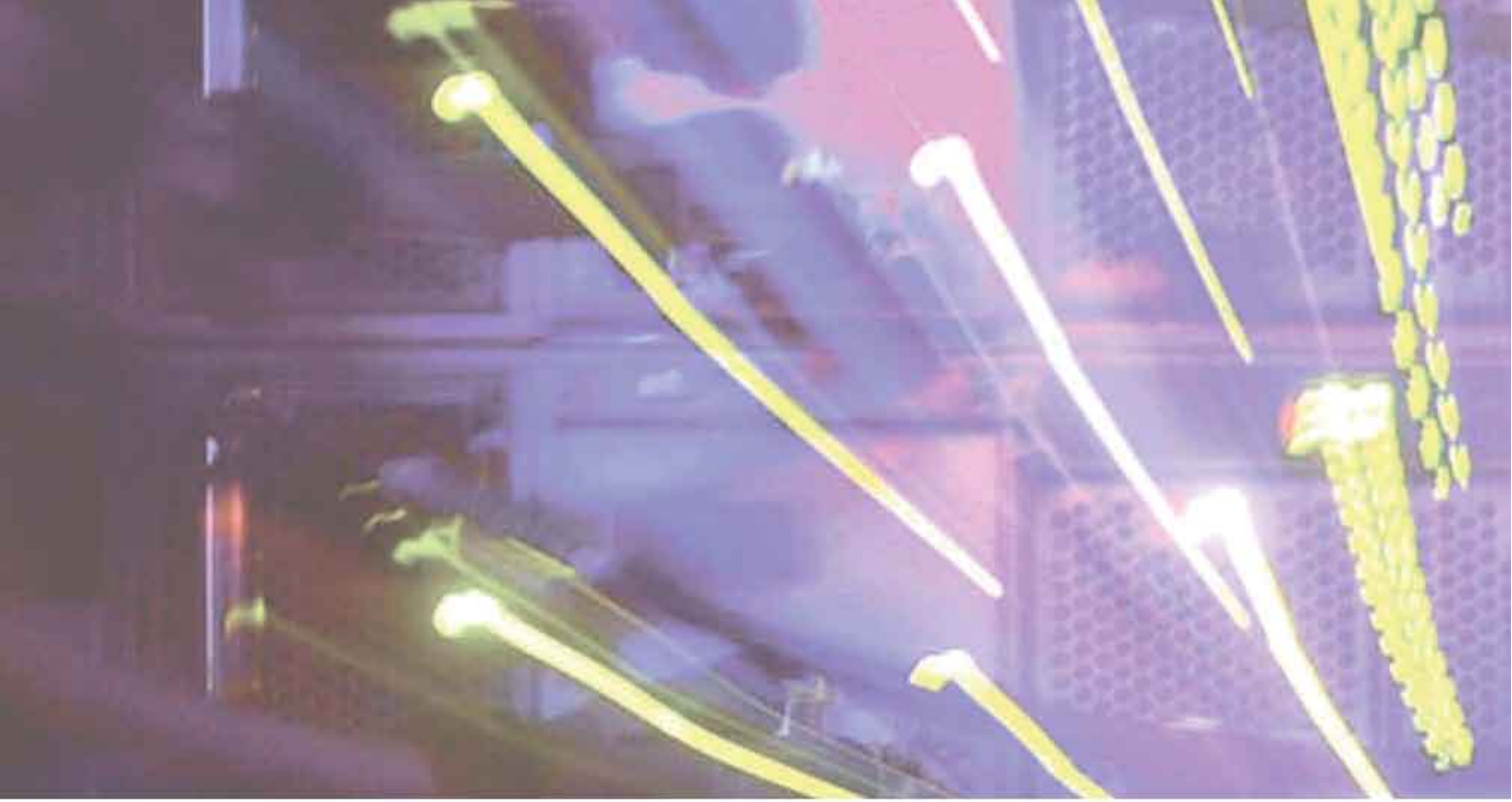# 2010 Annual Report

Galicia Supercomputing Centre

CESGA

GALICIA SUPERCOMPUTING CENTRE

CREDİTS

2010 CESGA ANNUAL REPORT

XUNTA DE GALICIA

CSIC
Consejo Superior de Investigaciones Científicas

GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

ERDF
EUROPEAN REGIONAL DEVELOPMENT FUND

CESGA Annual Activity Report 2010

Table of Contents

MESSAGES

MESSAGE FROM THE PRESIDENT

Ricardo Capilla Pueyo
Director General for Research, Development & Innovation
Regional Government of Galicia (Xunta de Galicia)

In 2010, CESGA carried out intensive work within the frame of important economic restrictions that were a result of necessary adjustments made by the practical totality of all Administrations. As a result, the Board of Trustees of the Foundation decided to postpone the construction of the new CESGA headquarters and to wait for an improvement in the economic situation that will enable the execution of said project, in consonance with the available budgets.

During 2010, CESGA in collaboration with RedIRIS, was able to advance in the coordinated deployment of dark fibre in order to interconnect the seven Galician cities and to establish lines dedicated for access to RedIRIS and to the Science and Technology Network of Portugal.

Another important accomplishment was the work carried out on the Unique Scientific-Technological Installation which provided an increase in the collaborations between the Centre and prestigious national and international institutions.

Looking ahead to 2011, CESGA will maintain its strategic lines of action which are moving internationalisation forward, increasing the transfer to industry, and continuing the pursuit of excellence in services as well as research in Computational Science. These priorities are specifically aligned with the role that the new "Galician Plan for Research, Innovation, and Growth, 2011-2015" reserves for technological centres and research centres as entities with a special responsibility in the transfer and evaluation of knowledge by means of the intensification of the relationship with the productive sector and, as a result, with the market.

The strong support provided to CESGA by the Regional Government of Galicia and CSIC as a Centre of services for RTD and Innovation as well as a research institution was reinforced through the renovation of infrastructures in 2011. The renovation consisted of the up-dating and enlargement of the data storage subsystem, the up-dating of distributed memory clusters, and the improvement of the network security system. All of these activities were supported by ERDF financing.

XUNTA DE GALICIA

MESSAGE FROM THE VİCE-PRESİDENT

"

Carmen Peláez Martínez
Vice-President for Scientific & Technical Research,
Spanish National Research Council (CSİC)

The year 2010 demanded significant efforts in order to maintain the Centre's high level of service as well as research activity, considering the budgetary limitations of the period.

Last year, Galicia gained recognition of a new International Campus of Excellence, the Campus do Mar, in which also participate CSIC, the Regional Government of Galicia, the University System of Galicia, and CESGA, among others.

CSIC
Consejo Superior de Investigaciones Científicas

I would like to point out the following accomplishments of 2010 as they are especially relevant.

The number of computing hours provided by CESGA surpassed 20 million for the first time in its history.

The scientific production declared by CESGA users, and CESGA itself, resulted in 245 articles, 121 conference presentations, 10 doctoral dissertations, 7 graduation projects and 5 books or chapters.

CESGA continued an important level of activity in terms of participation in RTD and Innovation projects. During the last year CESGA participated in 37 projects, 11 of them were financed by foreign institutions.

"

2010 HIGHLIGHTS

The year 2010 was characterised by a significant increase in support activities which was a result of the access to CESGA that was provided to new research groups such as ICTS (Unique Scientific-Technological Installation).

Similarly, the administrative and management actions of the Centre also intensified as a consequence of existing budgetary restrictions which obligated the delay of the construction of the new CESGA building.

The launching of the new RECETGA (the Network of Science and Technology of Galicia) along with RedIRIS Nova was a demanding task that will culminate in the activation of the new network in October, 2011.

As a result of the work carried out during 2010, the following achievements are most notable.

The number of computing hours increased by **5.2%** with respect to the prior year, reaching **20.5** million hours.

The Centre participated in **37** projects; 11 were financed by foreign institutions.

Traffic on RECETGA increased by **16.10%** with respect to the previous year.

CESGA signed **9** collaboration agreements with other institutions that benefit the Centre's services and activities.

The second edition of "CESGA Computational Science Summer School" was conducted. Twelve students were enrolled in the program.

The Universities of A Coruña and Santiago conducted the first edition of the HPC Master degree with the cooperation of CESGA.

CESGA

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

HPC, HTC, GRID, AND CLOUD COMPUTING

RESOURCES	SERVICES
HPC, HTC Servers, GRID Servers, Scientific Software Applications	Code Optimization Problem Definition Parallelisation User Support ...

DATA STORAGE

RESOURCES	SERVICES
Storage Servers	Critical Storage Systems

COMMUNICATIONS NETWORK

RESOURCES	SERVICES
RECETGA Science and Technology Network of Galicia	DNS, Hosting, Mail Servers, Mailing List, FTP, News, Mirrors, Multicast, Video-conference, MCU / Gateway, Proxycache, Network Management, Security Systems, Statistics...

RTD PROJECTS

Viability Analysis
Proposal Development
Consortium Creation
Project Negotiation
Management ...

TRAINING (EDUCATION)

Workshops and Training
Courses for Users

DISSEMINATION

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

e-LEARNING & COLLABORATION TOOLS

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

TECHNOLOGY TRANSFER & e-BUSINESS

RESOURCES	SERVICES
Galicia's e-Business Leveraging Centre	Viability Analysis Project writing Partnership Formation ...

GEOGRAPHIC INFORMATION SYSTEMS

RESOURCES	SERVICES
Map Servers, Geographical Data Bases	Analysis Development Implantation Lodging Solutions

BOARD
OF TRUSTEES OF
CESGA FOUNDATİON

CESGA's Work Force, İts Most Valuable Asset

CESGA FOUNDATION

Organisational Chart

```
                    BOARD OF
                    TRUSTEES
                        |
                   MANAGING
                   DIRECTOR
      QUALITY
      COMMITTEE                          SECRETARY

      RTD MANAGEMENT
      COMMITTEE

   DEPUTY              DEPUTY              DEPUTY
   TECHNICAL           ADMINISTRATIVE     INFO - SOCIETY
   DIRECTOR            DIRECTOR           DIRECTOR

SYSTEMS      COMMUNICATIONS   APPLICATIONS      TECHNOLOGY    E-LEARNING        GIS          PR &
DEPARTMENT   DEPARTMENT       & PROJECTS        TRANSFER &    & COLLABORATION   DEPARTMENT   COMMUNICATION
                              DEPARTMENT        E - BUSINESS  TOOLS                          DEPARTMENT
                                                DEPARTMENT    DEPARTMENT
```

CESGA'S PERSONNEL: CONTRACTS IN 2010

ACADEMIC TRAINING LEVEL	NUMBER	MALE	FEMALE	AGE AVERAGE
PhD (6 Year Higher Ed.+ Dissertation)	12	10	2	36.67
5 Year Higher Ed.Degree	29	18	11	34.07
3 Year Higher Ed.Degree	5	2	3	39.2
Secondary Ed. & Technical Schools (2 Year Degree)	11	9	2	31.9
Other	3	3	0	46.66
TOTAL	60	42	18	35.15

20%
of the Staff holds a Ph.D.

FİNANCİAL İNFORMATİON

2010 Operational İncome

24.09%

57.7%

11.88%

3.19%

3.12%

Galician Government

CSIC

Spanish Government

European Commission

Other (Applied for Amortisation)
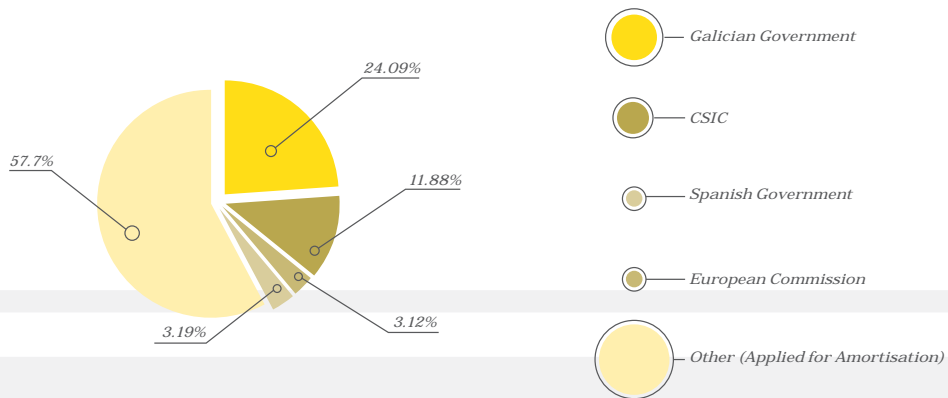
2010 Operational Expenses

21.07%

48.10%

30.82%

Personnel

Current Expenses and Taxes

Amortisation
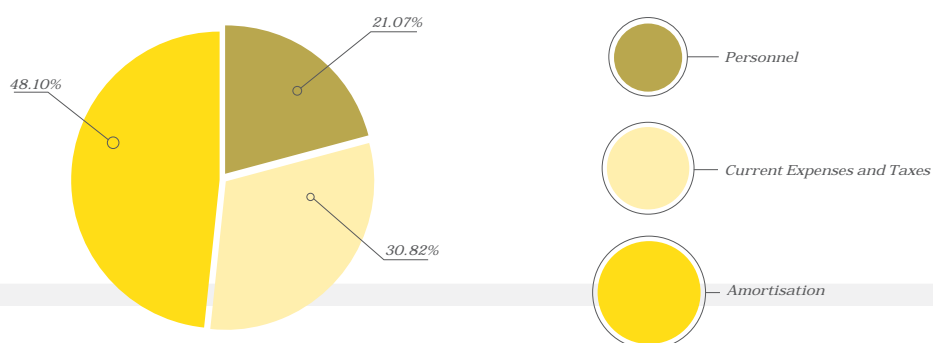
The following is a detailed description of CESGA Foundation accounts for the fiscal year 2010.

CESGA's main sources of operational income in 2010 came from the Galician Regional Government (Xunta de Galicia), the Spanish National Research Council (CSIC), the Spanish Ministry for Science and Innovation (MICINN), and from the European Commission. Of a total operational income in excess of 7.5 million euros, more than 3.5 million were applied for amortization of equipment and infrastructures in 2010.

Financial Accounts

2010 OPERATIONAL INCOME	GALICIAN GOVERNMENT	CSIC	SPANISH GOVERNMENT	EUROPEAN COMMISSION	OTHER	TOTAL
Services to User Community	1,284,177.57	919,131.29			83,684.05	2,286,992.91
Competitive projects	579,578.59		241,467.01	247,412.86	4,600.00	1,073,058.46
Finnancial and others					738,832.38	738,832.38
Applied for amortisation					3,636,389.81	3,636,389.81
TOTAL	1,863,756.16	919,131.29	241,467.01	247,412.86	4,463,506.24	7,735,273.56

2010 EXPENSES	
Personnel	1,600,049.77
Current expenses & taxes	2,340,289.30
Amortisation	3,652,205.26
TOTAL	7,592,544.33

EXTERNAL SERVİCES PROVİDED BY DEPARTMENTS

CESGA provides a varied repertoire of services to research users as well as to businesses and institutions. Here we present a list of the external services offered by each Department.

Systems Department

HPC, HTC, GRID, and CLOUD computing time

User technical support

Data Centre auditing and advanced services

Training

Scientific Applications and Projects Department

Scientific computing user support (parallelization, tuning, debugging, porting, algorithms).

User training

RTD & Innovation Project design and management

Project partnering

Project grant search

Project partner search

HPC advanced services

Collaboration Tools and e-Learning Department

Project design and management

Project partnering

Project grant search

Project partner search

e-Learning platform for courses and events

Virtual classroom for webinars

Access Grid rooms

Multicasting of events

e-Learning advanced services

Scientific conference and event organisation

Technology Transfer and e-Business Department

Project design and management

Project partnering

Technology transfer advanced services

Geographical Information Systems Department

GIS project design and management

GIS project partnering

Geo-referenced data production and analysis

Digital map processing

GIS application development

GIS advanced services

GIS user training

GIS platform

Cartographic service hosting

Network Communications Department

Centre connection: analysis and connection plan

Communications consulting: connectivity, security, and advanced services

Project partnering

Hosting of webs (contents of interest for researchers)

Videoconferencing

Management (e-mail, web, mailing lists, news, ftp, firewalls, security, virtualization,…)

Voice communications and videoconferencing management

IP address management

DNS administration

User support

Management of new services (IPv6, multicast, mobility,…)

Public Relations and Communication Department

PR services for researchers

Edition of scientific dissemination materials

Promotional space in CESGA's media (díxitos, web & others)

PR & communication advanced services for users and project partners

QUALİTY OF SERVİCES

PROCESS FLOW CHART

STRATEGIC PROCESSES

TECHNOLOGICAL OBSERVATORY	CREATION AND IMPROVEMENT OF THE QUALITY SYSTEM
MANAGEMENT PLANNING	QUALITY PLANNING

VALUE PROCESSES

COMPUTING

e-LEARNING & COLLABORATION TOOLS

TECHNOLOGY TRANSFER & e-BUSINESS

DATA STORAGE

GIS

CLIENT/ USER

USER MANAGEMENT

COMMUNICATIONS

PROMOTION AND DISSEMINATION

CLIENT/ USER

USER/ CLIENT SATISFACTION

PROJECT DESIGN AND DEVELOPMENT

TRAINING ACTIVITIES

TRAINING ACTIVITIES	INFRASTRUCTURES AND FACILITIES MAINTENANCE	HUMAN RESOURCE MANAGEMENT	FUND RAISING	ADMINISTRATIVE MANAGEMENT	SECURITY

İSO 9001:2008-CERTİFİED UNE 166002-Undergoing CERTİFİCATİON

Quality, a map of processes

During 2010, the CESGA Foundation again 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, 6 processes, 3 procedures, and 4 instructions were improved. CESGA was audited three times with successful results. Two of them were internal audits performed by external auditors and the other was the periodic external auditing process.

Additionally, in 2010, 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.

And last but not least, in 2010, CESGA prepared to obtain a new certification by March 2011: the UNE166002, related to research management, development, and innovation activities. Much work was required in order to adapt the existing procedures and to create new ones that describe precisely the R&D activity developed by CESGA's personnel. CESGA's Quality Management system will will be made up of these two certifications assuring an outstanding level of quality in CESGA's internal and external business processes.

Quality of services
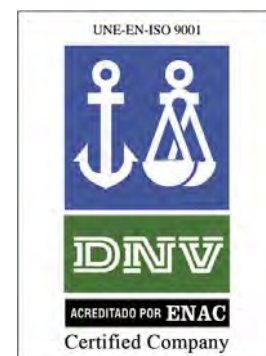
User satisfaction levels keep scoring high

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 we first started taking these measurements in 2007, 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 4.2 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, thereby demonstrating the highest standards of quality.

CESGA User Technical Helpdesk Service Requests in 2010

Most often, users interact with CESGA's technical helpdesk personnel through e-mail or by phone. Either way, requests are kept track of through an automated request tracker application called RT. Every time a user places a helpdesk service request, a ticket is opened in the RT application. This provides users and helpdesk personnel with an opportunity to track at all times how the request is being handled, which actions are taken, and when the actions are taken regarding the problem posed by the user.

Requests are categorized according to the type of service solicited and the technnical area involved in the provision of a solution. The following Table summarises the amount of service requests attended in 2010, categorized by service type.

User Support Activity 2010

Area	Number of requests
Communications	605
Applications	447
Systems	878
Infrastructures	68
GIS	46
General	22
TOTAL	**2,066**

User Satisfaction with Services Provided in 2010

Every year, CESGA conducts a survey to collect data relating to user satisfaction levels with the different services. It provides and requests user reflections and thoughts on how to improve services to them. To conduct this user satisfaction survey, an on-line questionnaire is made available for all users to declare their level of satisfaction with services and provide their views and insights on how to improve them. In order to encourage users to express whatever negative views they may have, answers are automatically collected anonymously. Here we account for the 2010 survey results.

HPC Services User Satisfaction Levels

Questions related to user satisfaction levels with computing, storage, and related support services were posed to 448 active user account holders. A total of 80 answers were collected through the 2010 survey (a 17.8% response rate). Satisfaction levels expressed through the survey scored high across all dimensions. The following Tables summarise the results of this survey.

COMPUTING — MEAN 4.38

STORAGE — MEAN 4.3

SUPPORT — MEAN 4.46

Very Poor 1 · Poor 2 · Average 3 · Good 4 · Excellent 5 · N/A* · * Non applicable
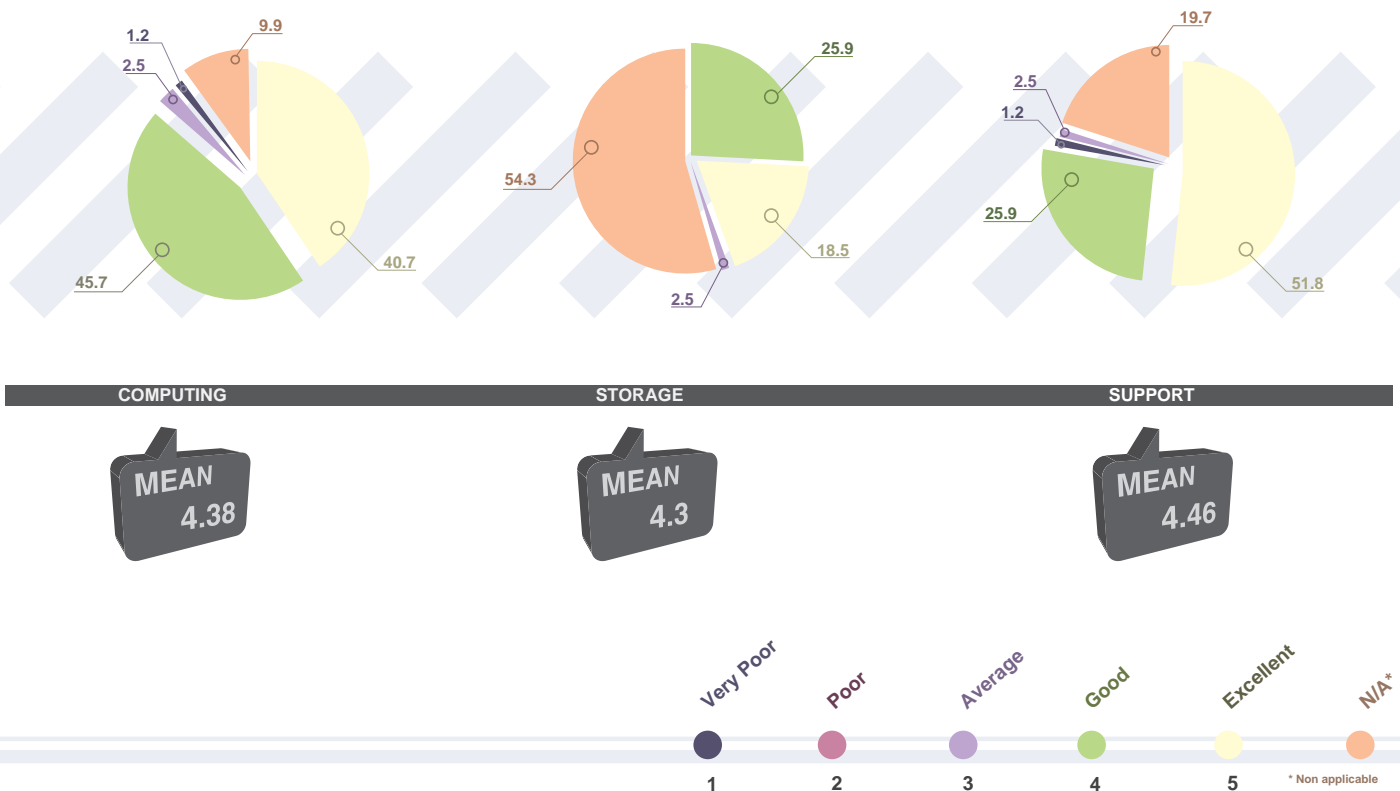
User Satisfaction: Well Above Average

Recetga Network Services User Satisfation Levels

Questions related to user satisfaction levels with RECET-GA network connectivity, RECETGA network services, and network support helpdesk services were posed to 37 contact persons in the different labs and centres that RECETGA interconnects.

