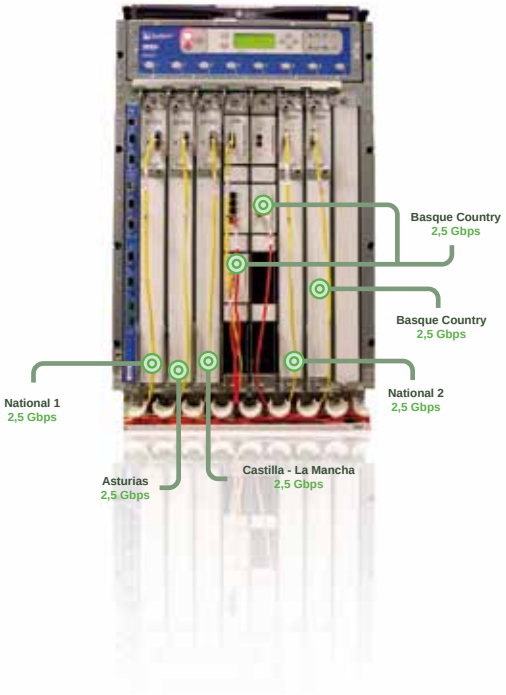
Dissemination and conference activity during 2009

1. Presentation of RECETGA and services during the guided tour following the RedIRIS JJTT to more than 200 people from industry and academe, during 4 days.
2. Remote participation via AccessGrid in the inauguration of the Board of Advanced Teaching of the Universidad de Sevilla.
3. Contribution to the deployment of the AccessGrid room at the Universidad de Cadiz.
4. Participation in the organizing committee of RedIRIS in Santiago de Compostela.
5. Attendance at RedIRIS JJTT and GGTT.
6. Attendance at the TERENA Networking Conference.
7. Presentation of CESGA and its services as well as a complete view of RECETGA for the conference, “Exercer a profesión de Enxeñeiro” (Engineering) in the School of Telecommunications Engineering of Vigo.

RECETGA-RedIris exchanged traffic in Mbps 2000-2009



RedIRIS PoP IN GALICIA (JUNIPER M40E)



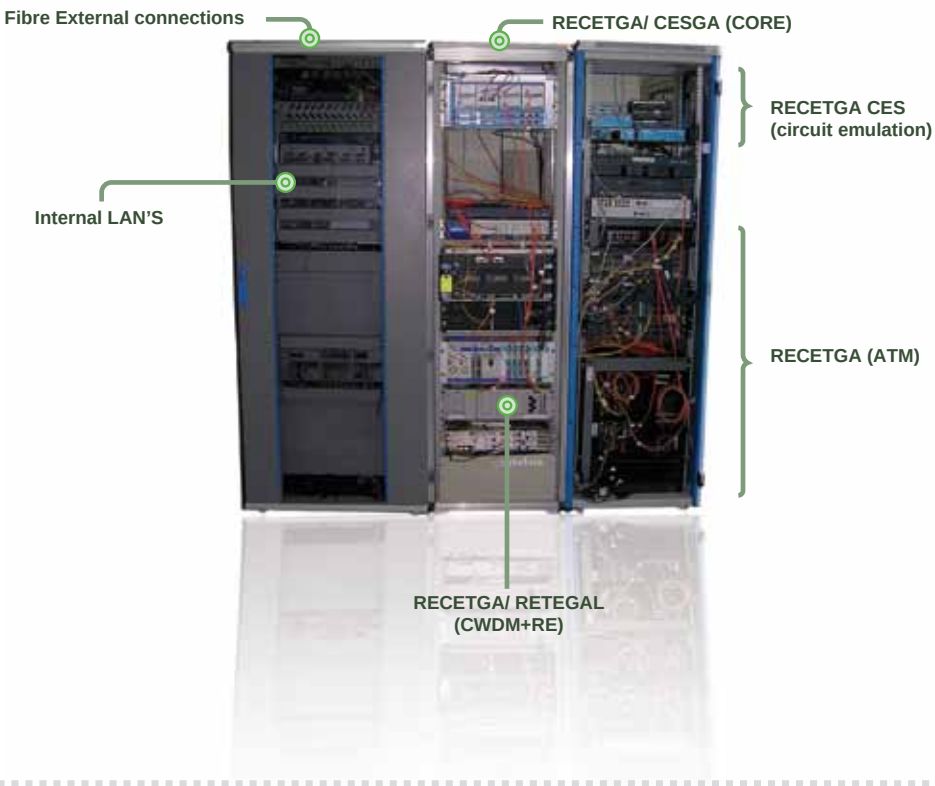
EXTERNAL CONNECTIONS THROUGH

RedIRIS

GÉANT2

TORGA net

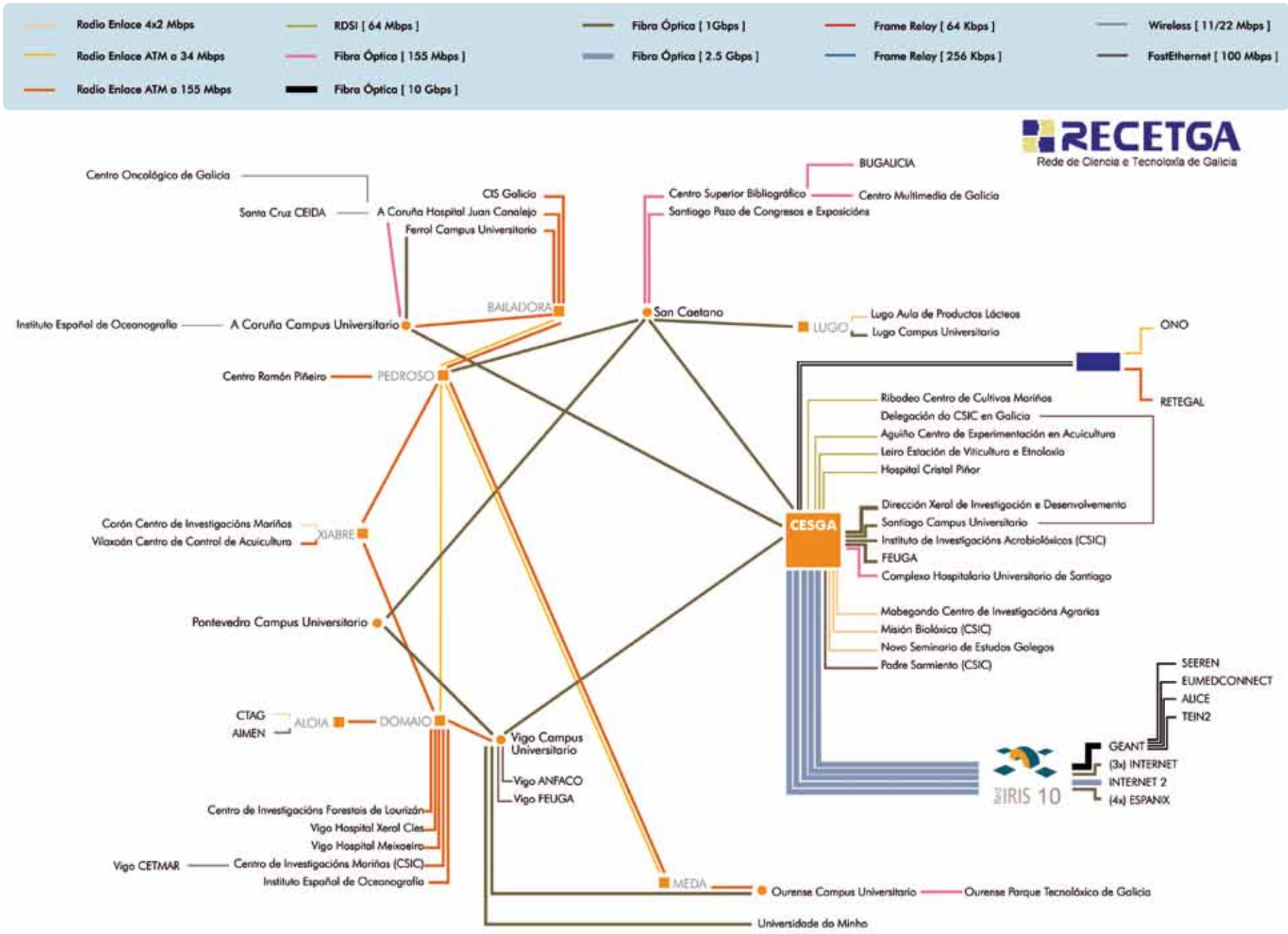
RECETGA CENTRAL NODE INSTALLED AT CESGA



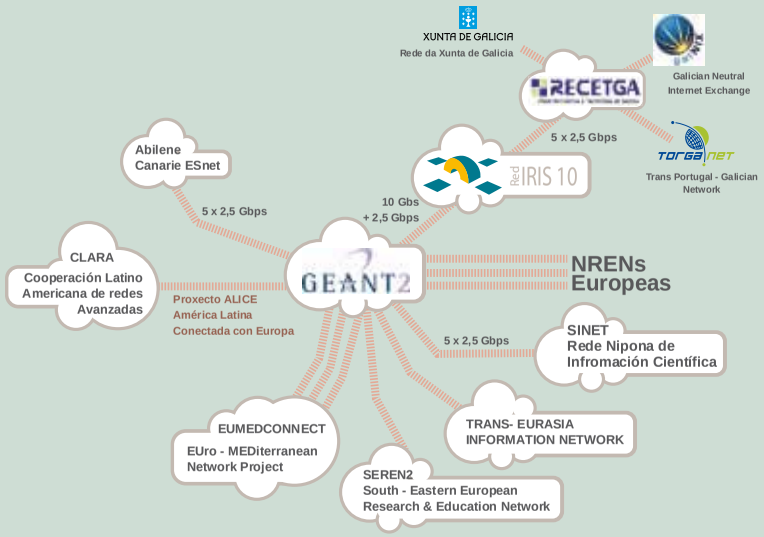
Centres Connected to RECETGA

CENTRE	LINK	AVAILABILITY
Universidade da Coruña (UDC)		
Coruña Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.994%
Ferrol Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.948%
Universidade de Santiago de Compostela (USC)		
Santiago Campus	2 Fibre Optics (1Gbps)	99.995%
Lugo Campus	Fibre Optics (155 Mbps)	99.463%
Universidade de Vigo (UVIGO)		
Vigo Campus	2 Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.988%
Pontevedra Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.975%
Ourense Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.988%
Universidade do Minho (UMINHO)	Fibre Optics (155 Mbps)	99.913%
BUGALICIA		
Consorcio de Bibliotecas Universitarias de Galicia	Fibre Optics (155 Mbps)	99.946%
RTD Centres		
ANFACO - CECOPESCA (Vigo)	FastEthernet (100 Mbps)	99.608%
Aula de Produtos Lácteos (USC - Lugo)	Radio Link 4x2 Mbps	99.981%
INIA - Centro de Investigacións Forestais (Lourizán)	ATM Radio Link at 155 Mbps	99.843%
Centro de Investigacións Lingüísticas “Ramón Piñeiro”	ATM Radio Link at 34 Mbps	99.994%
AIMEN - Centro Tecnolóxico Armando Priegue	Radio Link 4x2 Mbps	99.211%
CIAM - Centro de Investigacións Agrarias de Mabegondo	Radio Link 4x2 Mbps	99.859%
Centro de Control de Calidade do Medio Mariño (Vilaxoán)	ATM Radio Link at 155 Mbps	99.945%
Centro de Investigacións Mariñas (Corón)	Radio Link 4x2 Mbps	99.939%
CESGA Centro de Supercomputación de Galicia	1 Fibre Optics (1Gbps)	99.995%
CETMAR - Centro Tecnológico del Mar	Wireless (11/22 Mbps)	97.723%
Centro de Innovación e Servicios (Ferrol)	ATM Radio Link at 155 Mbps + Wireless (11/22 Mbps)	99.601%
FEUGA - Fundación Empresa - Universidade de Galicia (Vigo)	FastEthernet (100 Mbps)	99.608%
FEUGA -Fundación Empresa - Universidade de Galicia (Santiago)	Fibre Optics (16 Gbps)	99.979%
CEIDA (Santa Cruz)	Wireless (11/22 Mbps)	99.982%
Dirección Xeral de I+D+i	Fibre Optics (1 Gbps)	99.995%
CTAG - Centro Tecnológico del Automóvil	Radio Link 4x2 Mbps	99.943%
CMG - Centro Multimedia de Galicia	Fibre Optics (155 Mbps)	99.981%
Hospitals		
CHUS - Complexo Hospitalario Universitario de Santiago de Compostela	Fibre Optics (1 Gbps)	99.995%
CHUVI - Complexo Hospitalario Universitario de Vigo	Radio Link ATM at 155 Mbps	99.614%
CHUC - Complexo Hospitalario Universitario de A Coruña	Fibre Optics (155 Mbps)	99.995%
Unidade de Investigación do Hospital do Meixoeiro	ATM Radio Link at 155 Mbps	99.846%
COG - Centro Oncolóxico de Galicia	Wireless (11/22 Mbps)	99.982%
IEO		
I.E.O - Instituto Español de Oceanografía - A Coruña	Wireless (11/22 Mbps)	99.948%
I.E.O - Instituto Español de Oceanografía - Vigo	ATM Radio Link at 155 Mbps	99.833%
I.E.O - Delegación de Vigo sede Bouzas	WIMAX	99.661%
CSIC		
Misión Biológica de Galicia	Radio Link 4x2 Mbps	99.95%
Instituto de Investigaciones Agrobiológicas de Galicia	Fibre Optics (1 Gbps)	99.995%
Instituto de Investigaciones Marinas	ATM Radio Link at 155 Mbps	99.935%
IEGPS - Instituto de Estudos Galegos “Padre Sarmiento”	FastEthernet (100 Mbps)	99.995%
Delegación Institucional del CSIC en Galicia	2 Fibre Optics (1 Gbps)	99.946%
Other Centres		
Palacio de Exposicións e Congresos de Galicia *	Fibre Optics (155 Mbps)	100%
Parque Tecnolóxico de Galicia	Fibre Optics (155 Mbps)	99.975%
Meteogalicia	Fibre Optics (100 Mbps)	99.976%
Exchange with other Networks		
ONO	2x100 Mbps	99.976%
RedIRIS	5x2.5 Gbps	99.994%
RETEGAL	155 Mbps	99.975%
SERGAS	Fibre Optics (1 Gbps)	99.996%