A total of 11 persons completed the survey which represents a 29.7% response rate. RECETGA user satisfaction factors received high scores. The following pie charts summarize the results of the survey.
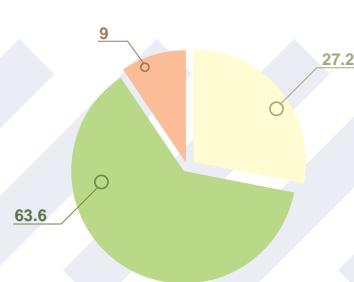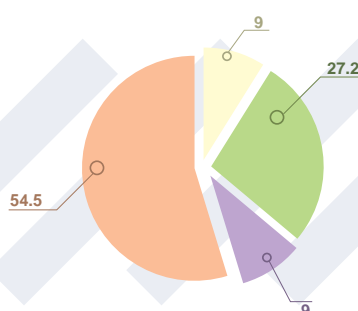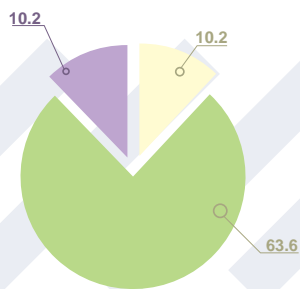
CONNECTIVITY	SERVICES	SUPPORT
MEAN 4	MEAN 4	MEAN 4.3

Very Poor Poor Average Good Excellent N/A*

1   2   3   4   5   * Not applicable
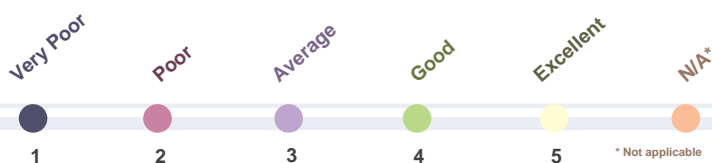
COMPUTING USERS
SCIENTIFIC PRODUCTION
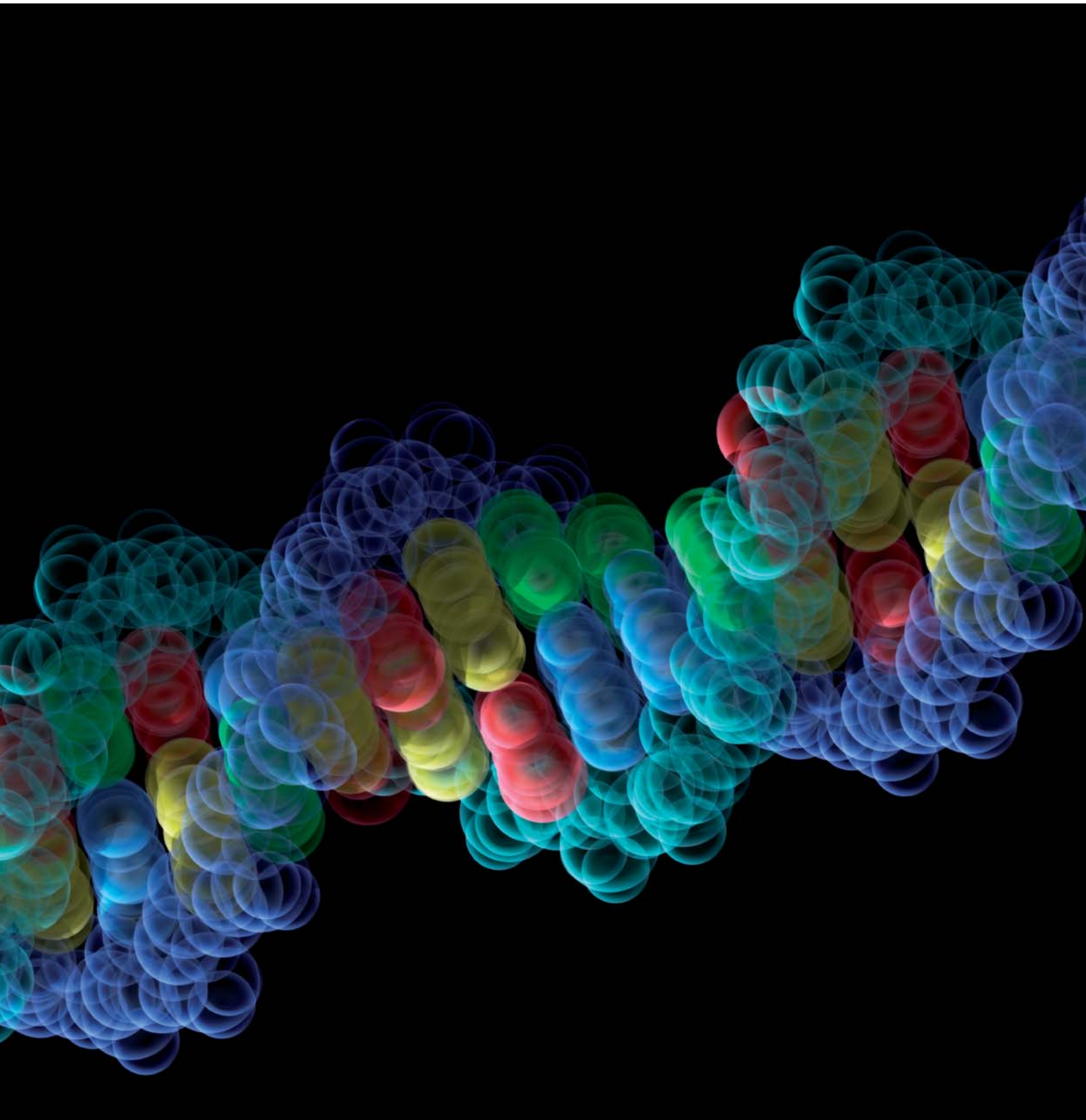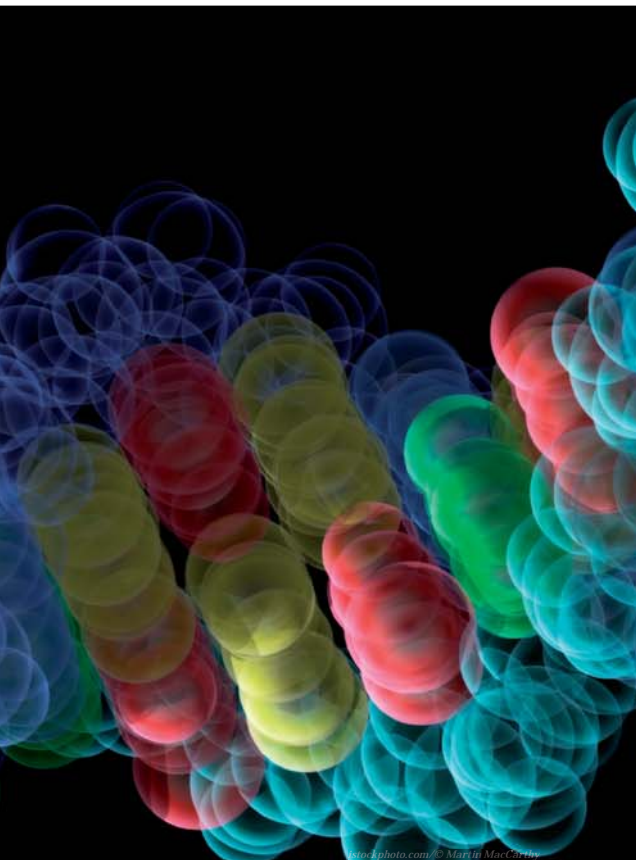
Scientific Production Reported by CESGA Users in 2010

The data summarising the scientific production reported by users is presented in the following Tables.

Articles increased by **27** &

Conferences decreased by **39**

Users Scientific Production

- Scientific Journal Articles
- Presentations at Conferences
- Doctoral Dissertations
- Master's theses/Final Projects
- Books/Chapters
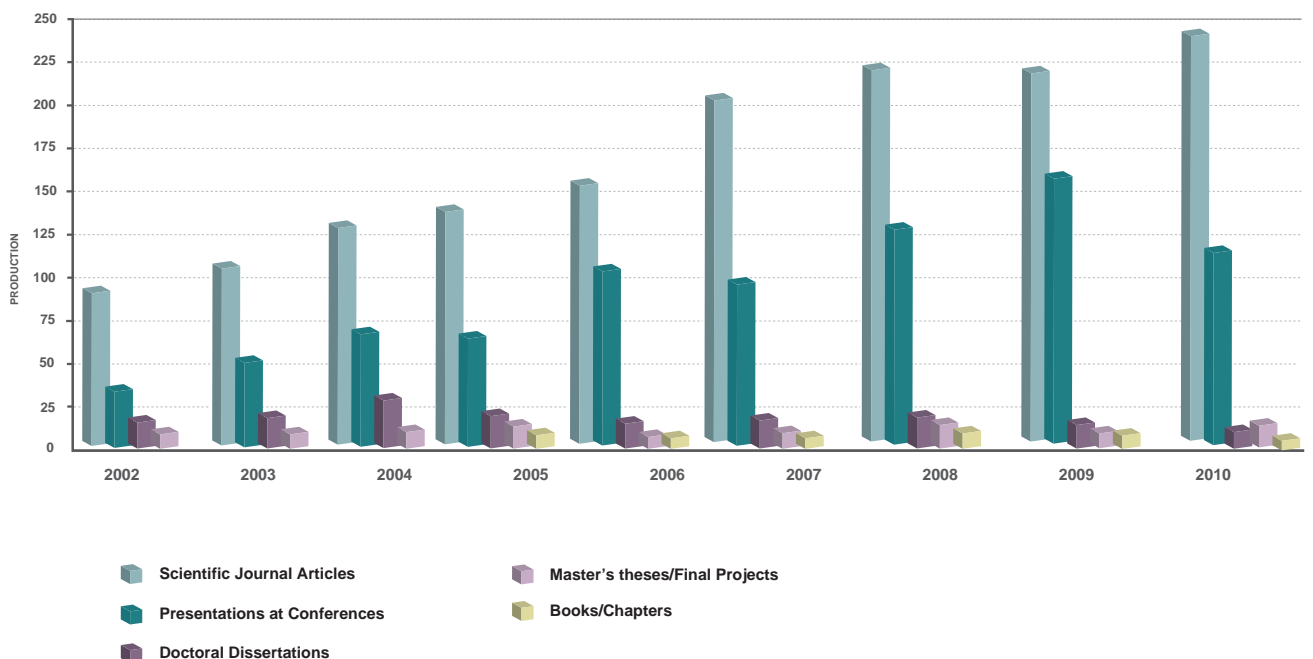
Users Published over

200

Scientific Articles

Distribution of all Users Scientific Production per Year

	2003	2004	2005	2006	2007	2008	2009	2010
SCIENTIFIC ARTICLES	107	134*	147	154	208	225	218	245
ACCEPTED / IN PRESS	8	20	16	26	19	21	24	22
SUBMITTED	29	26	27	23	24	31	14	20
PUBLISHED	70	91	104	105	165	173	180	203
CONFERENCE PRESENTATIONS	52	72*	65	105	101	148	160	121
DOCTORAL THESES	21	32	24	18	18	20	14	10
DEFENDED	4	5	9	10	11	10	10	7
PRESENTED	–	–	–	3	5	1	–	–
IN PROCESS	17	27	15	5	2	9	4	3
MASTER'S THESES GRADUATE PROJECTS	9	12	14	5	10	14	12	7
DEFENDED	4	5	13	3	8	10	12	7
IN PROCESS	5	7	1	2	2	4	–	–
BOOKS / CHAPTERS	NA**	NA**	5	4	3	9	13	5
ACCEPTED / IN PRESS	NA**	NA**	4	1	1	1	2	2
SUBMITTED	NA**	NA**	1	–	2	–	–	–
PUBLISHED	NA**	NA**	–	3	–	8	11	3
TOTAL	194	256	260	301	351	416	417	391

* 8 PUBLICATIONS & 16 CONFERENCES WITH AUTHORS FROM MORE THAN ONE INSTITUTION
** NA: Not Available

CSİC Users Published

95

Scientific Articles

Distribution of Scientific Production Declared by Users from CSİC and Galician Universities

	CSIC	UDC	USC	UVIGO
SCIENTIFIC ARTICLES	**130**	**18**	**43**	**40**
ACCEPTED/ IN PRESS	17	1	1	3
SUBMITTED	18	1	1	–
PUBLISHED	95	16	41	37
CONFERENCE PRESENTATIONS	**43**	**10**	**32**	**15**
DOCTORAL THESES	**2**	**3**	**3**	**2**
DEFENDED	2	2	2	1
PRESENTED	–	–	–	–
IN PROCESS	–	1	1	1
MASTER'S THESES / GRADUATE PROJECTS	**1**	**2**	**2**	**2**
DEFENDED	1	2	2	2
BOOKS / CHAPTERS	**1**	**–**	**–**	**3**
ACCEPTED/ IN PRESS	–	–	–	1
PUBLISHED	1	–	–	2
OTHER	**–**	**–**	**2**	**1**
TOTAL	**177**	**33**	**82**	**63**

COMPUTİNG USERS
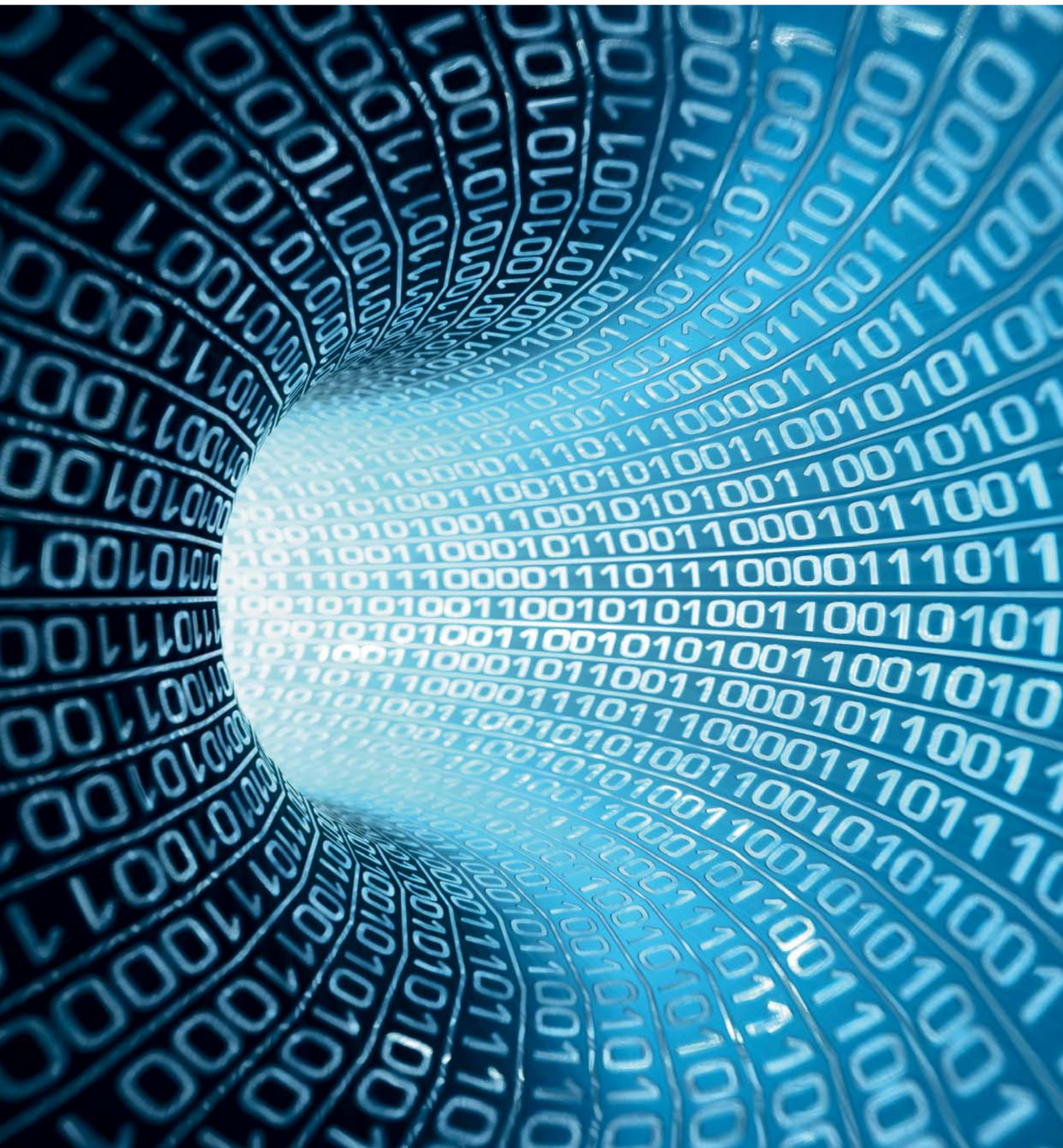
Most Active Users in 2010 by Institution

USER	DEPT / CENTRE	HOURS USED
UNIVERSIDADE DE SANTIAGO DE COMPOSTELA (USC)		
David Serantes Abalo	Applied Physics	476,838
Antonio Peón López	Organic Chemistry	364,163
Angel Piñeiro Guillén	Applied Physics	306,508
Jose Luís Domínguez Meijide	Condensed Matter Physics	284,838
Gonzalo Miguel Macho	Organic Chemistry	230,470
UNIVERSIDADE DA CORUÑA (UDC)		
Daniel Rivero Cebrián	Communications & Information Technologies	531,421
Ana Belén Porto Pazos	Communications & Information Technologies	118,294
Pablo Mesejo Santiago	Communications & Information Technologies	88,224
María Isabel Fernández Pérez	Chemistry, Physics, and Chemical Engineering I	85,824
Noha Veiguela Blanco	Communications & Information Technologies	78,015
UNIVERSIDADE DE VIGO (UVIGO)		
Juan Antonio Añel Cabanelas	Applied Physics	251,825
José Manuel Hermida Ramón	Chemistry Physics	189,460
Olalla Nieto Faza	Organic Chemistry	183,361
Laura Estévez Guiance	Chemistry Physics	110,041
Efrén Pérez Santín	Organic Chemistry	104,309
SPANISH NATIONAL RESEARCH COUNCIL (CSIC)		
María del Carmen San Martín Pastrana	Centro Nacional de Biotecnología	649,222
Víctur Cruz Cañas	Instituto de Física Fundamental	508,077
María Pilar De Lara Castells	Instituto de Estructura de la Materia	489,879
Otto Emiliano González Vázquez	Instituto de Física Fundamental	438,966
Carlos Calero Borrallo	Institut de Ciencia de Materials de Barcelona	405,805
UNIVERSITAT DE LES ILLES BALEARS (UIB)		
Juan Frau Munar	Chemistry	24,348
METEOGALICIA - XUNTA DE GALICIA WEATHER SERVICE (GALICIAN REGIONAL GOVERMENT)		
Vicente Pérez Muñuzuri	MeteoGalicia: Numerical Prediction and Research	154,955
TECHNOLOGY CENTRES (CTAG)		
Santiago Cabello Vieitez	Technological development in the automotive industry in Galicia	55,837
Manuel Ruíz Villareal	Grupo de Modelado Oceánico	31,660

Number of Active User Accounts

The number of active user accounts (that is, users with significant CPU time consumption throughout the year) continued to grow during 2010. User accounts associated with CSIC rose from 113 to 121. Active user accounts from Galician universities experienced a slight decrease from 294 to 290. The total number of active user accounts, including CSIC, universities, and other institutions, increased by 41, growing from 407 in 2009 to 448 in 2010. The bar chart below does not take into consideration active user accounts linked to projects in which CESGA participates such as EGI,EMI,EIMRT, or other Grid related projects.

FinisTerrae was the system with the greatest number of active user accounts (411). The SVG cluster registered 337 active user accounts, increasing by 20 from the previous year, in addition to Grid project users 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 the National Grid Initiative, RETELAB, CYTEDGRID, and regional projects such as FORMIGA and G-FLUXO).

The **total** amount of user accounts at CESGA is 748.

448 Active User Accounts in 2010

Active User Account Evolution by İnstitution per Year, 2000 - 2010

Active User Accounts

Legend:
- CSIC
- UDC, USC, UVIGO
- Total*
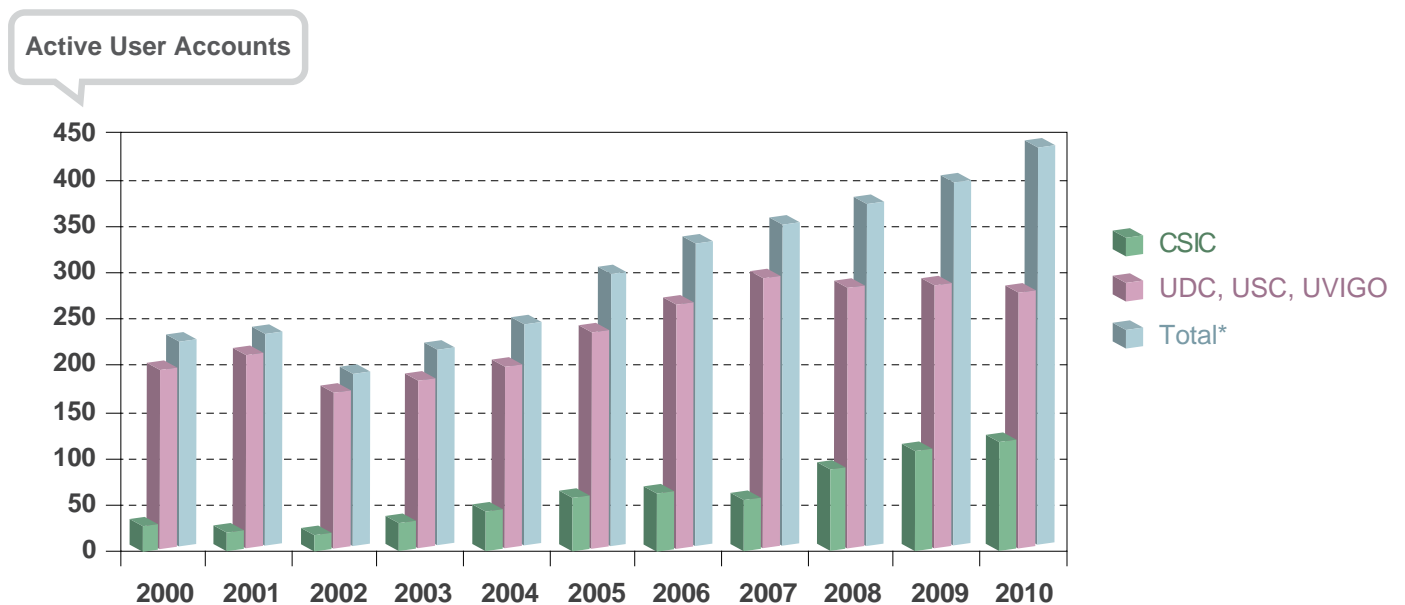
*Total Includes Technology Centres, IEO, UIB, Meteogalicia, PdE, ICTS, ...

Distribution by İnstitutions of the CPU Time Consumed in all systems

All user institutions increased the CPU time used with respect to the previous year. There was a 5.2% 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 21.1% of the total hours and increased the number of CPU hours from 3.9 million to 4.3 million this year. CSIC consumed 47.2% in 2010.

As a whole, the three Galician universities represent 37.5% of the total consumption. The projects in which CESGA participated were responsible for only 2.8% of the hours consumed. ICTS projects consumed 2 million hours, which represents 10.3% of usage.

CPU Hours Used

increased by 5.2%

% CPU Time Use Distribution by İnstitution in 2010

- Technological Centre
- CESGA
- CSIC
- Hospitals
- ICTS
- UDC
- UIB
- USC
- UVIGO
- Xunta de Galicia

Pie chart values: 0.8, 0.4, 8.7, 2.8, 21.1, 47.2, 0.1, 7.7, 0.9, 10.3
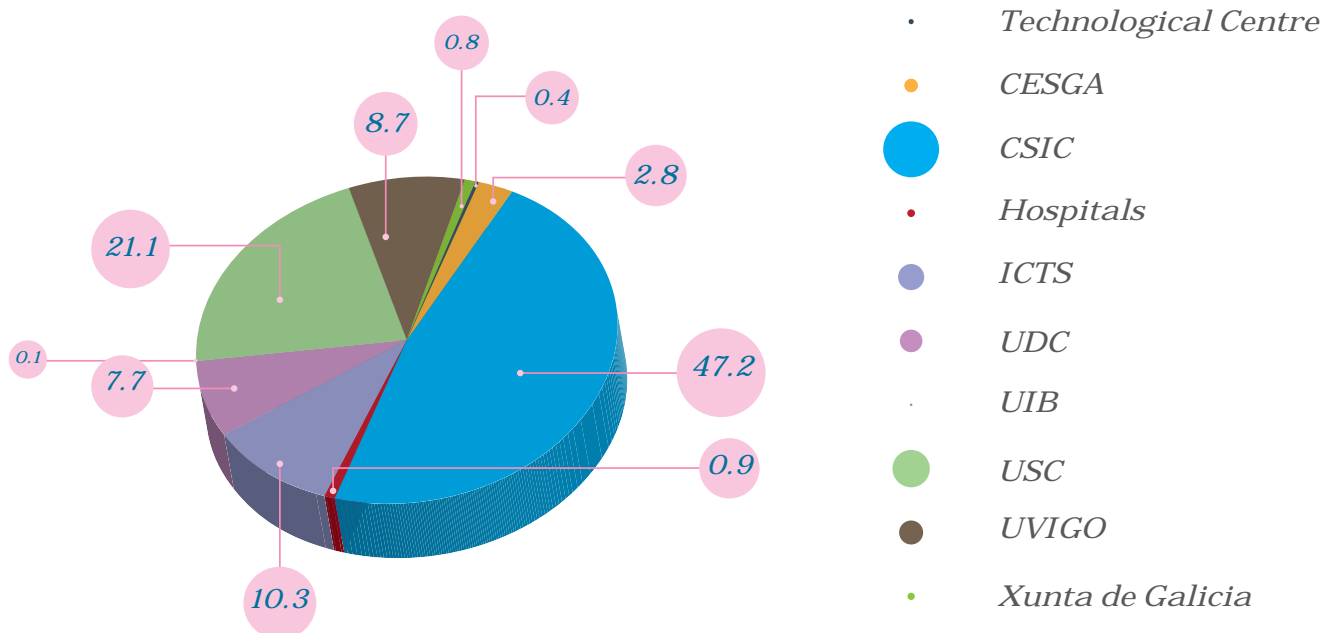
CPU Distribution by Research Area

The computing time related to Computational Physics research represented 36.6% of the consumption (down from previous year figures of 53.5%), surpassing Biochemical Modeling for the third time which represents 34.6% (11.1% more than in 2009). These two areas accounted for 71.2% of the total hours consumed.

CPU Use Distribution by Research Area, 2000 - 2010

	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
OTHER AREAS	15.1	11.7	11.7	16.7	6	8.1	5.6	2.2	6	3.2	5.8
BIOCHEMICAL MODELING	26.5	25.9	47.1	37.5	62	50.4	46.6	46.3	34.3	23.5	34.6
NUMERICAL METHODS	21.7	17.3	4.3	1.3	2	2.5	5.1	4.5	12.1	3.8	4
PHYSICS	15.6	22.1	21.8	39	27	30.7	30.7	28.4	34.8	53.5	36.6
EARTH SCIENCE	9.1	9.6	3.5	0.8	2	4.6	7.0	11	3.8	6.5	9.7
COMPUTER SCIENCE	12	20.8	11.7	4.7	1	3.7	5.1	7.6	9	9.5	9.2

Legend: OTHER AREAS · NUMERICAL METHODS · EARTH SCIENCE · BIOCHEMICAL MODELING · PHYSICS · COMPUTER SCIENCE

CSIC Researchers mainly Used FinisTerrae

CPU Usage Distribution by İnstitution and Machine

In this graph, we can see which of the systems were most demanded by each of the institutions that use the computing servers at CESGA. It can be easily appreciated that CSIC researchers mainly utilised the FinisTerrae server, registering nearly 50%, while the SVG was shared mainly by the researchers of the Universities of Santiago de Compostela and A Coruña, although there was an increase of CSIC usage in SVG from 19.3% to 35.4%.

Grid systems were fundamentally used by LHCb, Compchem, and Fusion international Virtual Organisations.

CPU Usage Distribution by İnstitution and Machine in 2010

FINISTERRAE
- XUNTA 0.6
- UVIGO 9.4
- USC 20.6
- UIB 0.1
- UDC 6.5
- CSIC 49.1
- CESGA 1
- TECH. CENTRES 0.9
- HOSPITALS 11.2
- ICTS 0.5

SVG_DELL
- XUNTA 2.6
- UVIGO 0.5
- USC 33.8
- UDC 27.1
- CSIC 35.4
- CESGA 0.5

GRID
- OTHER Vos 2
- VO LHCB 10
- VO Fusion 12
- VO Compchem 76
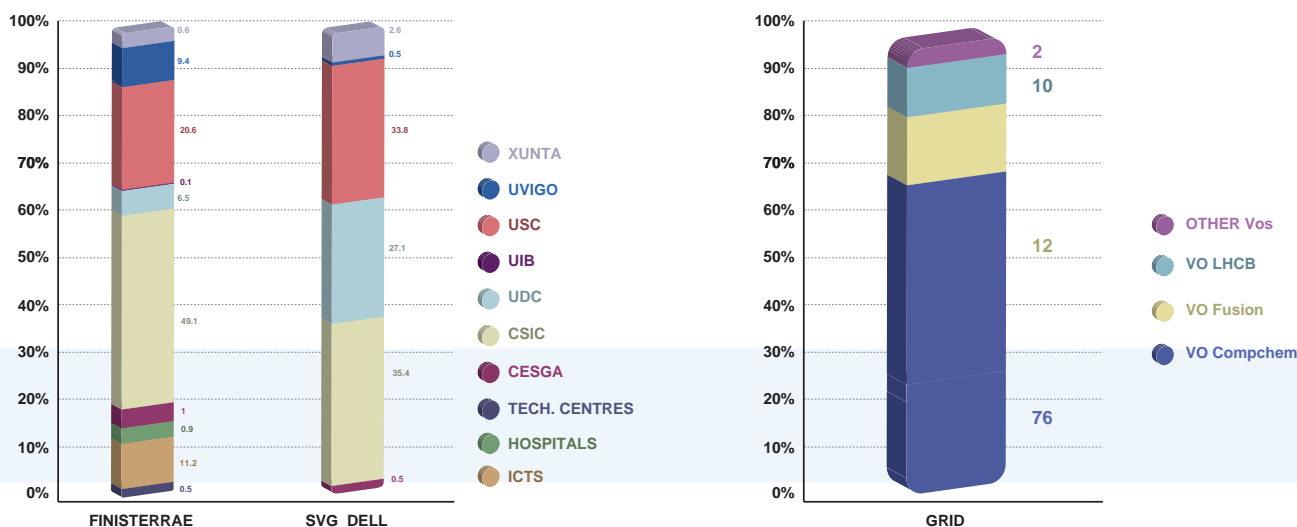
Application Use per Institution

Applications use by USC Users in 2010

Other Applications 1%
WRF 3%
Octopus 4%
SIESTA 4%
User Code 22%
Venus 9%
CHARMM 13%
Amber 11%
PARSEC 11%
g98/03/09 11%
Gromacs 11%
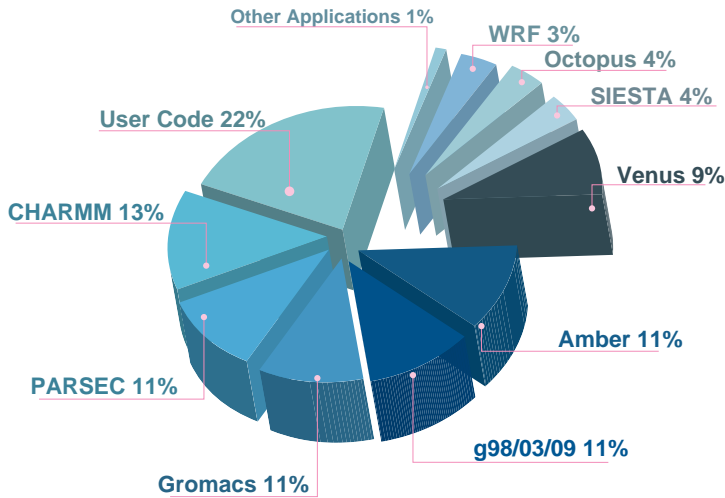
Applications use by UDC Users in 2010

Java 1.9%
Other Applications 0,1%
g98/03/09 33%
User Code 65%
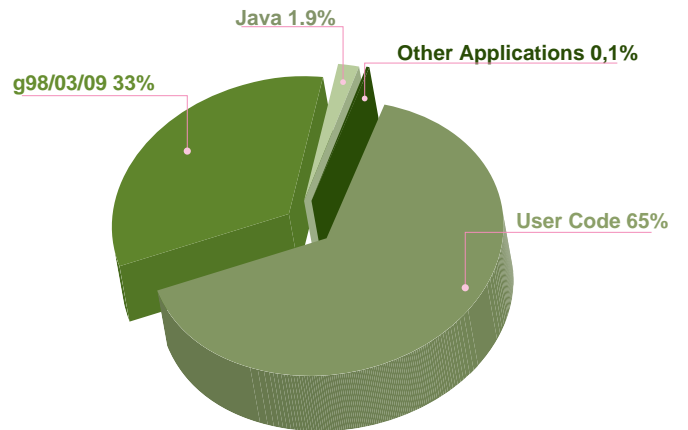
Application Usage Data reflects a Great Variety of Research Lines

• • •

Applications use by UVIGO Users in 2010

Other Applications 3%
WACCM 3%
g98/03/09 74%
Gamess 3%
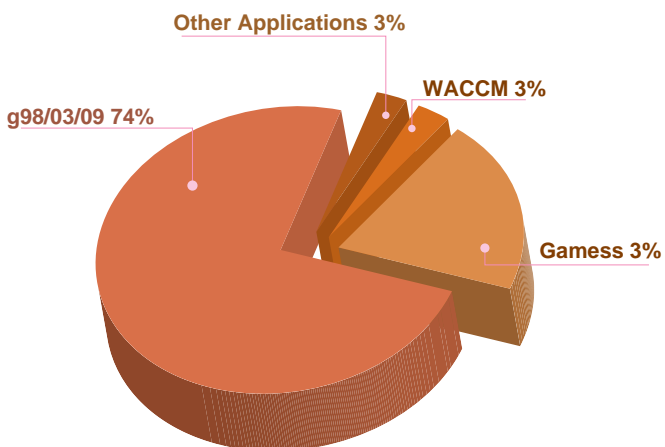
Applications use by CSIC Users in 2010

DYCI 3%
CPMD 2%
g98/03/09 4%
Other Applications 8%
Amber 5%
NAMD 6%
User Code 33%
SIESTA 8%
Xmipp 8%
VASP 13%
LAMMPS 10%
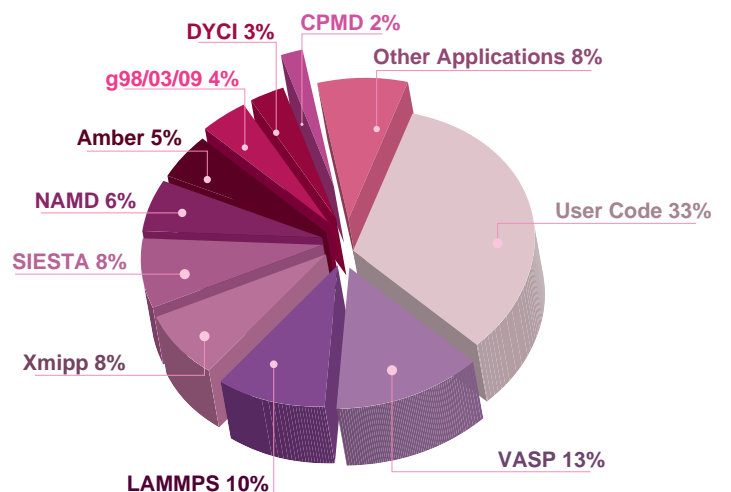
Application Use per System

Applications use in the FinisTerrae Server in 2010

DYCI 2%
WACMM 2%
Q 3%
Other Applications 9%
PARSEC 3%
CHARMM 3%
NAMD 4%
User Code 27%
Xmipp 4%
Gromacs 5%
SIESTA 5%
Amber 5%
g98/03/09 14%
LAMMPS 6%
VASP 8%
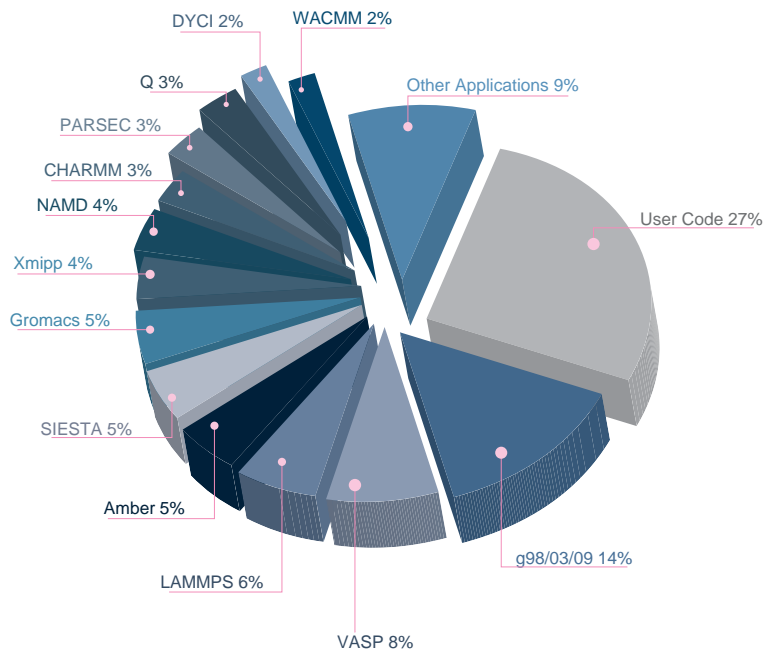
Applications use in the SVG Server in 2010
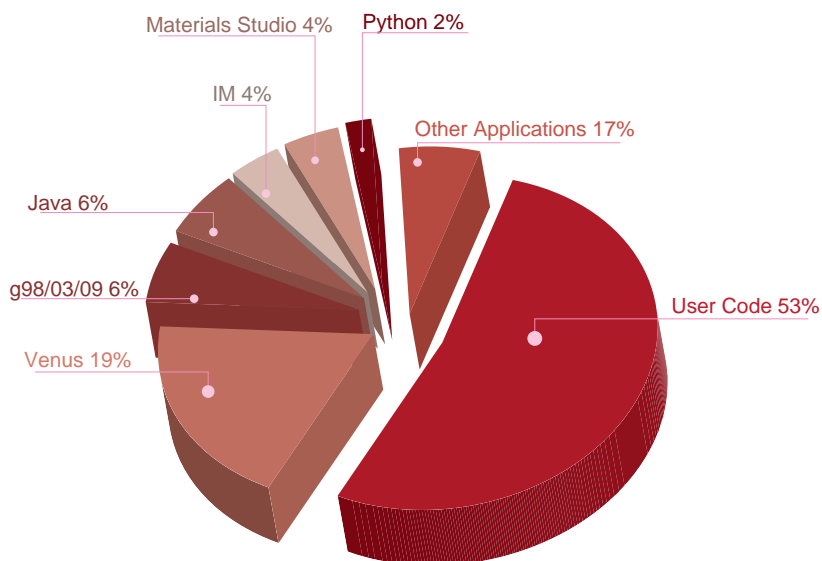
Materials Studio 4%
Python 2%
IM 4%
Other Applications 17%
Java 6%
g98/03/09 6%
User Code 53%
Venus 19%

CSIC USERS 2008-2010

CSIC CENTRES	Dept / Research Group	# active user accounts			CPU hours used		
		2008	2009	2010	2008	2009	2010

NATURAL RESOURCES AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Estación Biológica de Doñana (EBD)	Ecología de Humedales, Genética de la Conservación en Peces Litorales	1	0	1	623.6	0	0
	Biología Evolutiva; Integrative Ecology Group	4	5	7	27,268	52,631.9	210,859
	Genética de la Conservación	4	7	8	44,896.9	98,632.4	100,613.7
	Evolución de relaciones planta animal	2	1	4	982.8	170.9	2,590.6
	Departamento de Ecología Evolutiva. Grupo de Murciélagos	0	1	3	0	0	245
Institut Mediterrani d'Estudis Avançats (IMEDEA)	PANCODING	1	1	1	66.7	11,416.6	8.8
Centre d'Estudis Avançats de Blanes (CEAB)	Oceanografía Operacional	1	2	2	1,396.2	56,586.2	104,292.7

MATERIAL SCIENCE AND TECHNOLOGY AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Instituto de Ciencia de Materiales de Barcelona (ICMAB)	Estructura Electrónica de Materiales	12	12	13	665,772.1	2,122,972.1	1,774,629
	Departamento Teoría y Simulación de Materiales	2	4	4	15,402.6	726,992.9	1,030,246.5
	Nanociencia Molecular y Materiales Orgánicos	0	1	1	0	440.5	11,383.8
Instituto de Ciencia de Materiales de Aragón (ICMA)	Química Orgánica	1	1	1	7,869.7	71,391.5	46,988
	Química de los Compuestos Organometálicos	0	1	3	0	394.3	21,382.8
	Química/Grupo Síntesis Orgánica Estereoselectiva	1	1	1	79,617.3	98,746.7	142,833.3
	Grupo de Síntesis Química de la Rioja	0	2	2	0	34,993.1	30,730.3
Instituto de Ciencias de Materiales de Sevilla (ICMS)	FQM282	1	1	1	21,301.4	356,611.7	0
	Superficies, Intercapas y Capas Finas	1	2	2	181,804	288,658.5	106,077.3
Unidad Asociada CSIC-LABEIN	Unidad de Materiales Nanoestructurados y Ecoeficientes para Construcción	1	1	1	267,857.2	421,571.8	24,343.4
Instituto de Ciencia y Tecnología de Polímeros (ICTP)	Química Macromolecular	1	1	1	22,922.4	45,629.7	40,810.2
Centre d'Invstigació en Nanociéncia i Nanotecnologia (CIN2) Barcelona	CIN Theoria and Simulation	0	2	3	0	358,816.7	98,622.5
	Nanophononics and Nanophotonics	0	1	2	0	85.3	411.9
Instituto de Ciencia de Materiales de Madrid ICMM	Teoría Intercaras y Crecimiento	0	4	5	0	661,211.4	272,157.3
	Grupo de Simulación de Materiales	0	0	2	0	0	664

SOCIAL SCIENCE AND HUMANITIES AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Instituto de Análisis Económico (IAE)	Instituto de Análisis Económico	1	2	1	8,297.5	16,821.8	10,566.8

CSIC USERS 2008-2010

CSIC CENTRES	Dept / Research Group	# active user accounts			CPU hours used		
		2008	2009	2010	2008	2009	2010

CHEMICAL SCIENCE AND TECHNOLOGY AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Instituto de Investigaciones Químicas (IIQ)	Grupo de Carbohidratos	1	1	2	3,708.6	1,830.8	182,201.7
	Departamento de Química Inorgánica y Catálisis	0	1	1	0	15,895.2	81,884.5
	Grupo de Síntesis Orgánica y Reconocimiento Molecular	1	0	0	23.9	0	0
Instituto de Catálisis y Petroleoquímica (IPC)	Grupo de Catálisis Fundamental y Aplicada	1	1	1	1,510,868.7	197,777.8	17,391.2
Instituto de Investigaciones Químicas Avanzada de Cataluña	Química Teórica y Computacional	5	5	4	144,527.1	178,765.7	18,553.8
Instituto de Química Médica (IQM)	Quimioterapia	2	2	1	1,783.4	1,369.3	0
Instituto de Química Orgánica General (IQOG)	Química Orgánica Biológica	1	1	1	4,237.9	55,453	50,402.7
	Laboratorio de Radicales Libres y Química Computacional	2	4	1	4,659.7	65,054.3	0.1
	Productos Naturales	2	3	4	1,010	3,963	11,645.6
	Síntesis Asimétrica con sulfóxidos	0	0	1	0	0	1.3
Instituto Nacional del Carbón (INCAR)	Texture of Materials for Energetic Applications	2	2	0	4,906	46,100.2	0
Laboratorio de Investigación en Tecnologías de la Combustión	Grupo Fluidodinámica Numérica. Área Mecánica de Fluidos	0	1	1	0	0.6	1211.6

PHYSICS SCIENCE AND TECHNOLOGY AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Instituto de Física de Cantabria (IFCA)	Computación Distribuida	0	1	0	0	39.2	0
Instituto de Física Fundamental (IMAFF)	Departamento de Física Atómica y Molecular Teórica	12	10	7	848,010.4	1,372,621.7	1,863,913.1
Instituto de Matemáticas (ICMAT)	Matemáticas	4	5	8	119,518.1	483,849.6	828,729.1
Instituto de Física Teórica (IFTE)	Instituto de Física Teórica	0	1	1	0	188,009.1	0
Instituto de Investigación en Inteligencia Artificial (IIIA)	Multi-Agent Systems	0	3	4	0	33,053.8	287,431.8
Instituto de Ciencias del Cosmos (ICE-ICC)	Grupo formación de Galaxias	0	1	1	0	1,980	12,741.7
Instituto de Ciencias del Espacio (CSIC-IEEC)	Grupo de Astronomía de Ondas Gravitatorias - LISA	0	0	1	0	0	62,001.5
Instituto de Estructura de la Materia (IEM)	Departamento de Física Molecular	3	2	2	864,193.5	203,424	508,128.2
	Departamento de Química y Física Teóricas	7	4	4	547,787.8	491,767.1	297,421.8
	Física Macromolecular	0	1	1	0	487.3	149,984.1
	Gupo de Materia Condensada no Cristalina	1	0	0	10.2	0	0