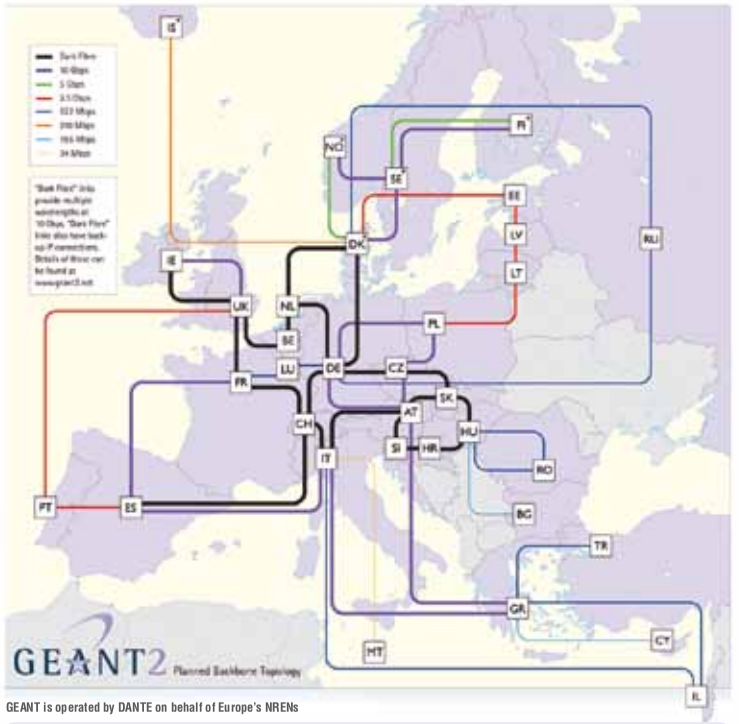
* 100% Conectivity provided on demand


Radio Enlace 4x2 Mbps
Radio Enlace ATM a 34 Mbps
Radio Enlace ATM a 155 Mbps
RDSI [64 Mbps]
Fibra Óptica [155 Mbps]
Fibra Óptica [10 Gbps]
Fibra Óptica [1Gbps]
Fibra Óptica [2.5 Gbps]
Frame Relay [64 Kbps]
Frame Relay [256 Kbps]
Wireless [11/22 Mbps]
FastEthernet [100 Mbps]
RECETGA
Rede de Ciencia e Tecnoloxía de Galicia
Centro Oncológico de Galicia
Santa Cruz CEIDA
A Coruña Hospital Juan Canalejo
CIS Galicia
Ferrol Campus Universitario
BAILADORA
Instituto Español de Oceanografía
A Coruña Campus Universitario
Centro Ramón Piñeiro
PEDROSO
BUGALICIA
Centro Superior Bibliográfico
Centro Multimedia de Galicia
Santiago Pazo de Congresos e Exposicións
San Caetano
LUGO
Lugo Aula de Productos Lácteos
Lugo Campus Universitario
ONO
RETEGAL
Ribadeo Centro de Cultivos Mariños
Delegación do CSIC en Galicia
Aguiño Centro de Experimentación en Acuicultura
Leiro Estación de Viticultura e Etnoloxía
Hospital Cristal Piñor
Dirección Xeral de Investigación e Desenvolvemento
Santiago Campus Universitario
Instituto de Investigacións Acrobiolóxicos (CSIC)
FEUGA
Complexo Hospitalario Universitario de Santiago
CESGA
Mabegondo Centro de Investigacións Agrarias
Misión Bioloxica (CSIC)
Novo Seminario de Estudos Galegos
Padre Sarmiento (CSIC)
Corón Centro de Investigacións Mariñas
Vilaxoán Centro de Control de Acuicultura
XIABRE
Pontevedra Campus Universitario
CTAG
AIMEN
ALOIA
DOMAIO
Vigo Campus Universitario
Vigo ANFACO
Vigo FEUGA
Centro de Investigacións Forestais de Lourizán
Vigo Hospital Xeral Cíes
Vigo Hospital Meixoeiro
Vigo CETMAR
Centro de Investigacións Mariñas (CSIC)
Instituto Español de Oceanografía
MEDA
Ourense Campus Universitario
Ourense Parque Tecnolóxico de Galicia
Universidade do Minho
IRIS 10
SEEREN
EUMEDCONNECT
ALICE
TEIN2
GÉANT
(3x) INTERNET
INTERNET 2
(4x) ESPANIX

CONNECTIONS THROUGH GEANT



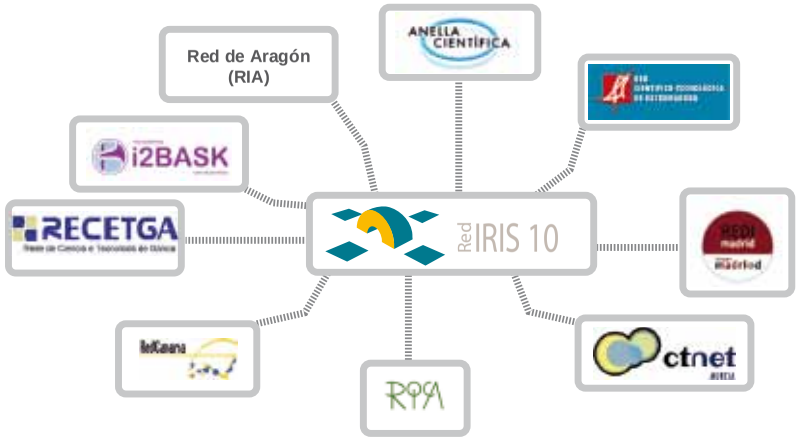
GEANT TOPOLOGY



GEANT is operated by DANTE on behalf of Europe's NRENs

RedIRIS TOPOLOGY

CONNECTION THROUGH REGIONAL NETWORKS



Projects

RESEARCH PROJECTS

The activity in the Projects Area has been intense during 2009. A total of 36 competitive RTD project grant applications were submitted in 2009. Fourteen of these were successful (50% of those evaluated in 2009). A Spanish national strategic project proposal in the ICT area, the NUBA project was successful and received funding for its development. In 2009, it is important to highlight the attainment of funding through the Spanish Science & Innovation Ministry's Scientific-Technological Infrastructures Programme (ICTS) which will open access to the FinisTerrae supercomputer to the entire European and Latin American scientific community. Additionally, ICTS funding will allow CESGA to host 18 research fellow visits in 2010. Also worthy of note is the geographic information systems department participation in an international research project. Among the project proposals presented which have not yet been resolved, four European Commission proposals are worth noting here: three have been proposed to the area of e-Infrastructures (two of these directly related to the new European infrastructure for distributed computing (EGI) and a proposal presented to the area of Health.

Finally, in 2009, a Computational Science Reseach sub-Unit was created under the Applications and Projects Department. A first researcher in Computational Condensed Matter Physics was hired. This sub-Unit represents the embryo of the new research division at CESGA.