CSIC USERS 2008-2010

CSIC CENTRES	Dept / Research Group	# active user accounts			CPU hours used		
		2008	2009	2010	2008	2009	2010

BIOLOGY AND BIOMEDICINE AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Centro Andaluz de Biología Molecular y Medicina Regenerativa (CABIMER)	Terapia Celular y Medicina Regenerativa	0	2	1	0	1,797.8	42.6
Centro de Investigaciones Biológicas (CIB)	Estructura y Función de Proteínas	1	1	1	126,914.2	19,849.6	0
	Microscopia Electrónica de Macromoléculas	1	0	0	4,965.8	0	0
	Grupo de Resonancia Magnética Nuclear	3	1	4	1,081.1	235.4	322,105.1
Centro Nacional de Biotecnología (CNB)	Servicio de Informática Científica	0	0	1	0	0	134.8
	Estructura de Adenovirus	1	2	1	318,126.3	228,972.3	649,222.5
	Departamento de Estructura Macromolecular	4	4	1	20,466	16,270.8	9.3
Instituto Cajal (IC)	Neurobiología del Desarrollo	1	2	2	464.5	82,586.4	162,539.1
Centro de Biología Molecular Severo Ochoa (CBM)	Diseño Racional de Encimas - BioWeb	1	1	0	27,472.8	69.2	0

AGRICULTURAL SCIENCE AREA

CSIC CENTRES	Dept / Research Group	2008	2009	2010	2008	2009	2010
Estación Experimental del Zaidin (EEZ)	Ciencias de la Tierra y Química Ambiental/Química Teórica y Modelización Molecular	3	2	3	8,353.1	106,594.8	117,954.1
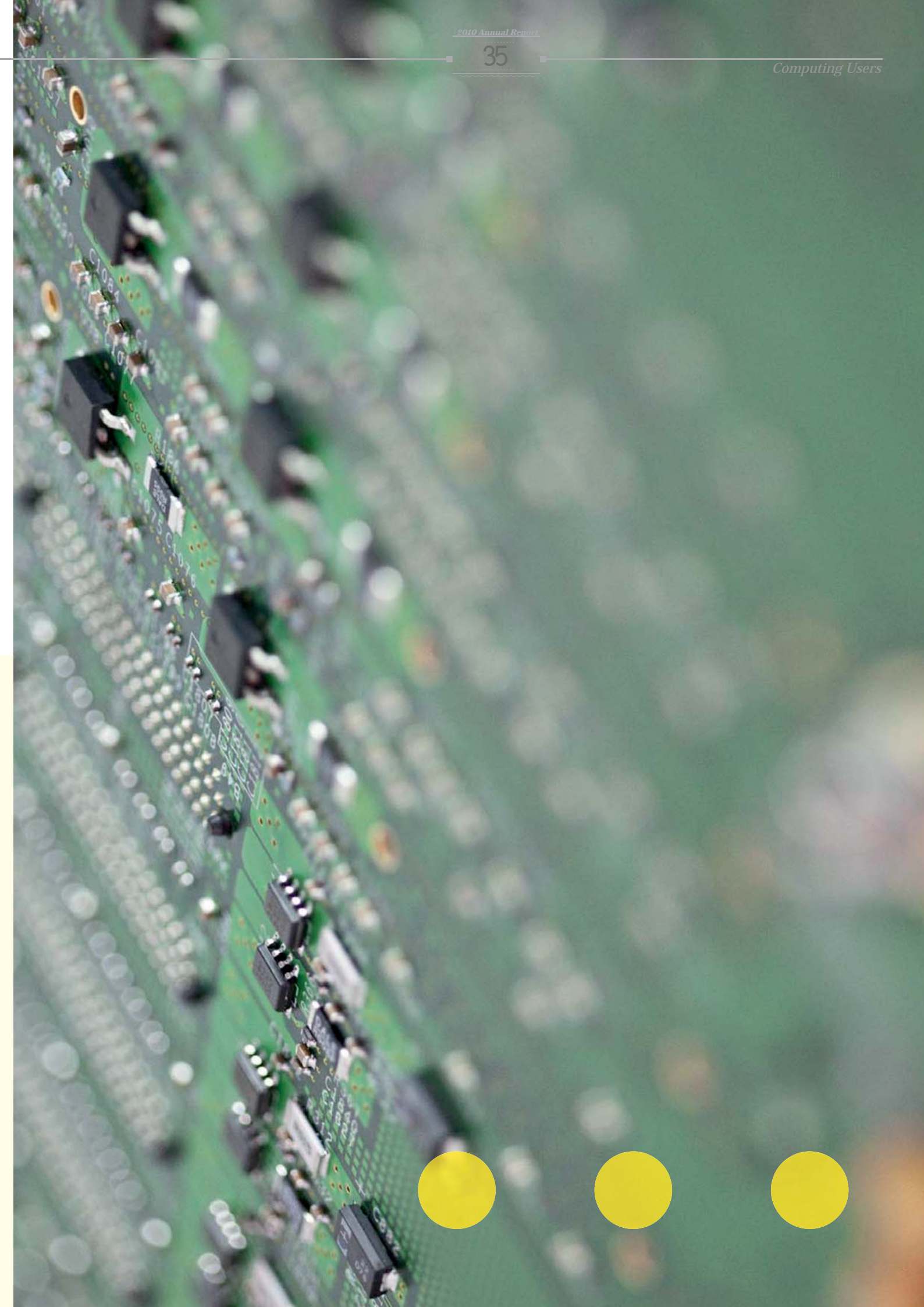
UNIVERSITY USERS 2008-2010

CENTERS	Department- Group	# of Active User Accounts			Hours used		
		2008	2009	2010	2008	2009	2010

UDC - Universidade da Coruña

CENTERS	Department- Group	2008	2009	2010	2008	2009	2010
Escuela Politécnica Superior	Enxeñaría Naval e Oceánica	1	2	2	7.8	1,262.8	3,143.2
	Enxeñaría Industrial	0	0	1	0	0	4,031.6
	Construccións Navais	0	0	1	0	0	12.9
Escuela Técnica Superior de Arquitectura	Tecnología de la Construcción	1	1	0	0	28.1	0
Escuela Técnica Superior de Ingenieros de Caminos, Canales y Puertos	Métodos Matemáticos	1	1	0	2,400.7	0	0
Facultad de Ciencias	Biología Animal	0	0	2	0	0	548.5
	Química, Física e Ingeniería Química I	9	9	8	314,442.9	373,984.4	242,268
	Química Fundamental	17	25	14	491,667.3	311,230.9	320,081.4
	Biología Molecular	0	1	1	0	0	4.7
Facultad de Informática	Computación	1	1	2	345.9	0	28,956.7
	Electrónica y Sistemas	15	16	16	170,264.8	315,190	24,470.8
	Tecnoloxías das Informacións e as Comunicacións	5	7	9	371,293.4	1,243,138	959,550.6
UDC Genérico	UDC Genérico	53	64	32	15,532.4	2,975.2	157

USC - Universidade de Santiago de Compostela

CENTERS	Department- Group	2008	2009	2010	2008	2009	2010
Escuela Técnica Superior de Ingeniería	Ingeniería Química	2	1	0	37.1	0	0
Facultad de Farmacia	Bioquímica y Biología Molecular	0	1	0	0	2.3	0
	Farmacología	2	2	1	53,414.1	233,731.5	4,721.4
Facultad de Física	Electrónica e Computación	17	15	21	83,287.2	112,415.3	209,830.5
	Física Aplicada	24	20	19	2,191,339.9	1,099,377.8	1,340,327.6
	Fisica de la Materia Condensada	14	15	15	1,501,689.7	1,908,033	994,757.5
	Física de Partículas	9	11	8	96,878.4	135,250.7	75,404.5

UNIVERSITY USERS 2008-2010

CENTERS	Department- Group	# of Active User Accounts			Hours used		
		2008	2009	2010	2008	2009	2010

USC - Universidade de Santiago de Compostela

CENTERS	Department- Group	2008	2009	2010	2008	2009	2010
Facultad de Matemáticas	Alxebra	1	1	0	2,765.4	574.3	0
	Operativa	1	0	0	1,303.7	0	0
	Matemáticas aplicadas	3	4	5	9.7	877.2	5,795.7
Facultad de Química	Química Física	20	20	20	627,722.7	729,864	644,962.7
	Química Inorgánica	1	1	6	60	0	4.1
	Química Orgánica	29	30	26	310,382	522,022	1,010,381.9
Instituto de Acuicultura	Instituto de Acuicultura	1	0	0	1.8	0	0
Instituto de Medicina Legal	Instituto de Medicina Legal	3	3	3	1,109.2	191,253.6	21,942
USC Genérico	USC Genérico	45	23	22	2,442.4	1,376.2	398

UVIGO - Universidade de Vigo

CENTERS	Department- Group	2008	2009	2010	2008	2009	2010
E.T.S. de Ingenieros de Telecomunicación	Ingeniería Telemática	1	1	1	7.7	833.3	0.1
	Matemática Aplicada	1	0	2	796	0	23,205.8
	Teoría de la Señal y Comunicaciones	3	2	5	13,280	1,471.6	2,290.2
E.T.S. de Ingenieros Industriales	Ingeniería Eléctrica	3	1	1	0.4	0.1	3
E.U. de Ingeniería Técnica Industrial	Departamento Informática y Diseño en Ingeniería	1	1	1	5.2	3	552.4
Facultad de Biología	Bioquímica, Genética e Inmunología	1	2	0	76	360.7	0
	Grupo de Bioinformática y Evolución Molecular	0	0	1	0	0	29
Facultad de Ciencias del Mar	Física Aplicada	11	12	7	63,373.5	690,664.8	257,603
Facultad de Química	Química Analítica y Alimentaria	12	11	9	183,064.7	659,079.6	301,187.5
	Química Física	1	6	9	26,027.7	175,144.2	263,445.5
	Química Inorgánica	1	1	4	1,398.9	3,321.6	117.9
	Química Orgánica	11	13	20	443,316.5	803,164.9	920,032.6
Facultad de Ciencias Económicas y Empresariales	Fundamentos de Análisis Económico, e Historia e Instituciones Económicas	0	1	0	0	0.8	0
UVI Genérico	UVI Genérico	0	11	0	0	155.6	0

OTHER USERS 2008-2010

CENTRES	Department- Group	# of Active User Accounts			Hours used		
		2008	2009	2010	2008	2009	2010

METEOGALICIA - Xunta de Galicia

METEOGALICIA	MeteoGalicia: Predicción e Investigación Numérica	3	3	6	162,797.4	105,719.4	154,960.4

CTAG - Centro Tecolóxico de Automoción de Galicia

Centro Tecnolóxico de Automoción de Galicia	Desarrollo Tecnológico en la Industria de la Automoción de Galicia	2	1	1	3,350.3	47,207.6	55,837.2

CESGA - Centro de Supercomputación de Galicia

CESGA	CESGA Genérico	305	411	324	499,694.5	454,573.6	576,405.8

UIB - Universitat de les Illes Balears

UIB	Física	0	2	2	0	42,201.5	22
	Química	0	1	1	0	5,401	24,348.1

IEO - Instituto Español de Oceanografía

Instituto Español de Oceanografía	Grupo de Modelado Oceánico	0	1	2	0	14,159.6	35,312.4
	Modelado y análisis de sistemas	0	0	1	0	0	585.5

İCTS · Access Programme 2010 · · · · ·
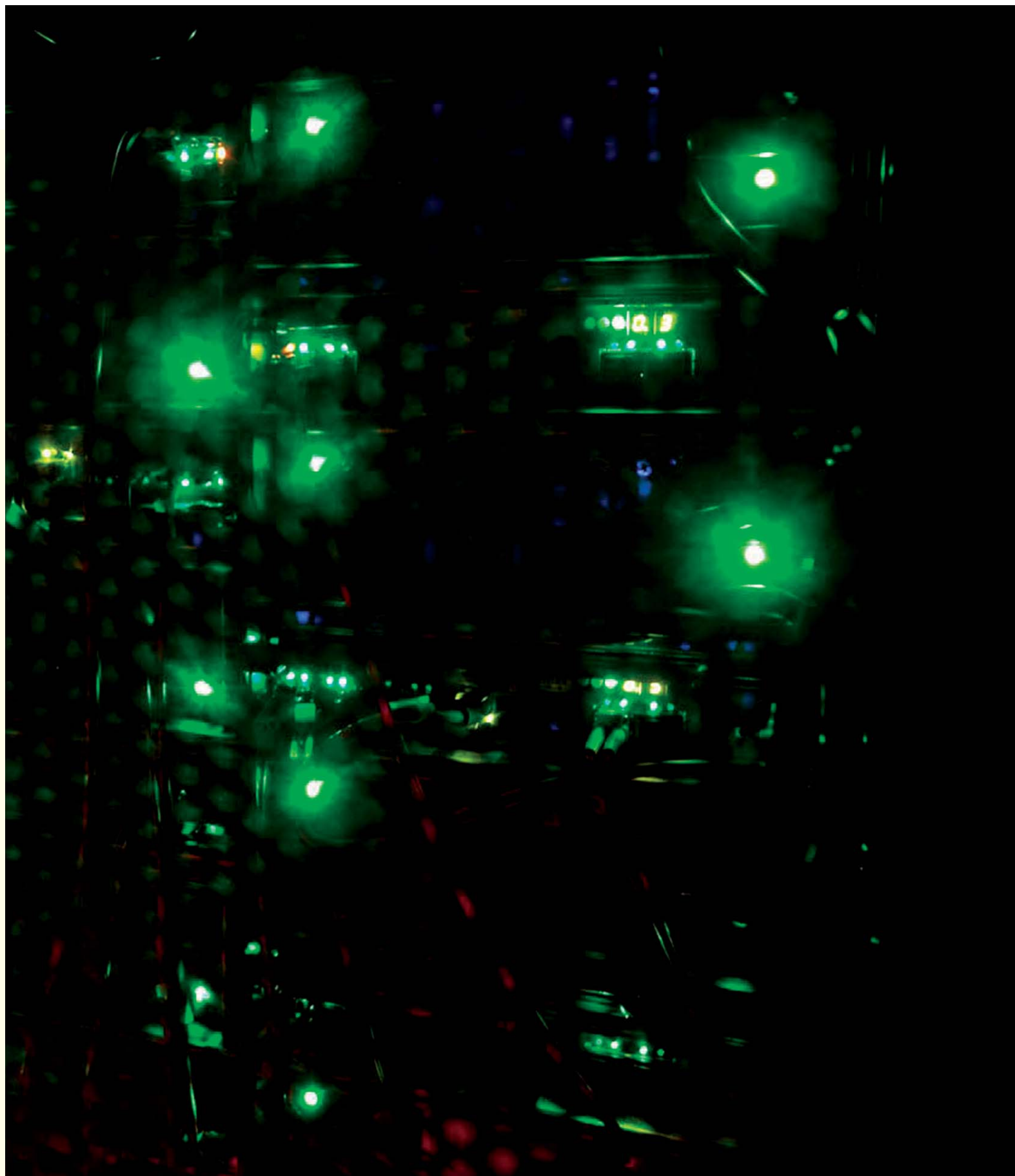
İCTS Access Programme

A a total of **38** proposals were aproved from researchers and research groups to grant access to ICTS-CESGA in order to carry out research projects, acquire knowledge, and receive training in technologies in use at the Centre.

Types of Access

Remote access to the FinisTerrae Supercomputer and research stays at CESGA.

Beneficiaries

Predoctoral students, Ph.D.s, and researchers with a minimum of three years research experience.

Access Procedure

Information and applications: all access requests were presented via an on-line application form available on the webpage, http://icts.cesga.es.

Proposals >> Geographical Distribution

ICTS access could be requested by researchers from the scientific community of EU countries, the European Economic Area, countries of the CYTED program, and also researchers with legal residence in any of these countries. Access requests during 2010 were primarily from Spain but almost 20% were from foreign research groups.
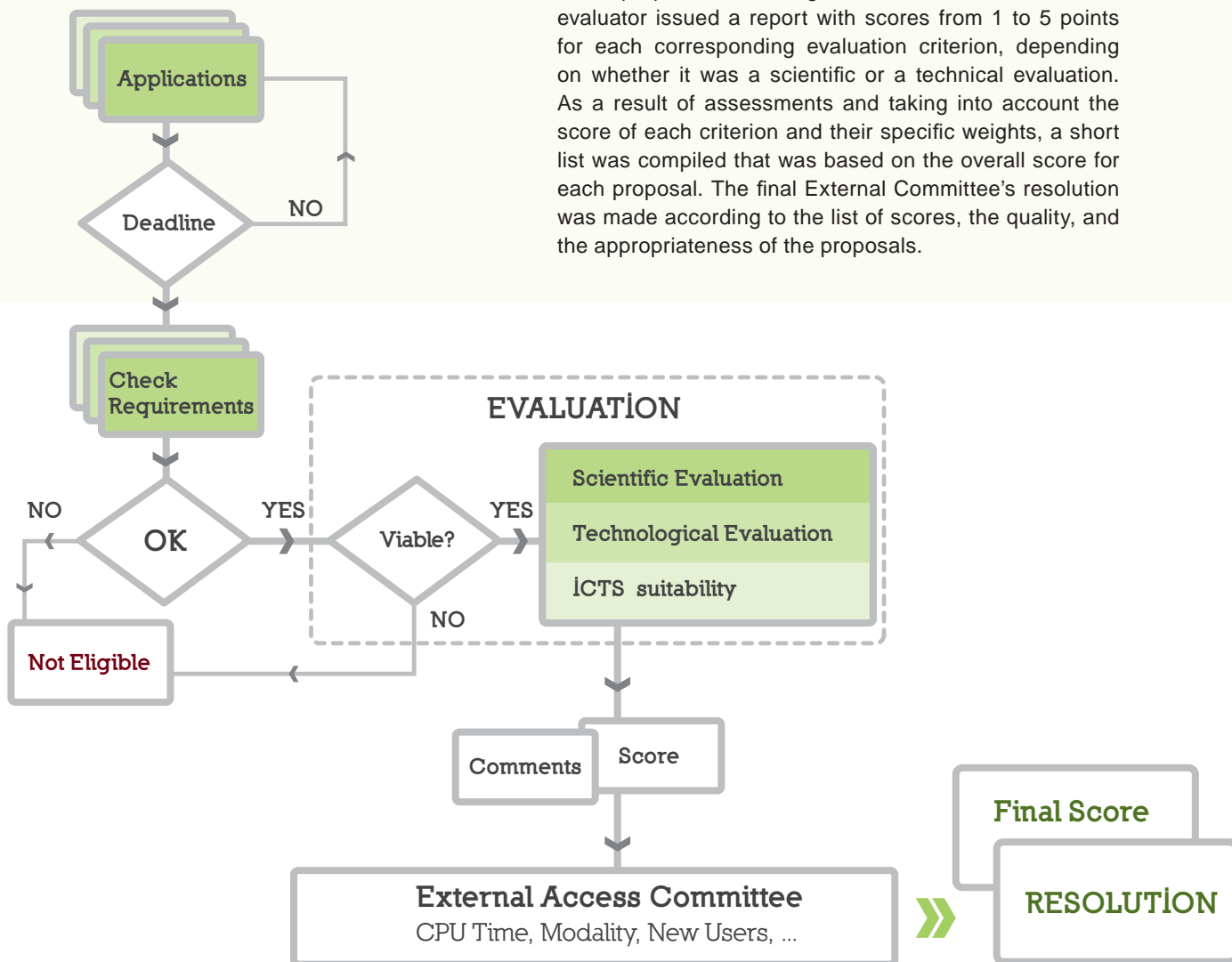
http://icts.cesga.es

38 Research Projects benefited from access to İCTS - CESGA

CESGA/FinisTerrae is a Unique Scientific Technological Infrastructure (ICTS). As such, in 2010, access to this infrastructure was financed by the Spanish Ministry for Science and Innovation (Reference ICTS-2009-40).

Evaluation and Review Process

More than **50** external reviewers, all experts in different scientific and technical areas, participated in the evaluation of proposals of access to FinisTerrae in 2010. Their work focused on the evaluation of proposals according to the criteria of the calls. Each evaluator issued a report with scores from 1 to 5 points for each corresponding evaluation criterion, depending on whether it was a scientific or a technical evaluation. As a result of assessments and taking into account the score of each criterion and their specific weights, a short list was compiled that was based on the overall score for each proposal. The final External Committee's resolution was made according to the list of scores, the quality, and the appropriateness of the proposals.

Applications

Deadline — NO

Check Requirements

NO — OK — YES

Not Eligible

Viable? — YES

NO

EVALUATION

Scientific Evaluation

Technological Evaluation

İCTS suitability

Comments   Score

External Access Committee
CPU Time, Modality, New Users, ...

Final Score

RESOLUTION

İCTS - 2010 Figures

The overall quality of proposals received in 2010 was remarkably high. Nevertheless, 24% of the remote access requests could not be granted, mainly because the requested computational time greatly exceeded the available time and not for reasons regarding scientific and/or technological quality.

REMOTE ACCESS

	Applications	Access	CPU time (h)		
			Prioritised	Non-Prioritised	TOTAL
Modality 1	7	7	483,000	228,000	711,000
Modality 2	35	19	2,087,202	1,236,838	3,324,040
TOTAL	42	26	2,570,202	2,464,838	4,035,040

RESEARCH VİSİTS

	Applications	Access	Weeks	CPU time (h)
Modality 1	4	4	18	40,000
Modality 2	8	8	25	80,000
TOTAL	12	12	43	120,000

Computing Time Granted

4 million hours of computing time were granted in 2010. There were two types of allocated computation time as indicated below.

64% **Prioritised hours** were guaranteed with the condition of having consumed them within the prescribed dates for each access period.