AREA	PROJECTS	
	2008	2009
Computing	19	19
Network Comunications	4	3
Collaboration Tools & e-Learning	3	9
Geographical Information Systems	4	3
Tecnology Transfer & e-Business	4	4
Other Grants for Research	4	6
TOTAL	38	44

GRANT SOURCE	PROJECTS	
	2008	2009
European Comission	10	10
Spanish Goverment	7	13
Galician Regional Goverment	17	19
Industry	4	2
TOTAL	38	44

Thematic Networks, Tecnological Platforms	19	19

COMPUTING

NUBA, Normalized Usage of Business-oriented Architectures

Partners: Telefónica I+D, Atos Origin, BSC, CESGA, UCM, Catón Sistemas Alternativos, Digital Bubble S.L., Xeridia SL.
Coordinator: Telefónica I+D
Principal Researcher: C. Fernández, CESGA
Financing: Avanza I+D
Project Code: TSI-020301-2009-30
Budget: 171638€
Period: 2009 - 2011
Objective: The project focuses research on the management of a cloud, service-oriented infrastructure that integrates different providers, on which service providers can define the requirements of their virtual environments and deploy and manage their services transparently. It also provides automated monitoring, scaling, cost control, and remote management.

RENDER: New model for remote render

Partners: Cluster Audiovisual Galego, CESGA, USC, Interacción, Ficción and R Cable
Coordinator: C. Reyes, Cluster Audiovisual Galego (CLAG)
Principal Researcher: C. Fernández, CESGA
Financing: Avanza I+D
Project Code: TSI-020110-2009-321
Budget: 55,188€
Period: 2009-2010
Objective: The project aims to analyse the technological viability and business models for a technological platform for remote rendering. This technology will allow animation companies to save on hardware, software, operational cost, and infrastructures. Remote Render Farms also have high availability of computing power to process Render providing flexibility, adaptability, and competitiveness to businesses while they implant and develop models of sustainability and energy efficiency.

Computational studies of strongly-correlated quantum systems

Partners: CESGA
Coordinator: I. González López del Castillo, CESGA
Principal Researcher: I. González López del Castillo
Financing: Spanish Ministry of Science and Innovation
Project Code: FIS2009-13520
Budget: 16,940 €
Period: 2010 - 2012
Objective: The goal of this project is to study the physics of strongly-correlated quantum systems using advanced numerical techniques and high-performance computing. The focus is on novel quantum properties of both traditional condensed matter systems, such as electronic liquids, and quantum magnets as well as non-traditional many-body systems, such as cold atoms in optical lattices and nanoscale conductors.

Optimization of irregular applications on emerging CPU/GPU high performance computing systems

Partners: CESGA, USC
Coordinator: J.C. Pichel, CESGA
Principal Researcher: J.C. Pichel
Financing: Directorate General for Research Development and Innovation (DXIDI), Galician Regional Government (Xunta de Galicia)
Project Code: 09TIC002CT
Budget: 78,890 €
Period: 2009 - 2012
Objective: The project offers the assessment of the GPUs as suitable platforms to develop/optimize irregular applications with extension of the memory hierarchy models previously developed by the researchers to the new hybrid architectures, CPU/GPU. The development of new tools for irregular applications that take advantage of the new levels of the memory hierarchy in these systems will be introduced. Moreover, these tools will make their programming easier. The knowledge acquired during the project about these hybrid architectures will provide a good starting point for the next FinisTerrae supercomputer.

FORMIGA-CLOUD: Fostering re-usage of computer labs through their integration in the Cloud

Partners: USC, CESGA
Coordinator: J. López Cacheiro, CESGA
Principal Researcher: J. López Cacheiro
Financing: Directorate General for Research Development and Innovation (DXIDI), Galician Regional Government (Xunta de Galicia)
Project Code: 09TIC001CT
Budget: 58,825.95 €
Period: 2009 - 2012
Objective: Creation of a cloud based on the resources of the computer labs of Galician universities extending the functionality of the existing FORMIGA platform.

GIS-OCEANO: Production, processing, and distribution of oceanographic multipurpose operational fields using open standards and web services

Partners: CESGA, Universidad Santiago de Compostela.
Coordinator: A. Gómez, CESGA
Principal Researcher: A. Gómez
Financing: Directorate General for Research Development and Innovation (DXIDI), Galician Regional Government (Xunta de Galicia)
Project Code: 09MDS009CT
Budget: 74,134.75 €
Period: 2009 - 2012
Objective: The objective of the project is the development and adjustment of the ROMS (Regional Ocean Model System) model to the Galician coast as well as making it operational so that Meteogalicia can use its results. Such results will be deployed using a data processing architecture and will generate products with added value starting from the output files, following an correct organization, management and dissemination procedures. The methods will satisfy the European directive, INSPIRE, and will use the web service standards proposed by the Open Geospatial Consortium (OGC).

EIMRT-II: Advanced Planning Systems for Radiotherapy by mean of Computing Environments

Partners: CESGA, USC, UVIGO, CHUVI
Coordinator: J.C. Mouriño, CESGA
Principal Researcher: J.C. Mouriño
Financing: Directorate General for Research Development and Innovation (DXIDI), Galician Regional Government (Xunta de Galicia)
Project Code: 09SIN007CT
Budget: 129432.5 €
Period: 2009 - 2012
Objective: The previous e-IMRT project has produced new remote services for the planning of radiotherapy treatments that require high computational capacity. This second project will develop new computational modules for treatment planning and optimization and their parallelization. We will use the Cloud Computing infrastructure as remote computational resources and the platform will be validated by the hospital Radiophysics staff.

Access and improvement of FinisTerrae, Infraestructura Científico Tecnológica Singular (ICTS)

Partners: CESGA
Coordinator: I. López, CESGA
Principal Researcher: I. López
Financing: The Ministry of Science and Innovation, Sub-Program for design, feasibility, access and improvement of Science and Technology Infrastructures CTS)
Project Code: ICST-2009-40.
Budget: 434,732€
Period: 2009-2010
Objective: To provide access to FinisTerrae in open calls, as Science and Technology Infrastructure (ICTS). To improve the FinisTerrae ICTS. To host research fellow visits to the Centre.

Enabling Grid for E-SciEnce III (EGEE III)

Partners: CERN, JKU, KFKI-RMKI, CESNET, II SAS, JSI, CYFRONET, SRCE, FOM, VUB, FZK, SWITCH, CNRS, CGGV, 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: INFSO-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 (HPUPC)

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, CESGA
Coordinator: C. Fernández Sánchez, CESGA
Principal Resarcher: C. Fernández Sánchez
Financing: Research Contract (Subject to an Agreement of Confidentiality)
Project Code: HP-002
Budget: 91,903.00 €
Períod: 2008-2011
Objective: The project aim is 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: European Commission - VII Framework Programme
Project Code: EU-FP7-223797
Budget: 66,000.00 €
Period: 2008 - 2010
Objective: The project aim is 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.

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

Partners: Universidad Santiago de Compostela, CESGA
Coordinator: J. J. Saborido Silva, Universidade de Santiago de Compostela, USC
Principal Investigator: C. Fernández Sánchez, CESGA
Financing: Spanish Ministry of Science and Innovation
Project Code: FPA2007-66437-C02-02
Budget: 13,797.00 €
Period: 2007-2010
Objective: The goal is to launch a GRID infrastructure for CERN's LHCb experiment.

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: PGIDIT04CS0137030PR
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 BeInEIMRT services to many European hospitals based on 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 Tecnologico 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 that is oriented toward those business models through the limits of the organisation.

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
Financing: Regional Government of Galicia (Xunta de Galicia)
Project Code: 07SIN012CT
Budget: 147,338.00 €
Period: 2007-2009
Objectives: This study of the design and development of a Qualified Electronic Signature Infrastructure (IfeC), sustained on the Management of Privileges Infraestructure (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.