36% **Non-prioritised hours** were to be used by the grantee once assigned prioritised hours were consumed as long as there were CPU hours still available that had not been used by the other applicants.
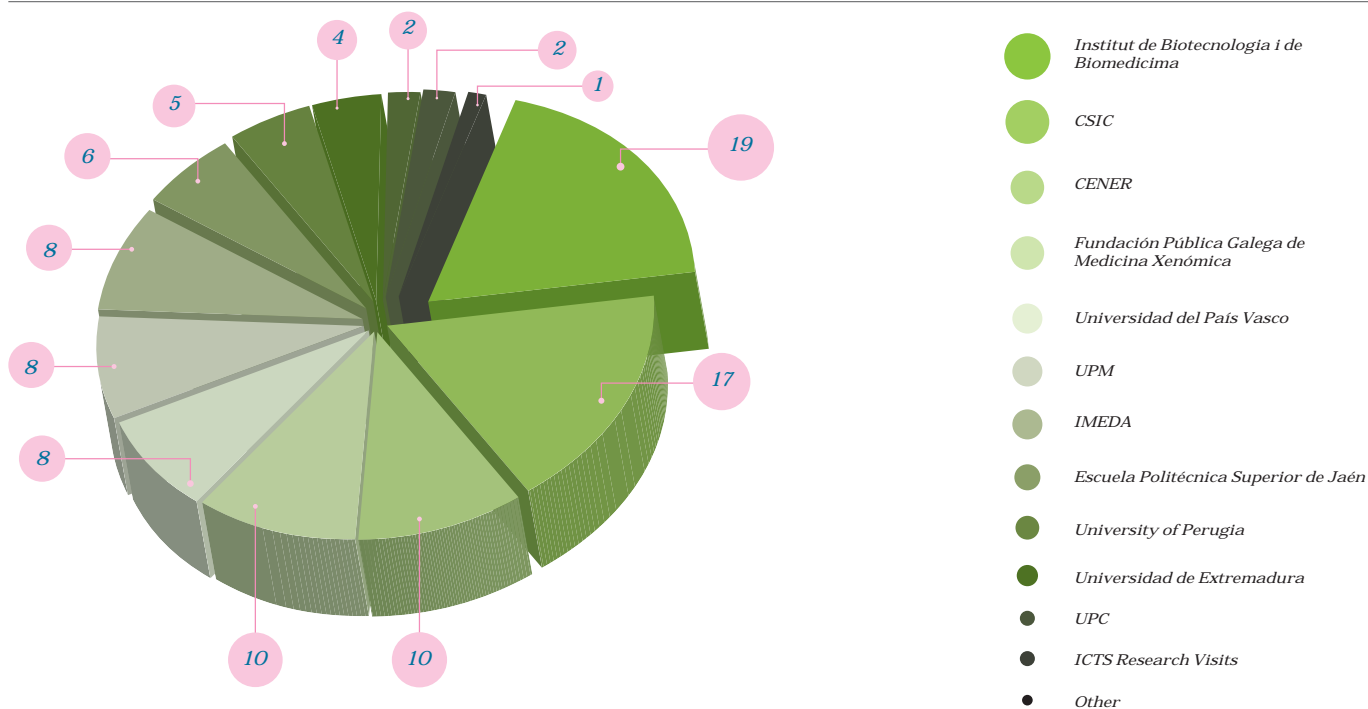
Administrative and Technical Support

CESGA provided administrative support to all of the proposals that obtained access and, in a more continual manner, to research visitors in terms of providing information, storage reservation, necessary equipment, etc.

The provision of technical support began at the moment at which the beneficiary signed the agreement of access to the infrastructure and requested a user account in said infrastructure or access from an existing account.

Each activity had specific needs regarding support related to applications or scientific libraries and/or the compilation of specific versions. In 2010, this resulted in 50 activities in the area of applications support. Additionally, a support technician was assigned to each research visitor according to the area of activity for the duration of the period of access.

ICTS % CPU Time Used Distribution by Institution 2010

- Institut de Biotecnologia i de Biomedicina
- CSIC
- CENER
- Fundación Pública Galega de Medicina Xenómica
- Universidad del País Vasco
- UPM
- IMEDA
- Escuela Politécnica Superior de Jaén
- University of Perugia
- Universidad de Extremadura
- UPC
- ICTS Research Visits
- Other

The scientific results obtained by the researchers in their first year of access to ICTS CESGA/FinisTerrae are now in the analysis phase as both periods of access terminated in December 2010. Nevertheless, some of the first scientific studies have already been completed, the majority of which have been presented for publication and are awaiting acceptance by the particular publication.

	Published / Accepted	Submitted
Articles	5	2
Conferences	2	8

ICTS - UNIQUE SCIENTIFIC TECHNOLOGICAL INFRASTRUCTURE 2010

CENTRES	Department- Group	# of Active User Accounts 2010	CPU Hours used 2010

CSIC - Consejo Superior de Investigaciones Científicas

Instituto de Investigaciones Químicas	Grupo de Carbohidratos	2	48,940.5
	Departamento de Física Atómica y Molecular Teórica	3	100,305.1
	Matemáticas	1	198,961.2
CSIC-UPV	Departamento de Matemáticas	1	191.2

HOSPITALS

Complexo Hospitalario Universitario de Santiago	Fundación Pública Galega de Medicina Xenómica	1	198,961.2

UDC - Universidade da Coruña

Facultad de Informática	Electrónica y Sistemas	4	1,987.8

ICTS - UNIQUE SCIENTIFIC TECHNOLOGICAL INFRASTRUCTURE 2010

CENTRES	Department- Group	# of Active User Accounts 2010	CPU Hours used 2010
ICTS			
CENER	Departamento de Energía Eólica	1	216,354.9
CESGA Estancias	Estancias ICTS	11	41,238.9
Escuela Politécnica Superior de Jaén	Departamento de Ingeniería Mecánica y Minera	1	130,000
Escuela Técnica Superior Ingenieros Aeronáuticos (UPM)	Motopropulsión y Termofluidodinámica	2	33,254.2
E.T.S.I. Navales (UPM)	Departamento de Ingeniería Nuclear	1	22,163.5
Fundación IMDEA Energía	Procesos Termoquímicos	1	162,022.2
Institut de Biotecnologia i de Biomedicina	Unidad de Bioinformática	1	394,944.1
Universidad Politécnica de Madrid	Instituto de Fusión Nuclear	3	113,070.6
IU. de Telecom. y Aplic. Multimedia (iTEAM)	Grupo de Comunicaciones Ópticas (GCO)	1	3,877
Karlsruhe Institute of Technology	Computational Nanophysics	1	7,952.1
Universdad del Pais Vasco	Química Física	1	174,988.2
Universidad de Extremadura	Tecnología de los Computadores y las Comunicaciones	1	90,090
Universitat Politecnica de Cataluña	Ingeniería Molecular	1	43,922,5
University of Perugia	Department of Chemistry	1	100,000

COMPUTİNG İNFRASTRUCTURE

Computing Servers

Different architectures of high-performance computing systems are available for CESGA's community of users. Depending upon the algorithms involved, users choose the computing architecture that is most appropriate for their needs. The highlights of 2010 regarding computing servers are listed below.

Users employed more than 20 million CPU hours.

Efforts were undertaken to improve energy efficiency.

New computing and storage platforms were designed.

In 2010, CESGA focused its efforts on improving FinisTerrae's service, user support, and building a Private Cloud.

FinisTerrae 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. FinisTerrae was made available to all users on April 1, 2008.

The computing servers available to users in 2010 appear in the chart below.

COMPUTING SERVERS IN 2010			
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	2004	DISTRIBUTED PC CLUSTER	50 CPU's, 0.5 -1 GB MEMORY CPU, 9.9 GFLOPS, 110 CPU, 300 GFLOPS
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 Performance

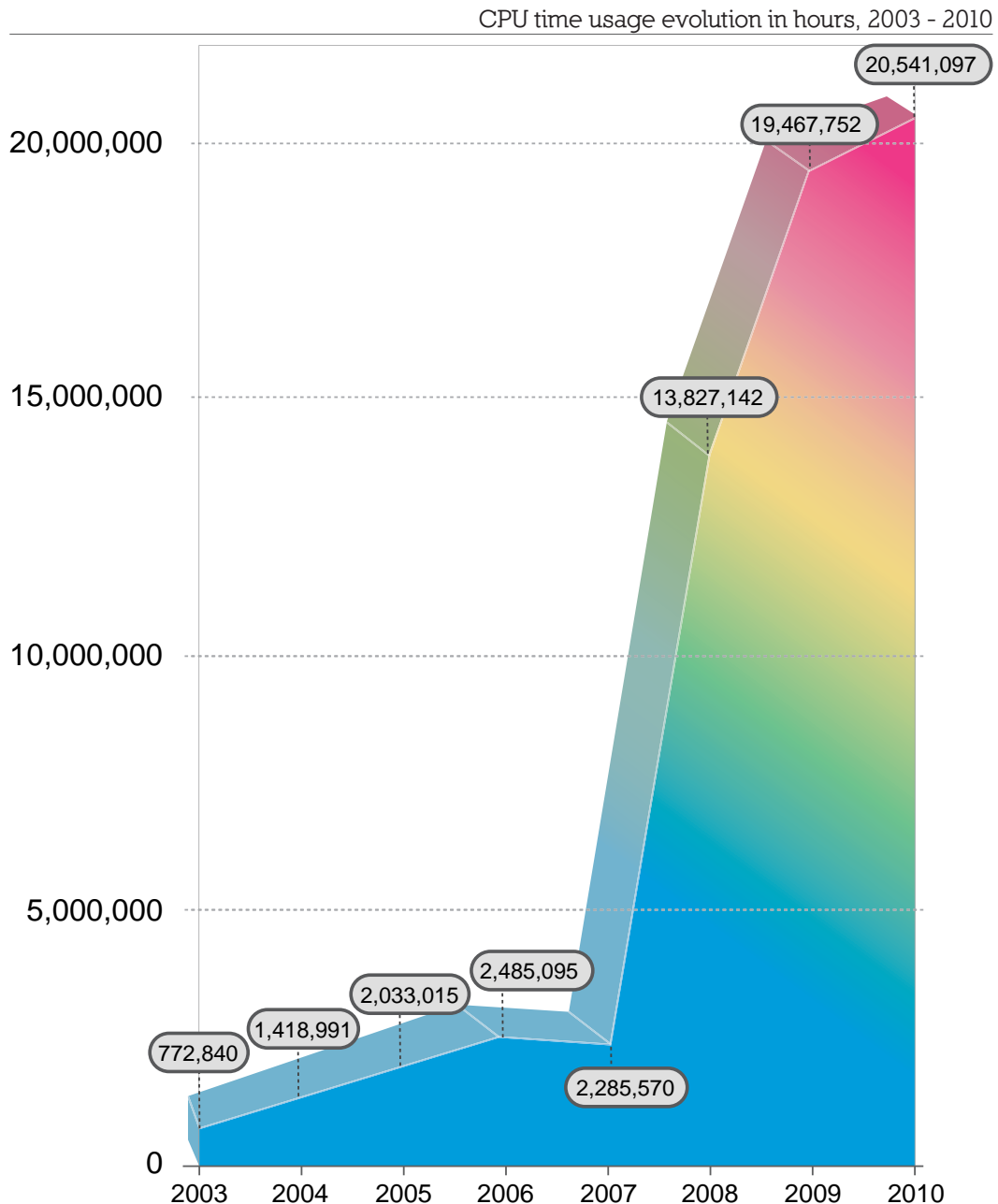Peak Perfomance Evolution at CESGA (in GFLOPS*)

x6.14

x10,278

26,000
25,000
24,000
23,000
22,000
21,000
20,000
19,000
18,000
17,000
16,000

25,696   25,696

21,000

7,500
6,000
6,500
6,000
5,500
5,000
4,500
4,000
3,500
3,000
2,500
2,000
1,500
1,000
500

x 15.5

x 10.5

YEAR 93 | 94 | 95 | 96 | 97 | 98 | 99 | 00 | 01 | 02 | 03 | 04 | 05 | 06 | 07 | 08 | 09 | **2010**
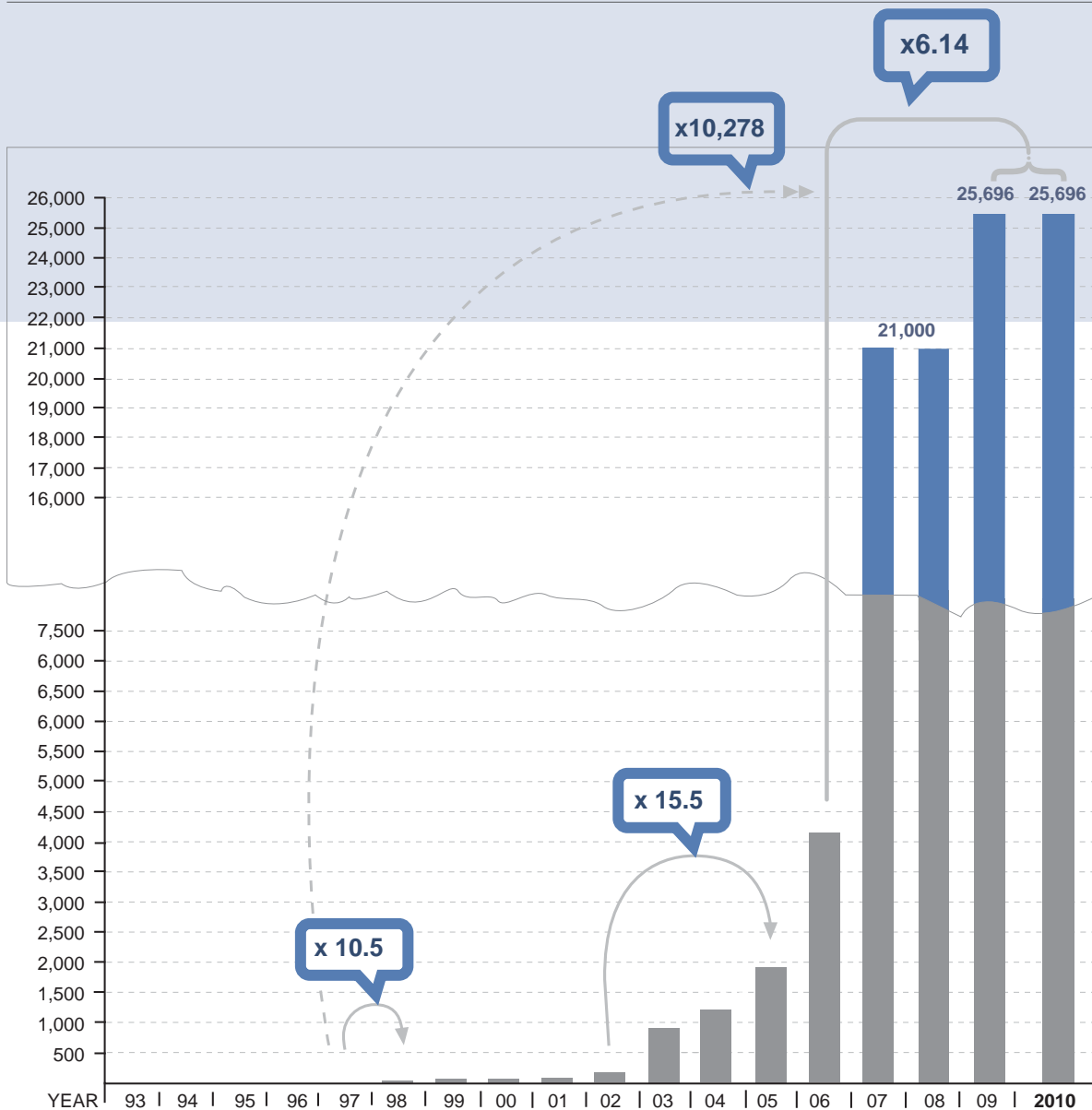
* 1GFLOPS= 1,073,741,824 (floating point operations per second)

Evolution of CPU Consumption

During 2010, the FinisTerrae system and the SVG cluster were the available servers at CESGA.

The number of hours consumed increased significantly from 19,467,752 hours in 2009 to 20,541,097 hours in 2010, incrementing the total by 5.2%.

20,541,097
hours in 2010

CPU time usage evolution in hours, 2003 - 2010

- 20,541,097
- 19,467,752
- 13,827,142
- 772,840
- 1,418,991
- 2,033,015
- 2,485,095
- 2,285,570

20,000,000

15,000,000

10,000,000

5,000,000

0

2003 2004 2005 2006 2007 2008 2009 2010

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 only depend on the available computing capacity but also on the resources necessary for the execution of simulations.

Simulation Jobs Executed by System per Month in 2010

JOBS

SVG_DELL

GRID

FinisTerrae

MONTH
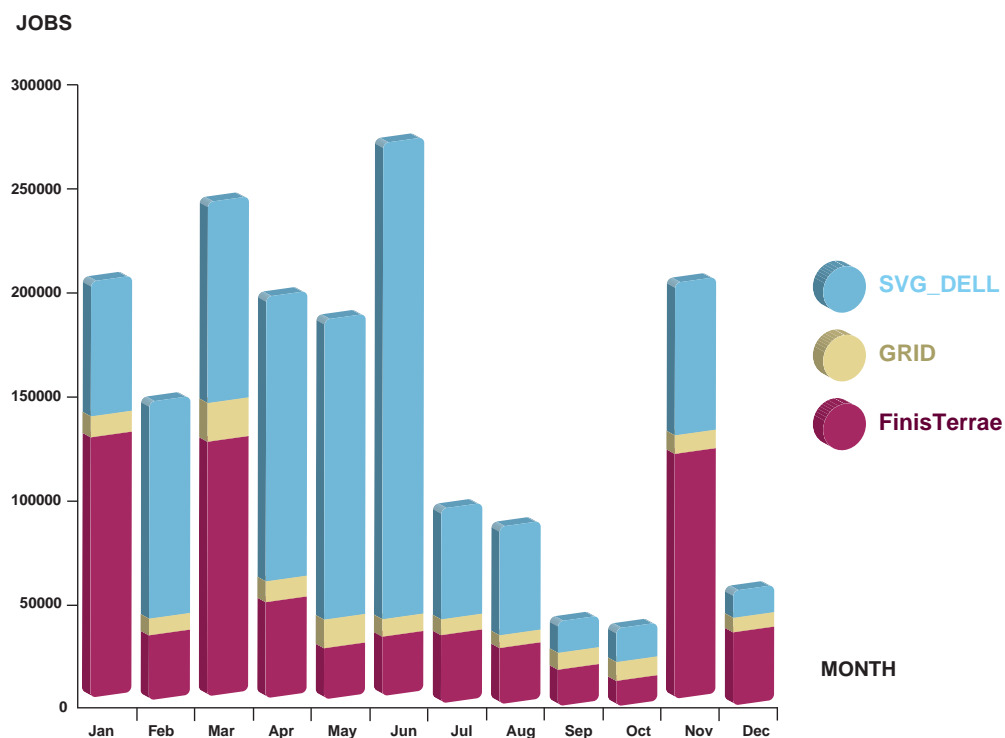
Average İn-Queue Time

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 as close as possible to zero so 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.

In summary, the waiting time increased last year. From an average of 3 hours in 2009, it increased to an average of 5 hours for all computing servers in 2010. In 2010, the FinisTerrae system experienced an increased demand and raised the waiting time to an average of 6 hours.

FinisTerrae
experienced an İncrease in Demand

Average İn-Queue Time for All Processes in All Systems (January 2001 - December 2010)
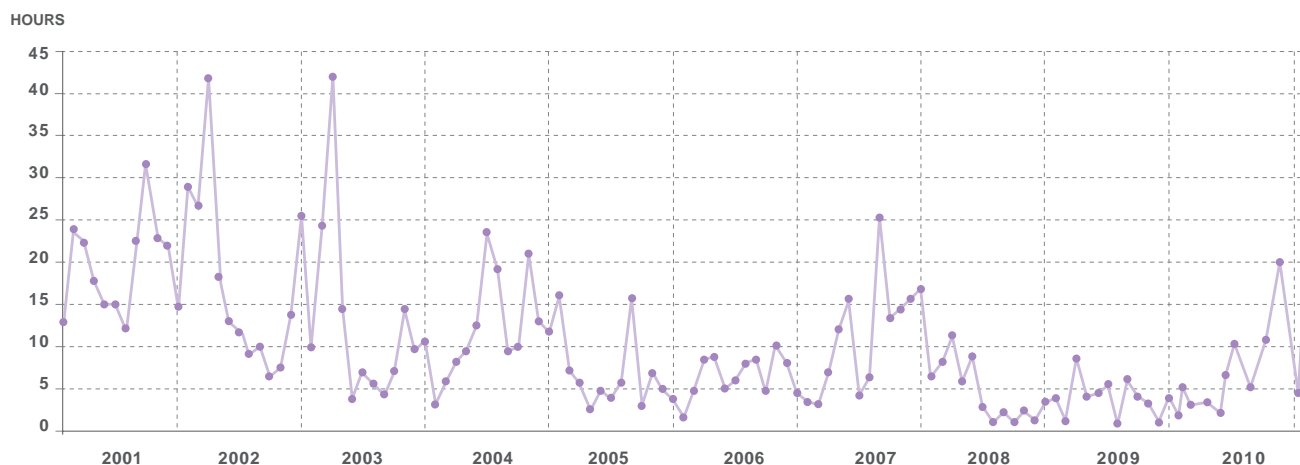
HPC: High Performance Computing Servers

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 low latency time and high transfer capacity.

During 2010, 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, ...
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 FinisTerrae supercomputer 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.

There are 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.

There is 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).

There is also an interconnect Infiniband 4x DDR at 20 Gbps and 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.

FINISTERRAE uses open software including Linux, Lustre, Grid Engine, and Globus.
The system has the following compilers, libraries, and development tools: Intel C/C and Fortran, Intel MKL, Vtune, HP-MPI, and HP UPC.

FINISTERRAE
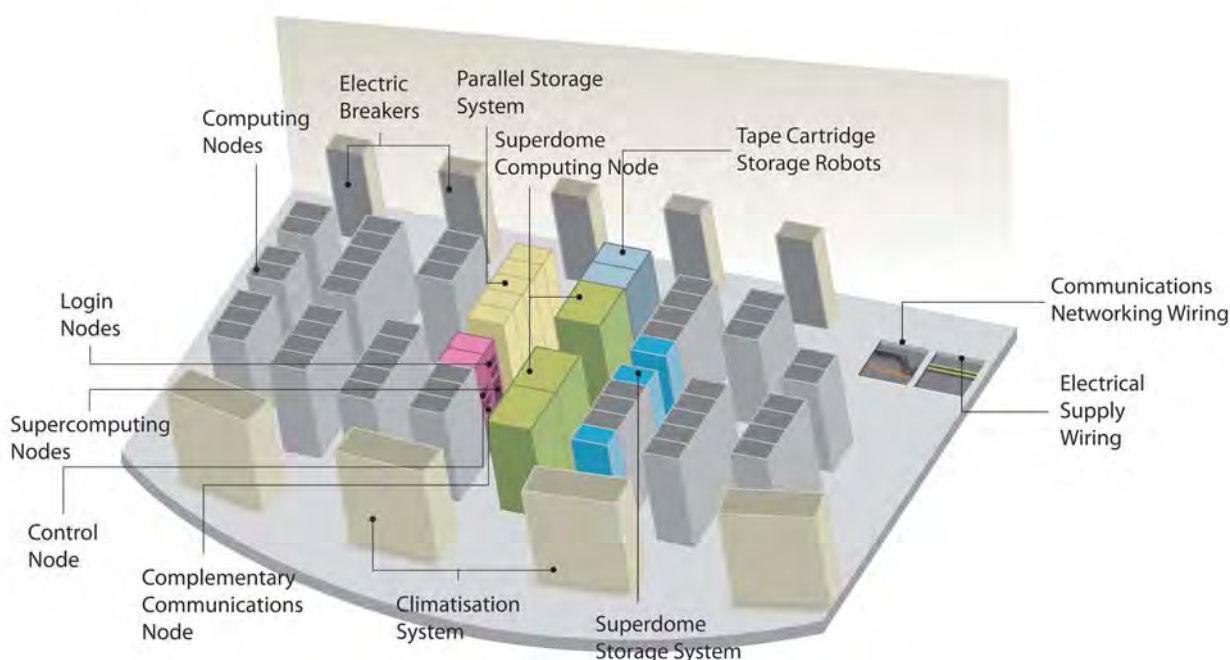
Cloud and HTC:

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 platforms 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)

The 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.
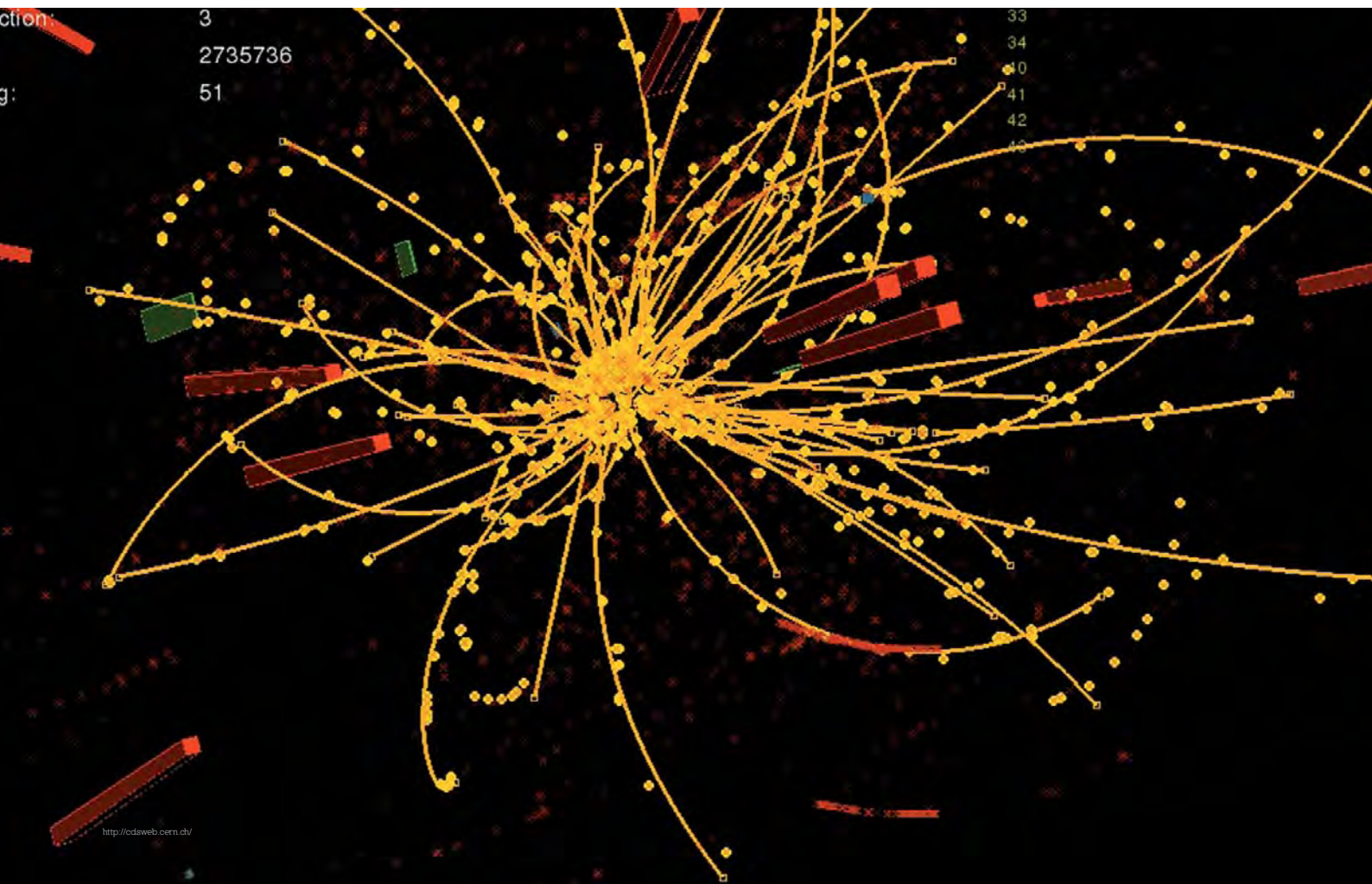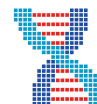
Servers for projects

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 HP ProLiant DL160G6 node with dual quad-core Intel X5570 (Nehalem) and 32GB of memory,

1 HP ProLiant DL165G6 node with two AMD Opteron 2435 six-core processors 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)
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
Industrial (Forest) Information System
**Number and type of processors, total
memory**: 2 Intel Xeon 3 GHz, 2 GB RAM
Number of servers: 1 Operating Sys-
tem: Microsoft Windows Server 2003

RETELAB

Project: RETELAB - A Virtual Labo-
ratory for the National Network for the
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 sub-
sequent 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 2010, there was no significant increase in data storage capacity. Available storage reached **1,739** Terabytes by the end of 2010.

The data storage service 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 89 requests for storage service demanding **63** TB of data storage.

Storage Service Criteria for the Classification of Information

In 2010, 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 analysed 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 utilised 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 systems in order to have a secure copy of their data. The availability of the service may be low.

Parallel Scratch (SFS) 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.
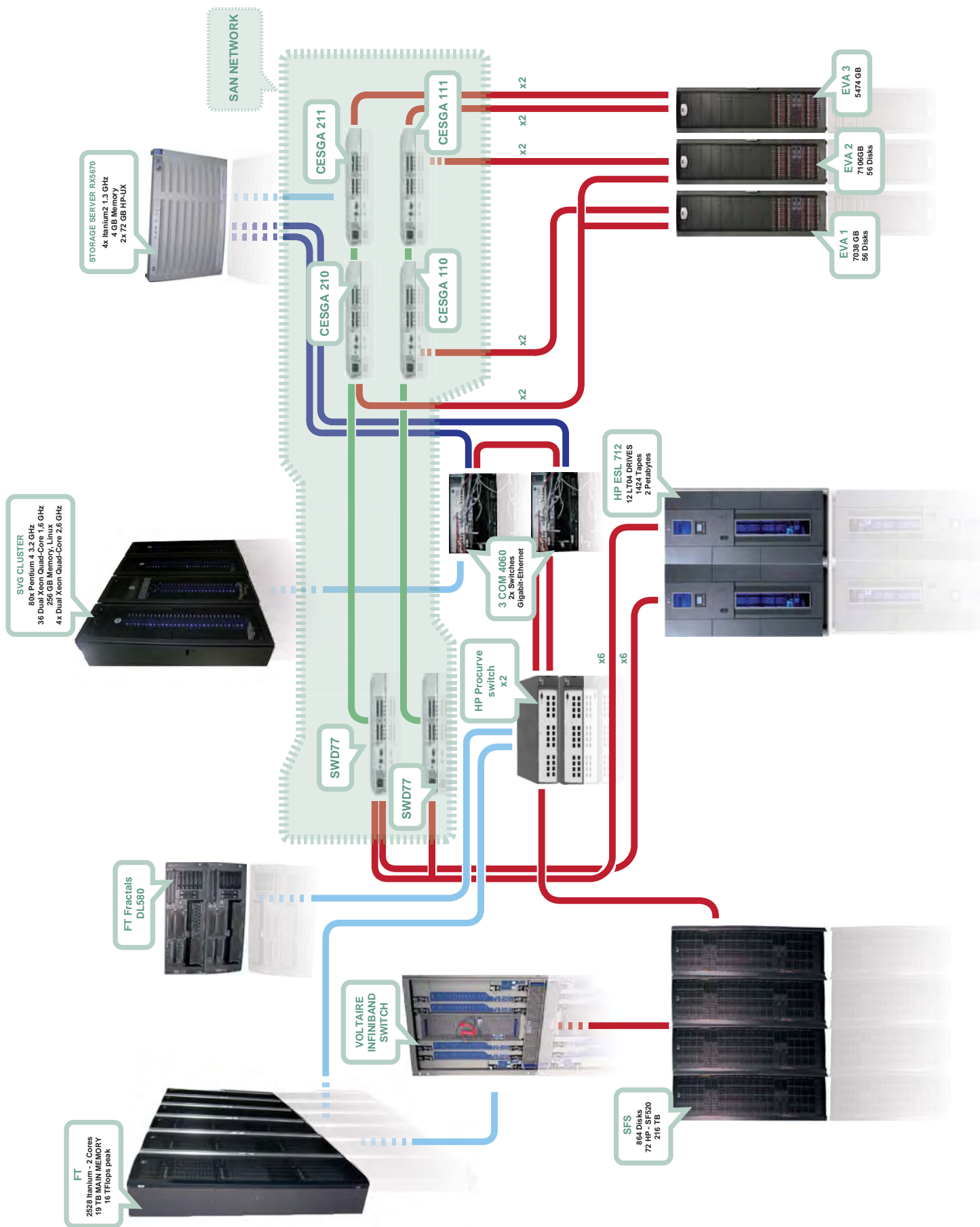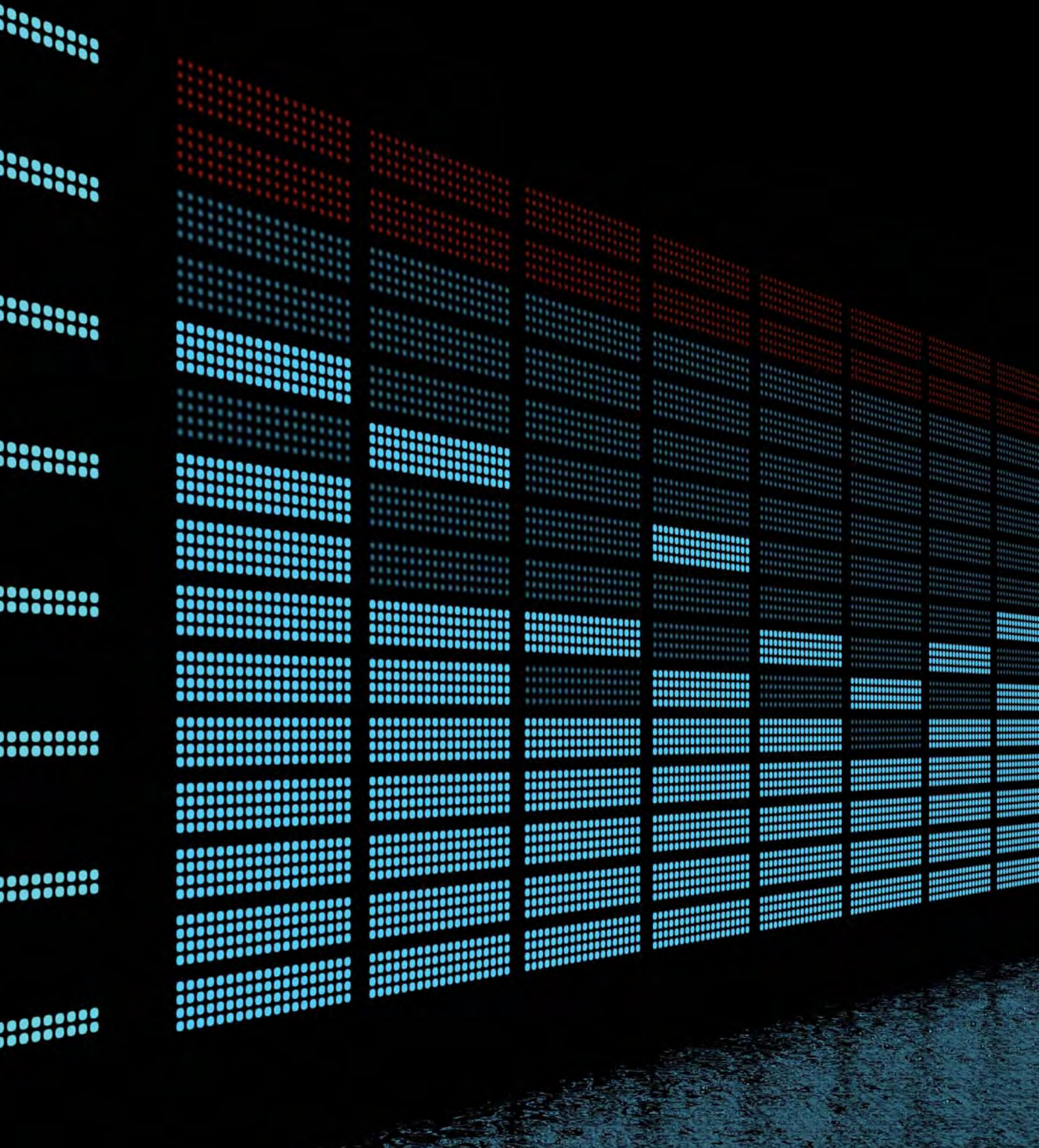
1,739 TB
used in 2010

Data Storage used in 2010

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

Data Storage Resources 2010

SAN NETWORK

STORAGE SERVER RX5670
4x Itanium2 1,3 GHz
4 GB Memory
2x 72 GB HP-UX

CESGA 211

CESGA 111

CESGA 210

CESGA 110

x2

x2

x2

x2

x2

EVA 3
5474 GB

EVA 2
7106GB
56 Disks

EVA 1
7038 GB
56 Disks

SVG CLUSTER
80x Pentium 4 3.2 GHz
36 Dual Xeon Quad-Core 1,6 GHz
256 GB Memory, Linux
4x Dual Xeon Quad-Core 2,6 GHz

HP ESL 712
12 LTO4 DRIVES
1424 Tapes
2 Petabytes

3 COM 4060
2x Switches
Gigabit-Ethernet

HP Procurve
switch
x2

x6

x6

SWD77

SWD77

FT Fractals
DL580

VOLTAIRE
INFINIBAND
SWITCH

SFS
864 Disks
72 HP - SF520
216 TB

FT
2528 Itanium - 2 Cores
19 TB MAIN MEMORY
16 TFlops peak

SCİENTİFİC APPLİCATİONS

The predominant activity in the Applications area during 2010 is listed below.

The completion of a very large number of user support activities.

The installation of all applications demanded by CESGA users along the year. A total of 116 new versions of applications, libraries, compilers, and development tools were installed.

Support for the deployment of a new operational oceanography tool based on the MyOcean fore-casting system for the Spanish Port System.

Testing of the development environment and portability of the applications that are most important for the future server, SVG, based on AMD Opteron(tm) processors.

Application activity is summarised below.

72 applications or scientific computing libraries were put into production. A total of 116 software versions were installed or updated.

447 requests for assistance were addressed (average interannual increase of 78% with respect to the previous year).

User Support Activities 2006-2010
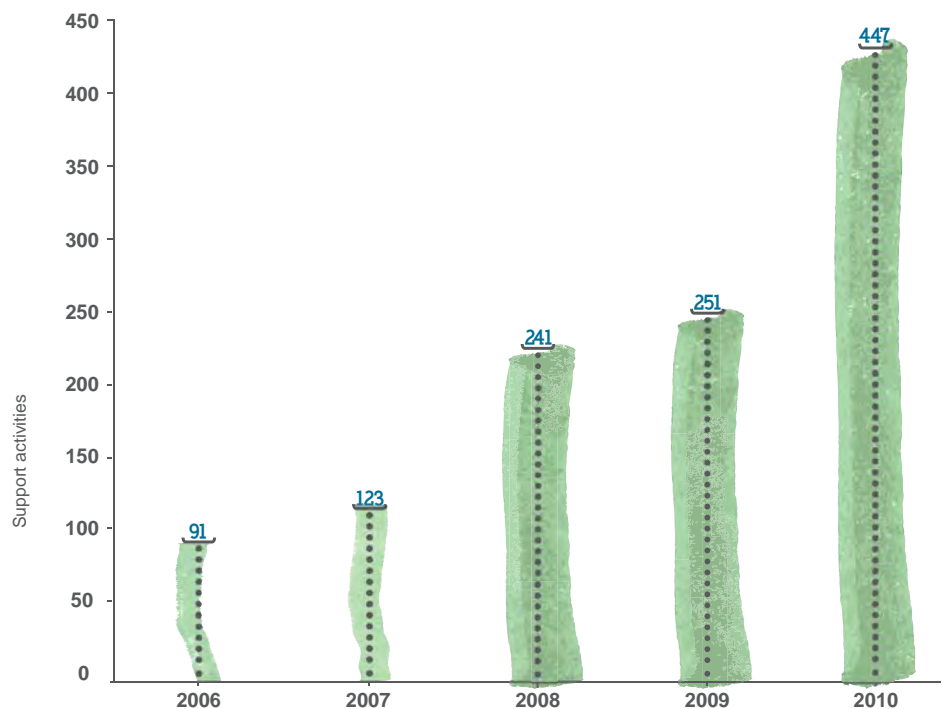
Ported Elements in 2010

Application	Version
Amber	6 & 11
BEAST	1.5.4 & 2.3
CDO	1.4.6
CLUMPP	1.1.2
cp2k	2.1.142 & 2.1.342
Crystal	9
CSD	v5.31(2010)
DL_POLY	2.2
Ferret	6.6.2
Gamess	12 Jan 2009 (R3)
Gaussian 03	E.01
Gaussian 09	A.02
gnuplot	4.2.6
Grads	2.0.a5
Gromacs	4.0.4, 4.0.5 & 4.0.7
HyperWorks	10
ILOG-CPLEX	12.1.0 & 12.2
JAGS	1.0.4
LAMMPS	21 May 2008 & 3 Jul 2010
Materials Studio	5
Matlab	R2009b
MEEP	1.1.1
Migrate	3.1.6
Molden	4.8
MrBayes	3.2
MSC-Nastran	2007
NAMD	2.7b1 & 2.7b2
Ncarg	5.2.0
NCO	4.0.1
OpenBUGS	3.1.2
OpenFOAM	1.5-dev & 1.6
ORCA	2.7
Panoply	2.9.2
R	2.12.0
Schrodinger Suite	2010
SIESTA	3.0-rc2
Structure	2.3.3
VASP	5.2

Library	Version
ACML	4.4.0
boost	1.41.0
FFTW	3.2.2
MKL	10.1.2, 10.2.1, 10.2.2, 10.2.6, 10.2.7 & 10.3.0.084
MUMPS	4.9.2
NumPy	1.5.0
octave	3.2.4
octcdf	1.0.12 & 1.0.17
PETSc	3.1
qhull	2009.1.1
ScaLAPACK	1.8.0
SciPy	0.8.0
SuiteSparse	3.4.0
HP MPI	2.3.1.0
Intel MPI Library	3.1.038, 3.2.1.009, 4.0.0.025 & 4.0.1.007
MPICH2	1.3.1
MVAPICH2	1.4 & 1.5
Platform MPI	7.1 & 8
ftgl	2.1.3-rc5
GMT	4.5.3
HDF5	1.8.4-patch1 1.8.4-parallel
NetCDF	4.0.1, 4.1.1 & 4.1.1-parallel
pgplot	5.2.2

Compilers and Development Tools	Version
CUDA	3.1
GNU Compilers	4.4.0
Intel C++ Compiler	9.1.052, 10.1.026, 11.1.046, 11.1.056, 11.1.073, 11.1.075 & 12.0.084
Intel Fortran Compiler	9.1.052, 10.1.026, 11.1.046, 11.1.056, 11.1.073, 11.1.075 & 12.0.084
Open64	4.2.3 & 4.2.4
PGI Compilers	7.2.5, 8.06, 9.04, 10.3 & 10.9
Sun JDK	1.6.0_20 & 1.6.0_22
HP-Caliper	5.2.0
PAPI	4.1.1
TotalView	8.8.0 & 8.9.0
git	1.7.0.5
subversion	1.6.13

Statistics of Applications Use During 2010

These statistics extracted from the accounting records summarise the use of applications from January 1, 2010 through December 31, 2010. Data collected for accounting purposes included only those entries with execution times greater than 30 seconds (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 due to the much shorter time used by this sort of applications.

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 Applications, 2010

KEY

Other, gg89/03/09, VASP, LAMMPS, amber, SIESTA, Gromacs, Xmipp, NAMD, CHARMM, parsec, Q, Venus, DYCI, waccm, WRF, dpmd, ILOG-CPLEX, octopus, java, ABC, OpenFoam, LAUTREC

gamess, IM, Molpro, Materials Studio, Cactus, ROMS, python, HEMCUVE, SYSTEM, HyperWorks, almpac, DL_POLY, Aires, batwing, structure, MM5, matlab, Leadmix, Nemo, pyMPI, CASTEP, Turbomole, MSC-Nastran

ORCA, Stata, cp2K, dalton, PHYML, MrBayes, MEEP, Eimer, Singular, Crystal, elmrt, nwchen, csd, BEAMnrc, abinit, blast, Grads, Schorodinger Suite, deMon2K, CDO, dock, Autodock, fluent, RAxML

molden, octave, perl, netckf, molcas, EMAN, R, VMD

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

Area	Application	FINISTERRAE	SVGD
Scientific Analysis	4ti2	✕	—
	R	✕	
	ROOT	—	✕
	Singular	✕	—
Scientific Databases	CSD	—	✕
Bioinformatics	batwing	—	✕
	BEAMnrc	—	✕
	BEAST	—	✕
	BEST	—	✕
	Blast	—	✕
	CLUMPP	—	✕
	Genehunter	✕	✕
	IM	—	✕
	IMa2	—	✕
	JAGS	✕	—
	Lamarc	—	✕
	Leadmix	✕	✕
	Migrate	✕	✕
	MrBayes	✕	✕
	MSVAR	—	✕
	OpenBUGS	—	✕
	phylobayes	—	✕
	PHYML	—	✕
	RAxML	—	✕
	Structure	—	✕
Structural Modeling, Fluids, and Magnetism	Elmer	✕	—
	OpenFOAM	✕	—
MPI	HP MPI	✕	—
	Intel MPI Library	✕	✕
	MVAPICH2	✕	—
	Platform MPI	✕	—
	pyMPI	✕	✕

Area	Application	FINISTERRAE	SVGD
Molecular Simulation	abinit	—	×
	Amber	×	×
	AutoDock	×	—
	cp2k	×	×
	CPMD	×	—
	Dalton	×	×
	Desmod Schrodinger	—	×
	Gamess	×	×
	Gaussian 03	×	×
	Gaussian 09	×	×
	Gaussian 98	—	×
	Gromacs	×	×
	LAMMPS	×	×
	Molden	×	×
	NAMD	×	×
	NWChem	×	×
	Octopus	×	—
	Schrodinger Suite	×	×
Compilers	Cmake	×	—
	CUDA	—	×
	GNU Compilers	×	×
	Intel C++ Compiler	×	×
	Intel Fortran Compiler	×	×
	Open64	×	—
	pcre	—	×
	PGI Compilers	—	×
	Python	—	×
	Sun JDK	×	×
Profiling Tools	HP-Caliper	×	—
	Intel Thread Checker	×	—
	Intel Thread Profiler	×	—
	Intel Trace Analyzer and Collector	×	—
	PAPI	×	—
	TotalView	×	×

Area	Application	FINISTERRAE	SVGD
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 Visualisation and Animation	CDO	✕	—
	Grace	—	✕
	Grads	✕	✕
	HDF	✕	—
	HDF5	✕	✕
	JasPer	—	✕
	Ncarg	✕	✕
	NCO	✕	—
	NetCDF	✕	✕
	szip	✕	—
	udunits	✕	—
	VMD	✕	✕
Software Management	Modules	✕	✕

Area	Application	FINISTERRAE	SVGD
Scientific Visualisation and Animation	CDO	✕	—
	etsf_io	✕	—
	ftgl	✕	✕
	GMT	✕	—
	gnuplot	✕	✕
	Grace	—	✕
	Grads	✕	✕
	HDF	✕	—
	HDF5	✕	✕
	JasPer	—	✕
	Ncarg	✕	✕
	NCO	✕	—
	NetCDF	✕	✕
	Panoply	✕	✕
	Parallel-NetCDF	✕	—
	pgplot	✕	—
	szip	✕	—
	udunits	✕	—
	VMD	✕	✕
Software Management	git	✕	—
	Modules	✕	✕

*Many new versions of **applications and libraries** were incorporated during 2010 at the request of users. They are listed below.*

SCİENTİFİC DATABASES

CSD (new version, 5.31 (2010) in SVG)

The Cambridge Structural Database (CSD) is the world repository of small molecule crystal structures. The CSD System is comprised of software for database access, structure visualisation and data analysis, and structural knowledge bases derived from the CSD. The CSD records bibliographic, chemical, and crystallographic information for organic molecules and metal-organic compounds whose 3D structures have been determined using X-ray diffraction or neutron diffraction.