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

Partners: USC, AZTI, ICCM, and CESGA
Coordinator: J.M. Cotos Yánez, 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 interdisciplinary projects related to oceanographic remote sensing.

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: Spanish Ministry of Science and Innovation
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: indefinitely
Objectives: The aim is to provide live multicasts 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: I. López Cabido, CESGA.
Financing: Regional Government of Galicia (Xunta de Galicia)
Project Code: (PGIDIT07TIC005105PR).
Budget: 96,002.00 €
Period: 2007-2010.
Objectives: The goal is 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: Spanish Ministry of Industry, Tourism and Trade
Budget total: 705,000.00 €
Period: 2008 – 2009.
Objectives: The project aim is the launching of a national communications network for the testing of new services.

E-LEARNING & COLLABORATION TOOLS

ABC: Learning based on competences: Intermediation system based on semantic web

Partners: CESGA, UVIGO
Coordinator: M.J. Rodríguez Malmierca, CESGA
Principal Researcher: M.J. Rodríguez Malmierca
Financing: Director General RTD, Galician Regional Government, Xunta de Galicia
Budget: 59800
Period: 2009 - 2012
Objectives: The ABC project goes deeper into E-procura project findings. It is focuses on learning that is based on competencies: Intermediation system based on semantic web technologies. It is financed by the Director General for RTD of the Galician Government.

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
Financing: Galician Regional Government (Xunta de Galicia)
Project Code: 08SIN004CT
Budget: 109,494.95 €
Period: 2008-2011
Objectives: The aim of the project is the design, development, and launching of an intermediation system specifically oriented toward the personalised search and localisation of courses that permits those in search of training to display the full 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, Austria, 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. Röhsner, 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: The project aims to provide 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, Associació Baobab, Spain, CESGA, Spain.
Coordinator: Academy of Management, Poland
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 aim of the project is to develop 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 Capacitación para la Industria Lactea - REDLECHE

Partners: USC, FEPALE y CESGA
Coordinator: J.M. Dónega, Universidad Santiago de Compostela
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: The aim of the project is to provide skill building for the Latin American dairy industry.

YES: Youth Employment Support

Partners: Die Berater, Austria, Local Mission Agenais and Albret, France, Glotta Nova, Slovenia, Furthter Training Centre for the Saxonian Eco¬nomy, Germany, Transfer, Slovakia, Reflexion Foundation, Netherlands, Meter Silesia, Czech Republic, and CESGA, Spain.
Coordinator: Die Berater, Austria
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 aim of the project includes 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 adapt the ICT to this context.

E-intervention
Partners: CESGA, USC, and UVIGO
Coordinator: A. Gómez Tato, CESGA
Principal Researcher: A. Gómez Tato
Financing: Galician Regional Government (Xunta de Galicia)
Project Code: PGIDIT05TIC00101CT
Budget: 70,000.00 €
Period: 2006-2009
Objectives: The aim of the project is the development of a technological platform for at-home gerontological attention.

GIS

METEO-XIS: Geographical Information System for Management and Distribution of Meteorological and Oceanographic Information of Galicia
Partners: METEOGALICIA, USC, UDC
Coordinator: J. F. Alonso Picón, LABORATORIO MEDIO AMBIENTE DE GALICIA (LMAG)
Principal Researcher: F. Landeira, CESGA
Financing: Directorate General for RTD, Galician Regional Government (Xunta de Galicia)
Project Code: 09MDS034522PR
Budget: 35172.75 €
Period: 2009 – 2012
Objective: This project aims to provide adequate organization, management, and dissemination of meteorological and oceanographic information in Galicia by implementing GIS-components and web services.

IDEPATRI: Design and Development of a Date Model for an Archaeological Age of Iron Age in Galicia
Partners: CESGA, Universidad Santiago de Compostela
Principal Researcher: F. Landeira Vega
Financing: Directorate General for RTD, Galician Regional Government (Xunta de Galicia)
Project Code: 09SEC002CT
Budget: 61180 €
Period: 2009-2012
Objective: This initiative aims to create an operational system of generation and supply of data from archaeological activities. The coordinated efforts of several research groups will design a platform for the exchange of archaeological themed geospatial information via the Internet.

Forest Industry Information System- SIFI Galicia
Partners: CIS Madera and CESGA
Coordinator: X.F. Pedras Saavedra, CIS Madera
Principal Researcher: F. Landeira Vega, CESGA
Financing: Galician Regional Government (Xunta de Galicia)
Project Code: PGIDIT06RF000301CT
Budget: 28,750.00 €
Period: 2006-2009
Objectives: The aim of the project is to elaborate a geographic information system for the industrial forestry sector of Galicia. The project was completed in 2009 and provided an application and web server for GIS data base management in the industrial lumber sector of Galicia.

TECHNOLOGY TRANSFER & E-BUSINESS

EVITA Exchange, Valorisation and Transfer of regional best policy measures for SME support on IT and e-business Adoption
Partners: CESGA, GRNET, COPCA, NUTEK, CCIMP, FTZ, eCLC SAITC, Southern Aegean Region, Sinergija DA, LTC- Latvia
Coordinator: Greek Research and Educational Network (GRNET)
Principal Researcher: R. Basanta, CESGA
Financing: INTERREG IVC
Project Code: Project 0226R1.
Budget: 135685 €
Period: 2008-2011
Objective: The main aim of the project is to reinforce social, economic, and territorial cohesion by making ICT products and services more accessible within less-developed regions, becoming an economic, social, ethical, and political imperative, according to the Lisbon Agenda.
Consequently, it is crucial that successful policy practices, recognized by the European Commission as "best practices" are transferred from the regions that have already successfully implemented them to regions that are just now designing policy measures for improvement of SME competitiveness through better access to the knowledge economy.
In addition to the exchange of know-how, EVITA proposes the pilot implementation of these practices, together with the development of new approaches, such as, the integration of e-learning techniques and methodologies for reaching SMEs in remote areas.

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

XesveTIC : Optimum design of the architecture of livestock exploitations integral veterinary control system
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: The aim is to provide an optimum design for the architecture of an integral veterinary control system for livestock operations.

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
Objectives: The aim is to provide strategic associative action focused on technological excellence for networking and software development.

OTHER GRANTS FOR RESEARCH

NextCESGA: Moving CSEGA forward as a Research Centre of Excellence

Partners: CESGA
Coordinator: J. García Tobío, CESGA
Principal Researcher: J. García Tobío
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.

unid-inv-09: Renewal contract for Consolidation and Structure of Competitive Research Units of the Galician I+D+i System

Partners: CESGA
Coordinator: J. García Tobío, CESGA
Principal Researcher: J. García Tobío, CESGA
Financing: Regional Government of Galicia (Xunta de Galicia)
Project Code: INCITE09E1R704062ES
Budget: 128,295 **€**
Period: 01/12/2009 -30/12/2009
Objectives: The aim of the project is to provide aid for research group consolidation.

Support Technicians II

Partners: CESGA
Coordinator: C. Fernández Sánchez, CESGA
Principal Researcher: C. Fernández Sánchez
Financing: Spanish Ministry of Science and Innovation
Project Code: PTA2007-0375-I
Budget: 54,000.00 **€**
Period: 2008-2011
Objectives: This project provides financing to contract HPC support technicians.

Isabel Barreto Program 07, Human Resources

Partners: CESGA
Coordinator: A. Gomez, CESGA
Principal Researcher: A. Gomez
Financing: Directorate General for Research Development and Innovation (DXIDI)
Project Code: Human Resources Program, Subprogram Isabel Barreto
Budget: 72,000.00 €
Period: 2008-2009
Objectives: This programme focuses on defining a scientific career that may provide opportunities for the training and consolidation of researchers and technicians and allow them to have a stable position in the Galician R+D+I system.

Lucas Labrada Program 08, Human Resources

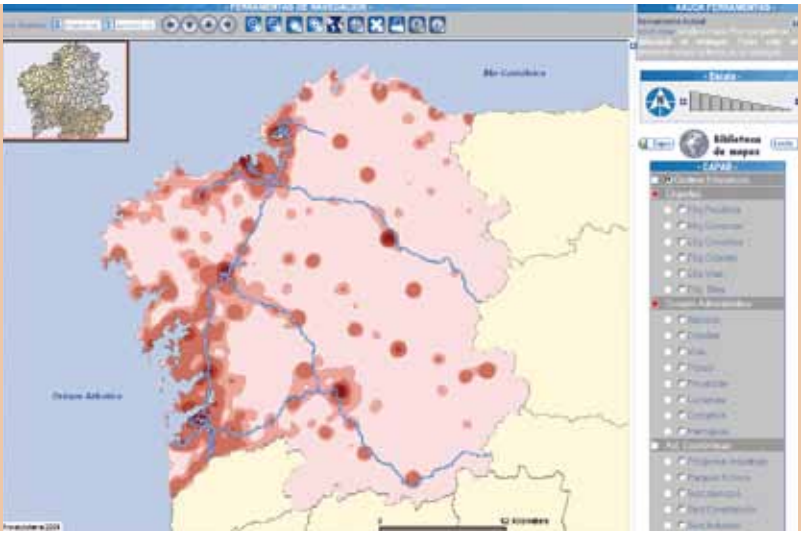
Partners: CESGA
Coordinator: J. García Tobio, CESGA
Principal Researcher: J. García Tobio
Financing: Directorate General for Research Development and Innovation (DXIDI)
Project Code: Human Resources Program, Subprogram Lucas Labrada
Budget: 84,000.00 €
Period: 2009-2010
Objectives: This programme focuses on defining a scientific career that may provide chances for training and consolidation of researchers and technitians that may allow them to have a stable position in the Galician R+D+I system.

Isidro Parga Pondal Program 08, Human Resources

Partners: CESGA
Coordinator: I. González López del Castillo, CESGA
Principal Researcher: I. González López del Castillo
Financing: Directorate General for Research Development and Innovation (DXIDI)
Project Code: Human Resources Program, Subprogram Isidro Parga Pondal
Budget: 108,000.00 €
Period: 2009-2011
Objectives: This programme focuses on defining a scientific career that may provide chances for training and consolidation of researchers and technitians that may allow them to have a stable position in the Galician R+D+I system.

GIS Geographic Information Systems

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



Noteworthy Activity in 2009

Projects

Forest Industry Information System- SIFI Galicia This project was completed in 2009. Both an application and a web server for data base management in the industrial lumber sector of Galicia were developed and put into production.

Archaeological Patrimony 2009 – Government of Galicia In 2009, goods and states declared of cultural interest (BIC) were located and delimited into a spatial database and integrated into a geographic information system application. Technical assistance was provided to elaborate an Archaeological Atlas of Galicia.

TERRA Project A map server of Galicia was developed for the educational project, TERRA, a teaching resource and tool for learning in primary and secondary Galician educational centres.

Participation in the Thematic Network of Geographic Information for Research in Galicia - REDIX A survey was conducted that concerned the use of GIS by local administrations in Galicia.

Dissemination Activities

Map Server of Surnames of Galicia The map of Surnames developed by the University of Santiago's Galician Language Institute (ILG) on Internet was maintained and fully operative.

Sueloempresarial.com The web of industrial parks developed for the Consortium Zona Franca de Vigo was maintained and fully operative.

Map of Gas Stations This GIS web application with the distribution of gas stations in Galicia was maintained and gas pricing information was updated weekly.

Training

Teacher Training course of the Regional Ministry of Education, "Opportunities posed by Networked Geographic Information Systems as a Learning Tool" 2009.

e-Learning & Collaboration Tools

Objectives

- To carry out research in the area of e-learning and collaborative applications in different environments.
- To promote and disseminate the use of ICT applied to learning and collaboration processes.
- To promote the use of e-learning and collaborative tools in research and education.

e-Learning Technological Resources

- e-Learning and collaboration on-line suite: 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 (Webminar).
- Hardware for mobile learning and T-learning.
- Web 2.0 tools for e-learning information and management.

2009 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, organized 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 OpenOffice and their 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 articles in international proceedings. Participation in the organizing committee of the IV Cibersociety Conference (Congreso de la Cibersociedad 2009). Presentations at 2 international conferences in the ICT and Education sectors.
- Analysis and implementation of an open source, on-line tool that allows virtual meetings and virtual seminars to be offered as a service to researchers.
- Participation in 8 e-learning projects during 2009, listed below.

e-Intervención: Analysis and impact of ICT use for people with special needs and their families, including quality of life and self-management. This is a project financed by the Directorate General for RTD&I of the Government of Galicia.

SUMA: Integration of e-learning services by means of standards. Suma is a project born within the eLearning group at the National Technological Platform (INES). The project is financed by Plan Avanza, and counts on the collaboration of other private and public institutions.

Parents: e-Learning training for parents as professional and vocational advisors of their children. Parents is a program financed by the European Commission, Long Life Learning Grundtvig Programme.

Yes: e-Learning training to support youth employment in SME. YES is a project financed by the European Commission, Long Life Learning Program -Leonardo-.

ICTeacher: Pilot course for the European Computer Driving Licence module to develop 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 and serves personalised training contents for television learning experiences (t-Learning). This is a project financed by the Directorate General for RTD&I of the Government of Galicia.

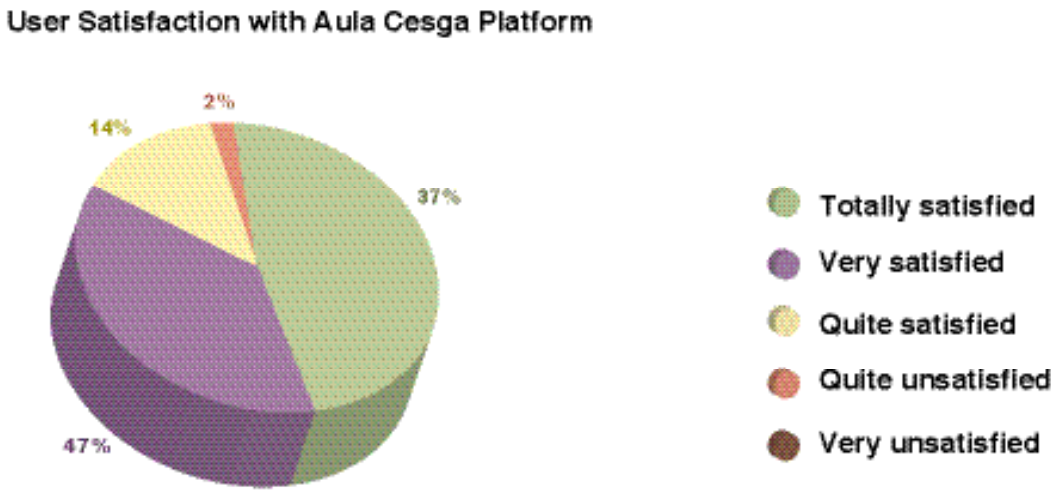
e-Procura: e-Procura is a system that permits on-line searches for personalised courses using semantic technologies. It is financed by the Directorate General for RTD&I of the Government of Galicia.