MOLECULAR SİMULATİON

Amber (new version, 11.0 in 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 sometimes used to refer to the empirical force fields that are implemented here. It should be recognised, however, that the code and force field are separate. Several other computer packages have implemented the Amber force fields and other force fields can be implemented with the Amber programs.

CP2K (new installation, versions 2.1.142 and 2.1.342 in FinisTerrae and SVG)

CP2K is a freely available (GPL) program, written in Fortran 95, to perform atomistic and molecular simulations of solid state, liquid, molecular, and biological systems. It provides a general framework for different methods such as density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW), classical pair, and many-body potentials.

Gamess (new version, 12 Jan 2009 (R3) in SVG)

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 03 (new version, E.01 testing in SVG2)

Gaussian 03 is used by chemists, chemical engineers, biochemists, physicists, and others for research in established and emerging areas of chemical interest. Starting from the basic laws of quantum mechanics, Gaussian predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types.

Gaussian 09 (new version, A.02 testing in SVG2)

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

Gromacs (new versions, 4.0.4, 4.0.5 and 4.07 in FinisTerrae)

GROMACS is a versatile package to perform molecular dynamics, i.e., 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. Since GROMACS is extremely fast at calculating the nonbonded interactions (that usually dominate simulations), many groups are also using it for research on non-biological systems, e.g., polymers.

LAMMPS (new installation, versions 21May2008 and 3Jul2010 in SVG; new version, 3Jul2010 in FinisTerrae)

LAMMPS is a molecular dynamics simulator. LAMMPS can run in monoprocessor machines or in parallel using message passing techniques and a decomposition of the simulation domain. The code is designed to be easily modified or to add new functionalities to it. It is distributed as an open source under the GPL license terms.

Molden (new installation, version 4.8 in SVG; new version, 4.8 in FinisTerrae)

Molden is a package for displaying Molecular Density from the *ab initio* packages (GAMESS-UK, GAMESS-US and GAUSSIAN) and the Semi-Empirical packages (Mopac/Ampac). It also supports a number of other programs via the Molden Format.

NAMD (new versions, 2.7b1 and 2.7b2 in SVG; new version, 2.7b2 in FinisTerrae)

NAMD is a parallel molecular dyamics code designed to obtain high performance in the simulation of large biomolecular systems.
Its programming is based on parallel Charm++ objects and it scales up to hundreds of processors in high-performance parallel platforms and up to tens of processors in common clusters with gigabit ethernet.

SIESTA (new version, 3.0-rc2 in FinisTerrae)

Siesta (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and 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

Amber (new version, 6.0 in SVG)

Specific user modified version of the Amber 6 suite of programmes.

Crystal (new version 9 in FinisTerrae)

CRYSTAL is a general-purpose program for the study of crystalline solids. The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations. The Bloch functions of the periodic systems are expanded as linear combinations of atom-centred Gaussian functions. Powerful screening techniques are used to exploit real space locality. Restricted (Closed Shell) and Unrestricted (Spin-polarised) calculations can be performed with all-electron and valence-only basis sets with effective core pseudo-potentials.

DL_POLY (new installation, version 2.2 in FinisTerrae)

DL_POLY is a package of subroutines, programs, and data files designed to facilitate molecular dynamics simulations of macromolecules, polymers, ionic systems, solutions, and other molecular systems on a distributed memory parallel computer.

Materials Studio (new version, 5 in SVG and FinisTerrae)

A comprehensive suite of modeling and simulation solutions for studying chemicals and materials including crystal structure and crystallisation processes, polymer properties, catalysis, and structure-activity relationships.

ORCA (new installation, version 2.7 in FinisTerrae)

ORCA is a flexible, efficient, and easy-to-use general purpose tool for quantum chemistry with specific emphasis on spectroscopic properties of open-shell molecules. It features a wide variety of standard quantum chemical methods ranging from semiempirical methods to DFT to single- and multireference correlated *ab initio* methods. It can also manage environmental and relativistic effects.

Schrodinger Suite (new version, 2010 in SVG)

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 modeling. QikProp is used 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 is used for focused library design. Epik is used for accurate enumeration of ligand protonation states in biological conditions. Jaguar is used the high-performance *ab initio* quantum mechanics application. MacroModel is a molecular modeling program 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 with a fully-integrated molecular visualisation and an analysis environment.

VASP (new version, 5.2 in 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 and an exact evaluation of the instantaneous electronic ground state at each.

BIOINFORMATICS

BEAST (new version, 1.5.4 in SVG)

BEAST is a cross-platform program for Bayesian MCMC analysis of molecular sequences. It is entirely orientated 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.

BEST (new installation, version 2.3 in SVG)

BEST is a free phylogenetics program written by Liang Liu to estimate the joint posterior distribution of gene trees and a species tree using multilocus molecular data that accounts for deep coalescence but not for other issues such as horizontal transfer or gene duplication. The program works within the popular Bayesian phylogenetics package, MrBayes (Ronquist and Huelsenbeck, Bioinformatics, 2003). BEST parameters are defined using the prset command in MrBayes.

CLUMPP (new installation, version 1.1.2 in SVG)

CLUMPP is a program that deals with label switching and multimodality problems in population-genetic cluster analyses. CLUMPP permutes the clusters output by independent runs of clustering programs such as structure, so that they match up as closely as possible. The user has the option of choosing one of three algorithms for aligning replicates, with a trade-off of speed and similarity to the optimal alignment. A program note describing CLUMPP was published in Bioinformatics 23: 1801-1806 (2007).

JAGS (new installation, version 1.0.4 in FinisTerrae)

JAGS is Just Another Gibbs Sampler. It is a program for analysis of Bayesian hierarchical models using Markov Chain Monte Carlo (MCMC) simulation not unlike BUGS.

Migrate (new version, 3.1.6 in 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.

OpenBUGS (new installation, version 3.1.2 in SVG)

BUGS is a software package for performing Bayesian inference Using Gibbs Sampling. The user specifies a statistical model of (almost) arbitrary complexity by simply stating the relationships between related variables. The software includes an 'expert system' which determines an appropriate MCMC (Markov Chain Monte Carlo) scheme (based on the Gibbs sampler) for analysing the specified model.

Structure (new version, 2.3.3 in SVG)

The program structure is a free software package for using multi-locus genotype data to investigate population structure. 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.

OpenFOAM (new installation, versions 10.5-dev and 1.6, in FinisTerrae)

The OpenFOAM® (Open Field Operation and Manipulation) CFD Toolbox is a free, open source CFD software package produced by a commercial company, OpenCFD Ltd. It has a large user base across most areas of engineering and science, from both commercial and academic organisations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence, and heat transfer to solid dynamics and electromagnetics.

HyperWorks (new version, 10.0 in FinisTerrae)

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

MSC-Nastran (new version, 2007 in 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 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.

SİMULATİON

MEEP (new installation, version 1.1.1 in FinisTerrae)

Meep is a free finite-difference time-domain (FDTD) simulation software package developed at MIT to model electromagnetic systems.

ILOG-CPLEX (new installation, versions 12.1.0 and 12.2 in SVG; version 12.1.0 in FinisTerrae)

IBM ILOG OPL-CPLEX Development Bundles is a modeling language and integrated development environment for optimisation and constraint programming models.

Matlab (new version, R2009b in SVG)

MATLAB is a high-performance language for technical computing. It integrates computation, visualisation, and programming in an easy-to-use environment where problems and solutions are expressed in familiar mathematical notation.

SCİENTİFİC VİSUALİSATİON AND ANİMATİON

CDO (new version, 1.4.6 in FinisTerrae)

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

Ferret (new installation, version 6.6.2 in FinisTerrae)

Ferret is an interactive computer visualisation and analysis environment designed to meet the needs of oceanographers and meteorologists analysing large and complex gridded data sets.

Ftgl (new installation, version 2.1.3-rc5 in SVG and FinisTerrae)

FTGL is a free, cross-platform Open Source C++ library that uses Freetype2 to simplify rendering fonts in OpenGL applications. FTGL supports bitmaps, pixmaps, texture maps, outlines, polygon mesh, and extruded polygon rendering modes.

GMT (new installation, version 4.5.3 in FinisTerrae)

GMT is an open source collection of ~60 tools for manipulating geographic and Cartesian data sets (including filtering, trend fitting, gridding, projecting, etc.) and producing Encapsulated PostScript File (EPS) illustrations ranging from simple x-y plots via contour maps to artificially illuminated surfaces and 3-D perspective views. GMT supports ~30 map projections and transformations and comes with support data such as GSHHS coastlines, rivers, and political boundaries.

Gnuplot (new installation, version 4.2.6 in SVG and FinisTerrae)

Gnuplot is a portable, command-line driven, graphing utility. It was originally created to allow scientists and students to visualise mathematical functions and data interactively but has grown to support many non-interactive uses such as web scripting. It is also used as a plotting engine by third-party applications like Octave. Gnuplot has been supported and under active development since 1986.

Grads (new version, 2.0a5 in FinisTerrae)

> The Grid Analysis and Display System (GrADS) is an interactive desktop tool that is used for easy access, manipulation, and visualisation of Earth science data. The format of the data may be either binary, GRIB, NetCDF, or HDF-SDS (Scientific Data Sets). GrADS has been implemented worldwide on a variety of commonly used operating systems and is freely distributed over the Internet.

HDF5 (new versions, 1.8.4-patch1 and 1.8.4-parallel in FinisTerrae)

> HDF5 is a unique technology suite for the management of extremely large and complex data collections. The HDF5 technology suite includes: 1) a versatile data model that can represent very complex data objects and a wide variety of metadata. 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 optimisations, 5) and tools and applications for managing, manipulating, viewing, and analysing the data in the collection.

Ncarg (new version, 5.2.0 in FinisTerrae)

> NCAR Graphics, a time-tested UNIX package, mainly consists of over two dozen Fortran/C utilities for drawing contours, maps, vectors, streamlines, weather maps, surfaces, histograms, X/Y plots, annotations, and more.

NCO (new version, 4.0.1 in 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 metadata manipulation) and produce a netCDF file as output. The operators are primarily designed to aid manipulation and analysis of gridded scientific data.

NetCDF (new version, 4.0.1 in SVG; new versions, 4.1.1 and 4.1.1-parallel in 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.

Pgplot (new installation, version 5.2.2 in FinisTerrae)

> The PGPLOT Graphics Subroutine Library is a Fortran- or C-callable, device-independent graphics package for making simple scientific graphs. It is intended for making graphical images of publication quality with minimum effort on the part of the user. For most applications, the program can be device-independent and the output can be directed to the appropriate device at run time.

Panoply (new installation, version 2.9.2 in SVG and FinisTerrae)

> Panoply is a cross-platform application which plots geo-gridded arrays from netCDF, HDF and GRIB datasets. One can slice and plot specific latitude-longitude, latitude-vertical, or time-latitude arrays from larger multidimensional variables; combine two arrays in one plot by differencing, summing, or averaging; plot lon-lat data on a global or regional map (using any of over 75 map projections) or make a zonal average lineplot, and overlay continent outlines or masks on lon-lat plots.

MATHEMATICAL LIBRARIES

ACML (new installation, version 4.4.0 testing in SVG2)

> ACML consists of the following main components: a full implementation of Level 1, 2 and 3 Basic Linear Algebra Subroutines (BLAS) with key routines optimised for high performance on AMD Opteron™ processors; a full suite of Linear Algebra (LAPACK) routines as well as taking advantage of the highly-tuned BLAS kernels (a key set of LAPACK routines has been further optimised to achieve considerably higher performance than standard LAPACK implementations); a comprehensive suite of Fast Fourier Transforms (FFTs) in both single-, double-, single-complex and double-complex data types and; fast scalar, vector, and array math transcendental library routines optimised for high performance on AMD Opteron processors. It has random number generators in both single-and double-precision.

BOOST (new installation, version 1.41.0 in SVG)

> 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 and usable across a broad spectrum of applications.

Octcdf (new installation, version 1.0.17 in SVG; versions 1.0.12 and 1.0.17 in FinisTerrae)

> Octcdf is a NetCDF interface for octave.

FFTW (new version, 3.2.2 in 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 of even/odd data, i.e., the discrete cosine/sine transforms or DCT/DST). According to some tests made by the manufacturer in several platforms, the FFTW yield is generally superior to thouse of other bookstores or software to calculate the FFT and is competitive with those that required payment. In addition, FFTW is portable; the same program can be executed in many architectures without modification.

MKL (new versions, 10.2.1 and 10.2.6 in SVG; 10.2.2 and 10.2.7 in FinisTerrae; 10.1.2, 10.2.6 and 10.3.0.084 testing in SVG2)

ACML includes a full implementation of Level 1, 2 and 3 Basic Linear Algebra Subroutines (BLAS) with key routines optimised for high performance on AMD Opteron™ processors and a full suite of Linear Algebra (LAPACK) routines. As well as taking advantage of the highly-tuned BLAS kernels, a key set of LAPACK routines has been further optimised to achieve considerably higher performance than standard LAPACK implementations. ACML also offers a comprehensive suite of Fast Fourier Transforms (FFTs) in both single-, double-, single-complex and double-complex data types and fast scalar, vector, and array math transcendental library routines optimised for high performance on AMD Opteron processors. It has random number generators in both single-and double-precision.

MUMPS (new installation, version 4.9.2 in FinisTerrae)

MUMPS is a parallel sparse direct solver that is used to provide solutions for large linear systems with symmetric positive definite matrices, general symmetric matrices, and general unsymmetric matrices. This version is for complex arithmetic; parallel factorisation and solve phases; iterative refinement and backward error analysis; various matrix input formats including assembled format, distributed assembled format, and elemental format; partial factorisation and Schur complement matrix; and several interfaced orderings: AMD, AMF, PORD, METIS, PARMETIS, SCOTCH, and PT-SCOTCH.

PETSc (new installation, version 3.1 in FinisTerrae)

PETSc (Portable, Extensible Toolkit for Scientific Computation), pronounced PET-see (the S is silent), is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. It employs the MPI standard for parallelism.

NumPy (new version, 1.5.0 in 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 Python-Numeric and F2PY packages.

Octave (new version, 3.2.4 in 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 2009.1.1 in FinisTerrae)

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.

ScaLAPACK (new installation, version 1.8.0 testing in SVG2)

The ScaLAPACK (or Scalable LAPACK) library includes a subset of LAPACK routines redesigned for distributed memory MIMD parallel computers. It is currently written in a Single-Program-Multiple-Data style using explicit message-passing for interprocessor communication. It assumes matrices are laid out in a two-dimensional block cyclic decomposition.

SciPy (new installation, version 0.8.0 in FinisTerrae)

SciPy is open-source software for mathematics, science, and engineering. The SciPy library depends on NumPy, which provides convenient and fast N-dimensional array manipulation. The SciPy library is built to work with NumPy arrays and provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimisation.

SuiteSparse (new installation, version 3.4.0 in FinisTerrae)

> The Suite of Sparse matrix packages includes the following features. AMD is a symmetric approximate minimum degree; BTF is a permutation to block triangular form; CAMD is a symmetric approximate minimum degree; CCOLAMD is a constrained column approximate minimum degree; COLAMD is a column approximate minimum degree; CHOLMOD is a sparse supernodal Cholesky factorization and update/downdate; CSparse is a concise sparse matrix package; CXSparse is an extended version of Csparse; KLU is sparse LU factorization, for circuit simulation; LDL is a simple LDL^T factorization; UMFPACK is a sparse multifrontal LU factorization; RBio is a MATLAB toolbox for reading/writing sparse matrices; UFconfig is a common configuration for all but Csparse; LINFACTOR solves Ax=b using LU or CHOL; MESHND is for 2D and 3D mesh generation and nested dissection; SSMULT is a sparse matrix times sparse matrix; SuiteSparseQR is a multifrontal sparse QR; UFcollection is software for managing the collection; MATLAB_Tools includes various m-file utilities.

SCIENTIFIC ANALYSIS

R (new version, 2.12.0 in SVG and FinisTerrae)

> R is a language and environment for statistical computing and graphics. R provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering, ...) and graphical techniques, and is highly extensible.

PARALLEL LBRARIES

HP MPI (new version, 2.3.1.0 in 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 the shared memory for intra-node communications.

MPICH2 (new installation, version 1.3.1 testing in SVG2)

> MPICH2 is a high-performance and widely portable implementation of the Message-Passing Interface (MPI) Standard, designed to implement all of MPI-1 and MPI-2 (including dynamic process management, one-sided operations, parallel I/O, and other extensions).

Intel MPI Library (new versions, 3.1.038, 3.2.1.009 and 4.0.0.025 in SVG; 4.0.1.007 testing in SVG2)

> 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. The Intel MPI Library enables you to quickly deliver maximum end user performance even if you change or upgrade to new interconnects, without requiring major changes to the software or to the operating environment. Intel also provides a free runtime environment kit for products developed with the Intel MPI library.

MVAPICH2 (new installation, versions 1.4 and 1.5 in FinisTerrae)

> The MVAPICH "MPI over InfiniBand, 10GigE/iWARP and RDMA over Converged Ethernet (RoCE)" project, lead by the Network-Based Computing Laboratory (NBCL) of the Ohio State University. MVAPICH/MVAPICH2 software delivers best performance, scalability, and fault tolerance for high-end computing systems and servers using InfiniBand, 10GigE/iWARP, and RoCE networking technologies. MVAPICH/MVAPICH2 software is powering several supercomputers in the TOP 500 list.

Platform MPI (new installation, versions 7.1 and 8 in FinisTerrae; version 8 testing in SVG2)

> Platform MPI™ is a high performance, production quality implementation of the Message-Passing Interface (MPI) standard for both the Linux and Microsoft® Windows operating systems. Platform MPI combines the broad adoption and scalability of HP-MPI with the performance of Scali-MPI and is fully compliant with the MPI 1.2 and 2.2 standards.

COMPILERS

CUDA (new version, 3.1 in 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.

GNU Compilers (new installation, versions 4.4.0 and 4.5.0 in SVG; version 4.4.0 in FinisTerrae.)

> The GNU Compiler Collection includes front ends for C, C++, Objective-C, Fortran, Java, and Ada, as well as libraries for these languages (libstdc++, libgcj, ...). GCC was originally written as the compiler for the GNU operating system.

Intel C++ Compiler (new versions, 9.1.052, 10.1.026, 11.1.046 and 11.1.073 in SVG; 11.1.026, 11.1.056, 11.1.073 and 11.1.075 in FinisTerrae; 9.1.052, 10.1.026, 11.1.073 and 12.0.084 testing in SVG2)

> The Intel C++ Compiler Professional Edition offers the best support for creating multi-threaded applications. It offers the breadth of advanced optimisation, multi-threading, and processor support that includes automatic processor dispatch, vectorization, auto-parallelization, OpenMP, data prefetching, and loop unrolling, along with highly optimised C++ templates for parallelism, math processing, and multimedia libraries.

Intel Fortran Compiler (new versions, 9.1.052, 10.1.026, 11.1.046 and 11.1.073 in SVG; 11.1.026, 11.1.056, 11.1.073 and 11.1.075, in FinisTerrae; 9.1.052, 10.1.026, 11.1.073 and 12.0.084 testing in SVG2)

> 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 optimises and parallelizes software to take best advantage of multi-core Intel processors including dual-core mobile, desktop, and enterprise platforms.

Open64 (new installation, versions 4.2.3 in FinisTerrae and 4.2.4 testing in SVG2)

> Open64 is an open source, optimising compiler for multiple architectures. Open64 supports Fortran 77/95/2003 and C/C++, as well as the shared memory programming model, OpenMP. Open64 derives from the SGI compilers for the MIPS called MIPSPro. It was released under the GNU GPL in 2000. The initial release of Open64 only supports Intel IA-64(Itanium). Now it has been extended to generate code for CISC, RISC, VLIW, GPU architectures, including IA-32/x86-64, MIPS, IA-64, CUDA, and others.

HP-Caliper (new installation, version 5.2.0 in FinisTerrae)

> HP Caliper is a general purpose performance analysis tool for applications, processes, and systems. It allows you to understand the performance and execution of an application and to identify ways to improve its run-time performance.

PGI Compilers (new versions, 8.0.6, 10.3 and 10.9 in SVG; 7.2.5, 8.0.6, 9.0.4 and 10.9 testing in SVG2)

> 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.

PAPI (new installation, version 4.1.1 in FinisTerrae)

> PAPI aims to provide the tool designer and application engineer with a consistent interface and methodology for use of the performance counter hardware found in most major microprocessors. PAPI enables software engineers to see, in near real time, the relation between software performance and processor events.

TotalView (new versions, 8.8.0 and 8.9.0 in SVG and FinisTerrae; 8.9.0 testing in SVG2)

> TotalView provides dynamic source code and memory debugging for C, C++ and Fortran applications. It is a GUI-based source code defect analysis tool that offers unprecedented control over processes and thread execution and visibility into program state and variables.

SOFTWARE MANAGEMENT

Git (new installation, version 1.7.0.5 in FinisTerrae)

> Git is a free & open source, distributed version control system designed to handle everything from small to very large projects with speed and efficiency.

**Subversion** (new version, 1.6.13 in FinisTerrae)

> Subversion is an open source version control system. Subversion is an open-source, centralized version control system characterized by its reliability as a safe haven for valuable data, the simplicity of its model and usage, and its ability to support the needs of a wide variety of users and projects, from individuals to large-scale enterprise operations.