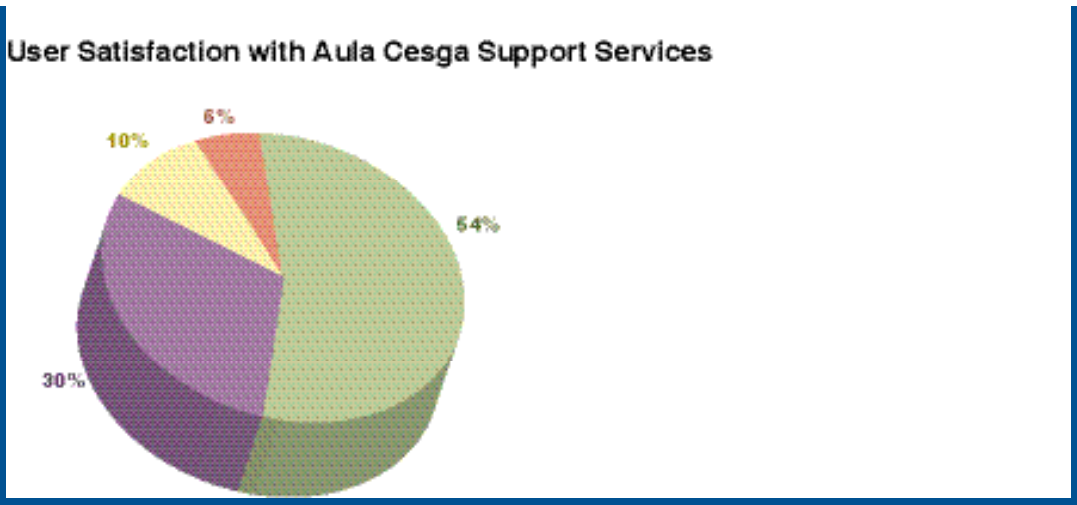
ABC: The ABC project aims to deepen on e-Procura project findings. It is focused at learning based on competencies: Intermediation system based on semantic web technologies. It is financed by the Directorate General for RTD&I of the Government of Galicia.

Aula CESGA Courses – 2009

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.

A user satisfaction survey carried out in January 2010 showed that our users were very satisfied both with the tool used and with the service provided:





The activity in the Aula CESGA platform during the period 2004-2009 is summarized below.

TRAINING COURSES AND COLLABORATIVE PLATFORMS IN AULA-CESGA

	2004	2005	2006	2008	2009
Number of Courses	108	162	235	461	626
Number of Users	1,583	2,533	4,378	6,748	10,302

Technology Transfer & e-Business

- Completion of contracted projects : XesveTIC, VINDEIRA-CMMI

- **Enforcement of the Quality Standard ISO9001**

- CAPITA Project: Development of the activities identified in the project plan for 2009

The most significant activities in the e-Business area in 2009

- ***Completion of International Projects***

  ICHNOS PLUS: Innovation and Change One-Stop Shops

  EVITA: Exchange Valorisation and Transfer of best of Regional Best Policy Measures for SME support on IT and e-Business Adoption.

- ***Participation in regional, national and international events***

  EVITA: study-visit to initiatives and projects of COPCA (Regional Development Agency of Catalonia) on May 7th and 8th 2009 in Barcelona.

  EVITA: study-visit to initiatives and projects of the Marseille Chamber of Commerce on May 25th, 2009 in Marseille.

  ICHNOS Plus: Staff exchange between Galicia and Estonia, Santiago de compostela, June, 17th, 2009

  Closing event of VINDEIRA-CMMi Project, on June 17th 2009, Santiago de Compostela

  ICHNOS Plus: Project Committee Meeting on June 18th 2009, Santiago de Compostela

  EVITA: Committee Meeting, on September 17th , 2009, Santiago de Compostela

  EVITA: study-visit to initiatives and projects of IGAPE, September 18th, in Santiago de Compostela

  ICHNOS Plus: Project 2nd International Conference, in Mytilene, Greece, on September 21st and 22nd, 2009.

  EVITA: study-visit to initiatives and projects of the Regional Development Agency of Stockholm on October 5th 2009, Stockholm.

  International Event eBSN: meeting of the participants in the network “European e-Business Support Network for SMEs” on October 6th 2009 in Stockholm

- ***International events Organisation***

  ICHNOS Plus: Organisation of the inter-regional seminar “Supporting Innovative Entrepreneurship and Innovation in Galician SMEs”, June, 19th, 2009, in Santiago de Compostela.

Training Activities

CESGA provides training opportunities for Users and Personnel. CESGA's users, RTD Companies personnel, public administration officials, university teachers, researchers, students, and the Centre's personnel all have benefited from training activities carried out in 2009. The Annual Training Plan is the keystone around which the organisation of these activities is structured.

During 2009, the Centre participated in the organization of a total of 55 training activities, distributed as indicated in the table below. The vast 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.

As a novelty in 2009, we highlight the celebration of the first edition of the CESGA Computational Science Summer School which took place with training sessions, speakers, and students of the highest quality.

SUMMARY OF TRAINING EVENTS	2004	2005	2006	2007	2008	2009
COURSES	16	21	22	16	49	39
SESSIONS AND SEMINARS	8	7	8	11	7	16
CONFERENCES	1	3	2	1	2	0
	25	31	32	28	58	55

TRAINING FOR USERS

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
C Programming	Course	CESGA	22/06/09	26/06/09	20
Fortran Programming	Course	CESGA	16/06/09	19/06/09	20
2nd Edition: Access to and Use of FinisTerrae Supercomputer	Course	CESGA	05/03/09	05/03/09	5
Open Source Tools for Debugging and Application Performance Analysis	Course	CESGA	07/09/09	11/09/09	20
Introduction to Algorithms for Scientific Applications	Course	CESGA	06/07/09	10/07/09	20
Computational Maths: Programs Compilations, Execution and Optimisation	Course	CESGA	29/06/09	03/07/09	20
Parallel Programming Using OpenMP Directives	Course	CESGA	27/07/09	31/07/09	20
Introduction to MPI Programming	Course	CESGA	20/07/09	24/07/09	20

TRAINING FOR CESGA STAFF

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
Senior Course for E-Learning Projects Direction and Management	Course	Global Estrategias	31/10/08	30/04/09	250
English Language	Course	Picadilly Academia	01/01/09	31/12/09	56
Operational Systems Networks and Linux Servers Administrator. Advanced	Course	CNTG	05/01/09	05/02/09	64
Web Accessibility Workshop	Course	Asociación Galega de Empresas TIC - AGESTIC - INTECO	21/01/09	29/01/09	10
Applications Developer with BBDD Oracle. Forms Developer. OCP (Oracle Certified Professional)	Course	Centro de Novas Tecnoloxías de Galicia	26/01/09	12/03/09	96
Installation and Configuration with VMWARE infraestructure 3	Course	Centro de Novas Tecnoloxías de Galicia	02/03/09	12/03/09	36
SIG Applications Programming	Course	Universitat de Girona	02/03/09	19/04/09	120
Tools for Scientific Dissemination in Galicia	Course	DXID	04/03/09	04/03/09	4
High Performance Interconection Systems. Infiniband	Course	HP	01/04/09	01/04/09	7
CCNP Module BSCI: Building Scalable Cisco Internetworks v5.0	Course	Centro de Novas Tecnoloxías de Galicia	13/04/09	08/05/09	80
Implementing and Efficient Services Center in ITIL Framework	Course	CESGA	20/04/09	22/04/09	16
Labor Productivity and Absenteeism Reduction. Towards Greater Efficiency in Managing People	Course	APD	28/04/09	28/04/09	5
Training the Trainers	Course	EGEE-III	06/05/09	06/05/09	8
Ocupational Hazard Prevention	Course	CESGA	15/05/09	15/05/09	2
Storage Systems. EVA Storage	Course	CNTG and HP	18/05/09	04/06/09	72
Spring School in Advanced Computing, TACC@UP	Course	Univ. Oporto	28/05/2009	28/05/2009	16

TRAINING FOR CESGA STAFF

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
Process of Management and Organisational Development in CESGA	Course	CESGA	28/05/09	31/12/09	72
Advanced Seminar on Multicore Platforms	Course	Universidade do Minho	01/06/09	04/06/09	24
Multiescale Systems	Course	USC	17/07/09	25/07/09	16
R Estatistical Environment	Course	Nodo CESGA I-MATH	07/09/09	11/09/09	20
GPUs Programming (General Purpose Computation on Graphics Processing)	Course	Red G-HPC	28/09/09	30/09/09	15
Effective Preparation and Delivery Skills for Business Presentations	Course	CESGA	05/10/09	08/10/09	16
Optimizing the Use of Memory Hierarchy	Course	Red G-HPC	13/10/09	15/10/09	15
Advanced Administration of Linux Operating Systems- LPIC 2 Ceráfication	Course	Centro de Novas Tecnoloxías de Galicia	26/10/09	19/11/09	64
Introduction to Portlets Programming	Course	Fundación CESGA	26/10/09	30/10/09	15
After Effects	Course	ARTEnet	02/12/09	04/12/09	14

SEMINARS

Activity	Type	Responsible Organisation	Date	Hours
New Algorithmic Solutions for Global Navigation Satellite Systems Modelling	Seminary	CESGA Computational Summer School	13/07/09	2
Interconnection Networks for Supercomputing: an Introduction	Seminary	CESGA Computational Summer School	14/07/09	2
Irregular Codes in High Performance Systems: The Sparse Matrix-Vector Product as a Case	Seminary	CESGA Computational Summer School	15/07/09	2
Simulation of "Quantum" Meterials Using "Chessic" Supercomputers	Seminary	CESGA Computational Summer School	16/07/09	2
Introduction of HPC Programming Through PGAS Paradigm with UPC	Seminary	CESGA	17/07/09	2

Mathematica.nodo.cesga.es Outreach Activities in 2009

Activity	Type	Responsible Organisation	Date
2nd i-MATH Free/Open Software for Science and Engineering Intensive Course	Course	UDC, UCA, UC, USC, UVIGO, CESGA	07/06/09-09/11/09
Mathematical Transfer Course	Course	USC, UDC, UVIGO	09/25/09-11/03/09
i-MATH Consulting for Industry and Public Administration	Industry Days	USC	03/25/09-03/27/09
Applied Math and Industry Interaction Day	Forum	UVIGO	04/17/09
Statistics in Quality Control Methods	Forum	UDC	06/11/09
Mathematics & Wind Energy	Forum	USC	05/29/09
Open Software for Science and Engineering Forum	Forum	UDC	03/13/09
Workshop: Statistics and Computational Oceanography and Hydraulics	Workshop	USC, UVIGO	11/27/09
Modelling and Numerical Techniques in Quantitative Finance	Workshop	UDC	10/14/09-10/16/09
Workshop on Mathematical Technology Transfer Experience	Workshop	EHU	06/15/09-06/16/09
CESGA Computational Science Summer School	Course	CESGA	06/15/09-09/30/09

Dissemination

Objectives

• Planning, coordination, and execution of CESGA dissemination activities.

• Development and maintenance of communication tools (website, “Díxitos” magazine, annual workshop, annual report, etc.).

• Edition of CESGA’s publications.

• Organization and logistics of the Annual Training Plan for CESGA personnel and users.

2009 Highlights

• Publication of the periodical magazine, “Díxitos”.

• Publication of the 2008 CESGA Annual Activity Report.

• Maintenance of the content management application for www.cesga.es

• Planning and development of a new content management system together with IMAXIN Software Company.

• Participation in the organisation and dissemination of courses, workshops, and seminars for CESGA users.

• Implementation of CESGA’s Communication Plan.

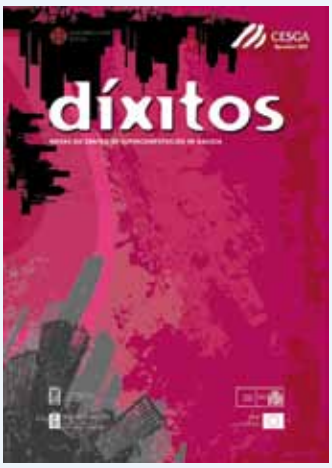
• Preparation of presentations, dossiers, and reports for CESGA, including The Annual Activity Report for CSIC’s Delegation in Galicia.

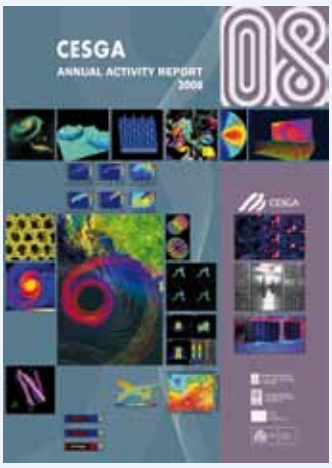
• Communication, public relations and dissemination support for the Centre’s projects and activities including: NextCESGA, IEMath, EGEE, e-HOSPITAL, Formiga, T-MAESTRO, MANCOMUN, ISOC, the USC ConCiencia Program, eIMRT, RECETGA, i-Math, and FinisTerrae.

• 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), and CSIC-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.

• Collaboration and participation with CSIC officials in Exper-i-Ciencia dissemination activity in 2009.

• Planning together with the consultancy firm, Cidadania, for the execution in 2010 of a thorough user satisfaction survey, regarding computing and storage services.

• Compilation of users' scientific production data from 2008 and preparation for the collection campaign of the same type of data for 2009.

• Planning of the Bibliometric Study of Scientific Production of the Users between 2002 and 2008 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 in the maintenance of CESGA's on-demand video repository for training and dissemination activities, tv.cesga.es.

• The organisation of institutional and educational visits to CESGA.

• Organization and attention to the 949 visitors from 30 different educational and technological institutions with a total of more than 33 visits during the year.