GALICIAN SCIENCE & TECHNOLOGY NETWORK

RECETGA
Rede de Ciencia e Tecnoloxía de Galicia

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 41 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 for research, development, and innovation in the field of communications.
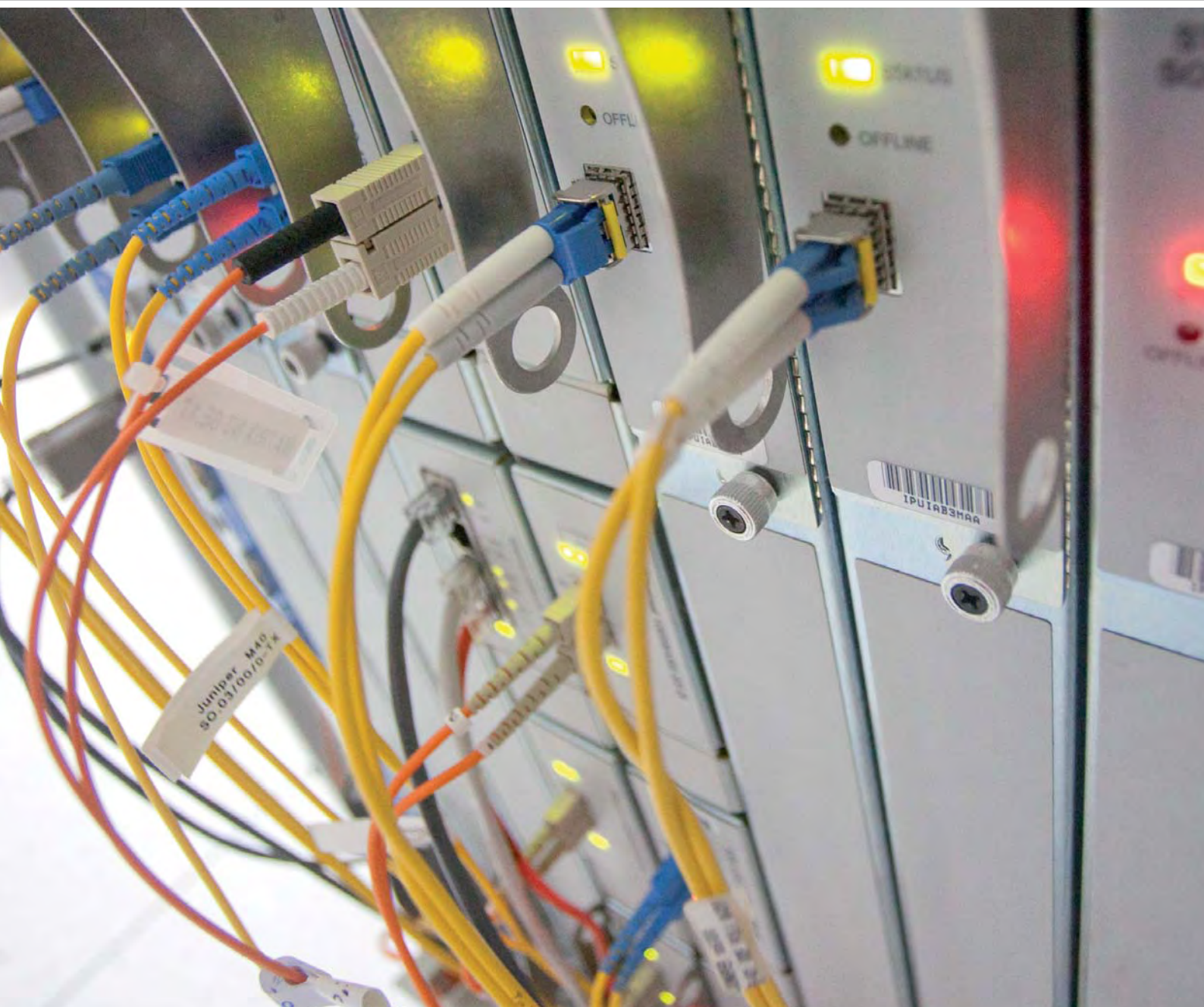
RECETGA is managed by CESGA which is licensed as a Class C Internet Service Provider by the Spanish Telecommunications Authority (CMT).

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.

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)

The University System of Galicia

The 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 2010

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
- SECURITY SERVICES (audits,incident management)
- HOUSING
- VIRTUAL PRIVATE SERVERS

RECETGA TECHNICAL SPECIFICATIONS

BACKBONE NETWORK	Based on Dark Fibre, leased lines, and SDH Radio Links
	Gigabit and ATM Links
	JUNIPER M20, M10 & M10i Gigarouters
	FORE ATM Switches
ACCESS NETWORK	Based on Fibre Optics, SDH Radio Links, and other technologies such as WIFI, WIMAX, etc...
	Up to multiple Gigabit Ethernet as needed
	JUNIPER Gigarouters, FORE, CISCO, and ENTERASYS Switches
NETWORK MANAGEMENT	Developments based on open source software
CONNECTION TO RedIRIS	Five links at 2.5 Gbps
CESGA INTERNAL NETWORK	Gigabit Ethernet, Fast Ethernet, 10 Gigabit Ethernet
	3COM, JUNIPER & ENTERASYS Switches
	DELL, HP & Alcatel Switches
	JUNIPER, ENTERASYS, CISCO Switchrouters

Network Management and Monitoring

The Galician Science and Technology Network offered its services with 99.881% availability.

Main Highlights

A list of the main activities undertaken in 2010 to guarantee the evolution and improvement of the network is presented below.

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 fibre 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 for 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

The RecetgaNova/RedirisNova backbone network was designed.

Dark fibre was deployed with a double coupling among the different PdP´s included in Rediris Nova.

DWM Alcatel 1626LM optical equipment was installed at the Lugo Campus (USC), the Elviña Campus (UDC), the Ourense Campus (Uvigo), and CESGA.

Static pathways were established in order to improve traffic management in case of failures in the main lines.

Alternatives were analysed for the interconnection of nodes pending connection and that are not included in the Rediris Nova backbone network.

4,466 Tbytes exchanged in RECETGA in 2010

Traffic exchanged in RECETGA in Terabytes, 1999 - 2010

4,466 Tbytes

	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010
Tbytes	39	290	414	429	988	1152	1384	1946	2588	3216	3745	4466
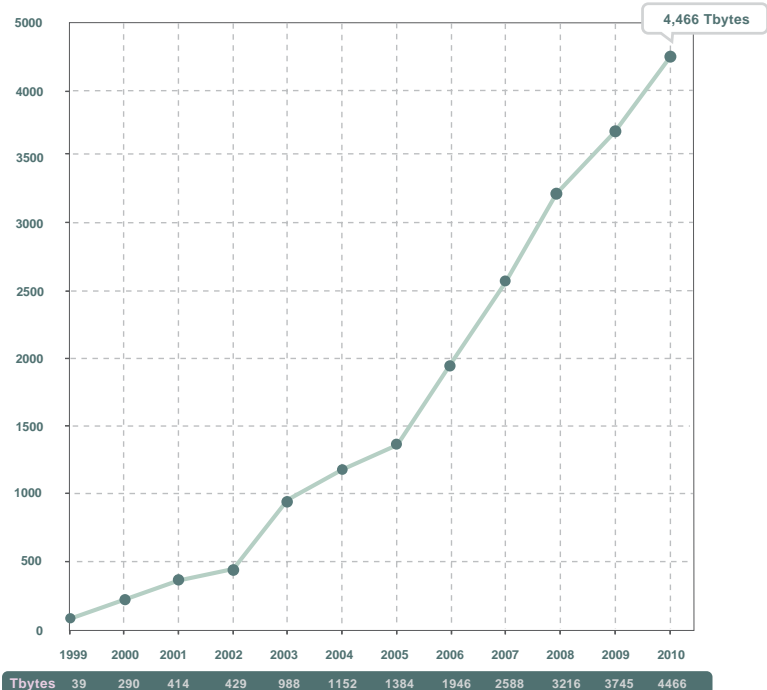
Access Network Highlights

1. The switches backbone was reconfigured after the IFGAE-USC servers were taken off-line. A new VLAN was created to collect them (they now reach us via USC).

2. CISGALICIA changed its access radio link and now uses UDC as transport to the PdP CESGA in UDC.

3. The RAGC (Real Academia Galega das Ciencias), located at the IEGPS site, was connected to the network and given an IP address.

4. Connectivity was provided to CLAG (Cluster Audiovisual Galego) and red Emprendia, both housed at FEUGA.

Dissemination and Conference Activity During 2010

1. Attendance at both GGTT and JJTT, RedIRIS.

2. Presentation: "Massive transfers of information" at GGTT, RedIRIS.

3. CESGA/RECETGA Presentation to the NCOs of the Marín Naval Academy (Escuela Naval Militar de Marín), associated with Vigo University.

RECETGA-RedIris exchanged traffic in Mbps, 2000 - 2010

Max.Outgoing   Max. Incoming   Average Outgoing   Average Incoming
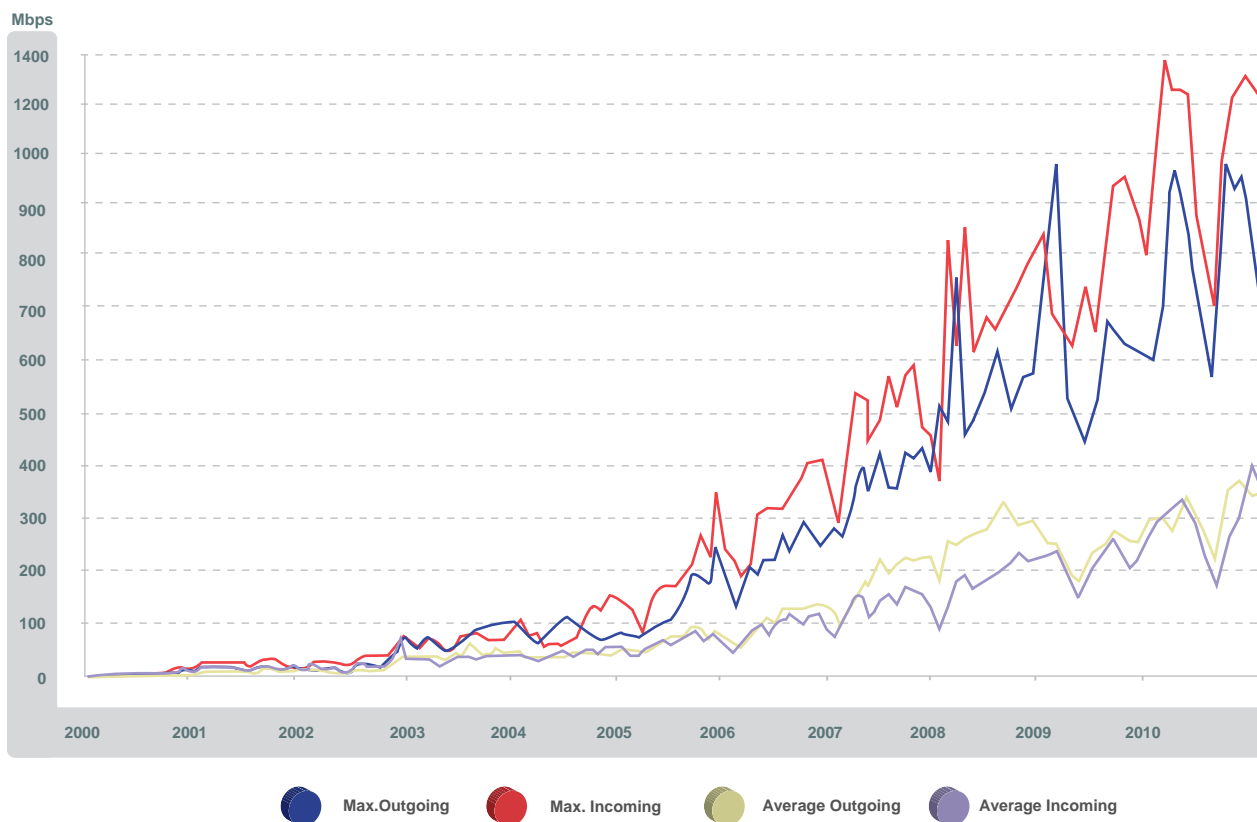
RedIRIS PoP IN GALICIA

EXTERNAL CONNECTIONS THROUGH

Red IRIS

GEANT2

TORGA.net

ESpanix

RECETGA CENTRAL NODE INSTALLED AT CESGA

External Fibre connections

RECETGA/ CESGA (CORE)

RECETGA CES
(circuit emulation)

Internal LAN'S

RECETGA (ATM)

RECETGA/ RETEGAL
(CWDM+RE)
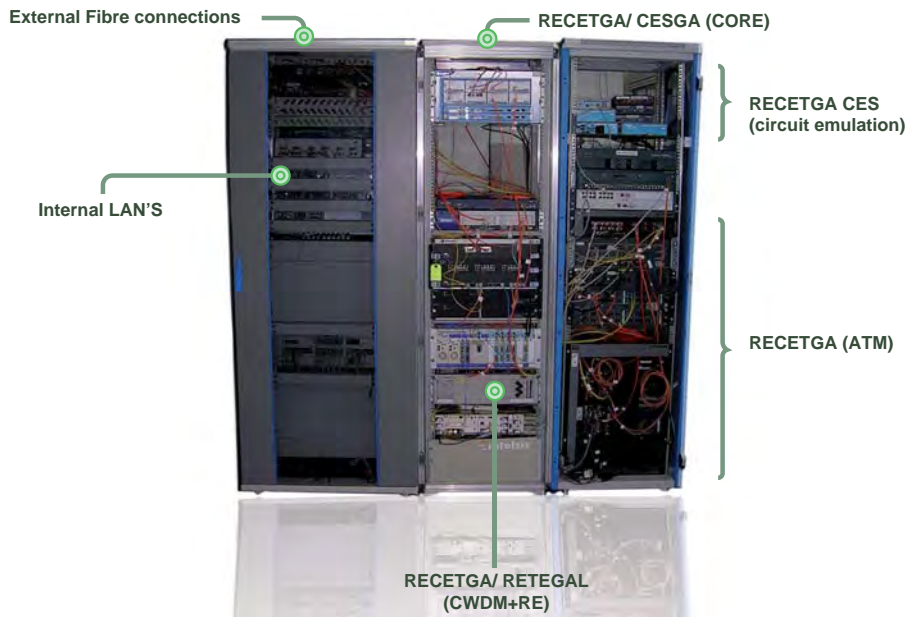
Centres Connected to RECETGA

CENTRE	LINK	AVAILABILITY
Universidade da Coruña (UDC)		
Coruña Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.997%
Ferrol Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.957%
Universidade de Santiago de Compostela (USC)		
Santiago Campus	2 Fibre Optics (1Gbps)	99.948%
Lugo Campus	Fibre Optics (155 Mbps)	99.939%
Universidade de Vigo (UVIGO)		
Vigo Campus	2 Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.989%
Pontevedra Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.99%
Ourense Campus	Fibre Optics (1Gbps) + ATM Radio Link at 155 Mbps	99.994%
Universidade do Minho (UMINHO)	Fibre Optics (155 Mbps)	99.988%
BUGALICIA		
Consorcio de Bibliotecas Universitarias de Galicia	Fibre Optics (155 Mbps)	99.983%
RTD Centres		
ANFACO - CECOPESCA (Vigo)	FastEthernet (100 Mbps)	99.54%
Aula de Produtos Lácteos (USC - Lugo)	Radio Link 4x2 Mbps	99.762%
INIA - Centro de Investigacións Forestais (Lourizán)	ATM Radio Link at 155 Mbps	99.927%
Centro de Investigacións Lingüísticas "Ramón Piñeiro"	ATM Radio Link at 34 Mbps	99.998%
AIMEN - Centro Tecnolóxico Armando Priegue	Radio Link 4x2 Mbps	99.791%
CIAM - Centro de Investigacións Agrarias de Mabegondo	Radio Link 4x2 Mbps	99.152%
Centro de Control de Calidade do Medio Mariño (Vilaxoán)	ATM Radio Link at 155 Mbps	99.85%
Centro de Investigacións Mariñas (Corón)	Radio Link 4x2 Mbps	99.816%
CESGA Centro de Supercomputación de Galicia	1 Fibre Optics (1Gbps)	99.985%
CETMAR - Centro Tecnológico del Mar	Wireless (11/22 Mbps)	97.883%
Centro de Innovación e Servicios (Ferrol)	ATM Radio Link at 155 Mbps + Wireless (11/22 Mbps)	99.851%
FEUGA - Fundación Empresa - Universidade de Galicia (Vigo)	FastEthernet (100 Mbps)	99.989%
FEUGA -Fundación Empresa - Universidade de Galicia (Santiago)	Fibre Optics (1 Gbps)	99.989%
CEIDA (Santa Cruz)	Wireless (11/22 Mbps)	99.978%
Dirección Xeral de I+D+i	Fibre Optics (1 Gbps)	99.998%
CTAG - Centro Tecnológico del Automóvil	Radio Link 4x2 Mbps	99.984%
CMG - Centro Multimedia de Galicia	Fibre Optics (155 Mbps)	99.983%
Hospitals		
CHUS - Complexo Hospitalario Universitario de Santiago de Compostela	Fibre Optics (1 Gbps)	99.992%
CHUVI - Complexo Hospitalario Universitario de Vigo	Radio Link ATM at 155 Mbps	99.686%
CHUC - Complexo Hospitalario Universitario de A Coruña	Fibre Optics (155 Mbps)	99.996%
Unidade de Investigación do Hospital do Meixoeiro	ATM Radio Link at 155 Mbps	99.974%
COG - Centro Oncolóxico de Galicia	Wireless (11/22 Mbps)	99.979%
IEO		
I.E.O - Instituto Español de Oceanografía - A Coruña	Wireless (11/22 Mbps)	99.986%
I.E.O - Instituto Español de Oceanografía - Vigo	ATM Radio Link at 155 Mbps	99.876%
I.E.O - Delegación de Vigo sede Bouzas	WIMAX	99.981%
CSIC		
Misión Biológica de Galicia	Radio Link 4x2 Mbps	98.29%
Instituto de Investigaciones Agrobiológicas de Galicia	Fibre Optics (1 Gbps)	99.998%
Instituto de Investigaciones Marinas	ATM Radio Link at 155 Mbps	99.995%
IEGPS - Instituto de Estudos Galegos "Padre Sarmiento"	FastEthernet (100 Mbps)	99.998%
Delegación Institucional del CSIC en Galicia	2 Fibre Optics (1 Gbps)	99.948%
Other Centres		
Palacio de Exposicións e Congresos de Galicia *	Fibre Optics (155 Mbps)	100%
Parque Tecnolóxico de Galicia	Fibre Optics (155 Mbps)	99.986%
Meteogalicia	Fibre Optics (100 Mbps)	99.992%
Exchange with other Networks		
RedIRIS	5x2.5 Gbps	99.985%
RETEGAL	155 Mbps	99.992%
SERGAS	Fibre Optics (1 Gbps)	99.999%

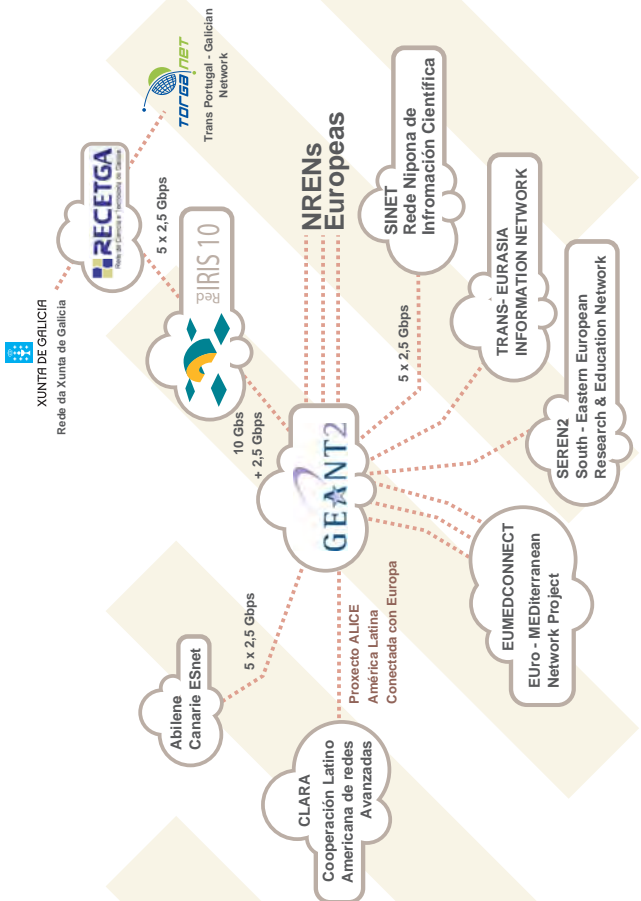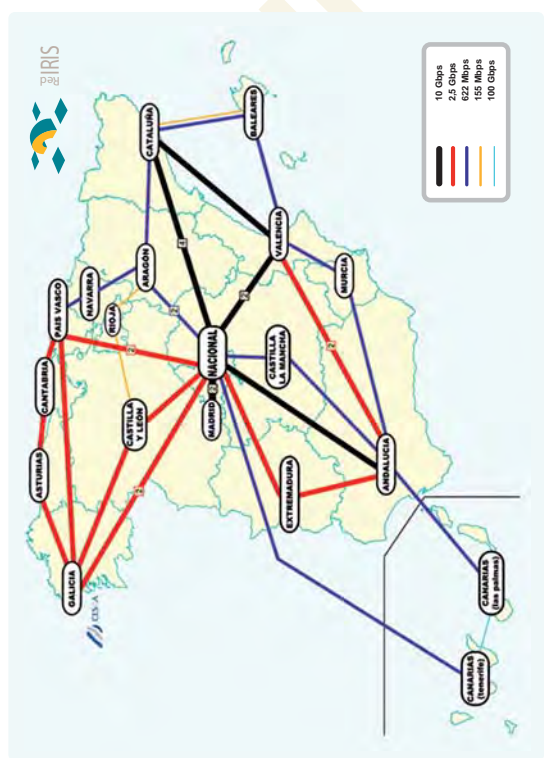* 100% Connectivity provided on demand

RECETGA
Rede de Ciencia e Tecnoloxía de Galicia

Legend:

- Radio Link 4x2 Mbps
- Radio Link ATM a 34 Mbps
- Radio Link ATM a 155 Mbps
- IDSN [64 Mbps]
- Fiber Optics [155 Mbps]
- Fiber Optics [10 Mbps]
- Frame Relay [64 Kbps]
- Frame Relay [256 Kbps]
- Fiber Optics [1 Gbps]
- Fiber Optics [2.5 Gbps]
- Wireless [11/22 Mbps]
- FastEthernet [100 Mbps]

Nodes and connections:

RETEGAL

BUGALICIA
Centro Multimedia de Galicia
Centro Superior Bibliográfico
Santiago Pazo de Congresos e Exposicións

Lugo Aula de Productos Lácteos
Lugo Campus Universitario
LUGO

San Coetano

Ribadeo Centro de Cultivos Mariños
Delegación do CSIC en Galicia
Aguiño Centro de Experimentación en Acuicultura
Leiro Estación de Viticultura e Enoloxía
Hospital Cristal Piñor
Dirección Xeral de Investigación e Desenvolvemento
Santiago Campus Universitario
Instituto de Investigacións Acrobiolóxicas (CSIC)
FEUGA
Complexo Hospitalario Universitario de Santiago
Mabegondo Centro de Investigacións Agrarias
Misión Biolóxica (CSIC)
Novo Seminario de Estudos Galegos
Padre Sarmiento (CSIC)

CESGA

SEEREN
EUMEDCONNECT
ALICE
TEIN2
GEANT
(3x) INTERNET
INTERNET 2
(4x) ESPANIX
IRIS 10

Ourense Campus Universitario — Ourense Parque Tecnolóxico de Galicia
Universidade do Minho
MEDA

Centro Oncológico de Galicia
Santa Cruz CEIDA
Instituto Español de Oceanografía — A Coruña Campus Universitario
CTS Galicia
C. H. Universitario de A Coruña
Ferrol Campus Universitario
BAILADORA

Centro Ramón Piñeiro
PEDROSO

Vigo Campus Universitario
Vigo ANFACO
Vigo FEUGA

Corón Centro de Investigacións Mariñas
Vilaxoán Centro de Control de Acuicultura
XIABRE

Pontevedra Campus Universitario

CTAG
AIMEN
ALOIA
DOMAIO

Centro de Investigacións Forestais de Lourizán
Vigo Hospital Xeral Cies
Vigo Hospital Meixoeiro
Centro de Investigacións Mariñas (CSIC)
Instituto Español de Oceanografía
Vigo CETMAR

Geant Topology

Connection through Regional Networks

Connections through Geant

RedIRIS Topology

ENERGY SAVİNGS AND EFFİCİENCY PLAN
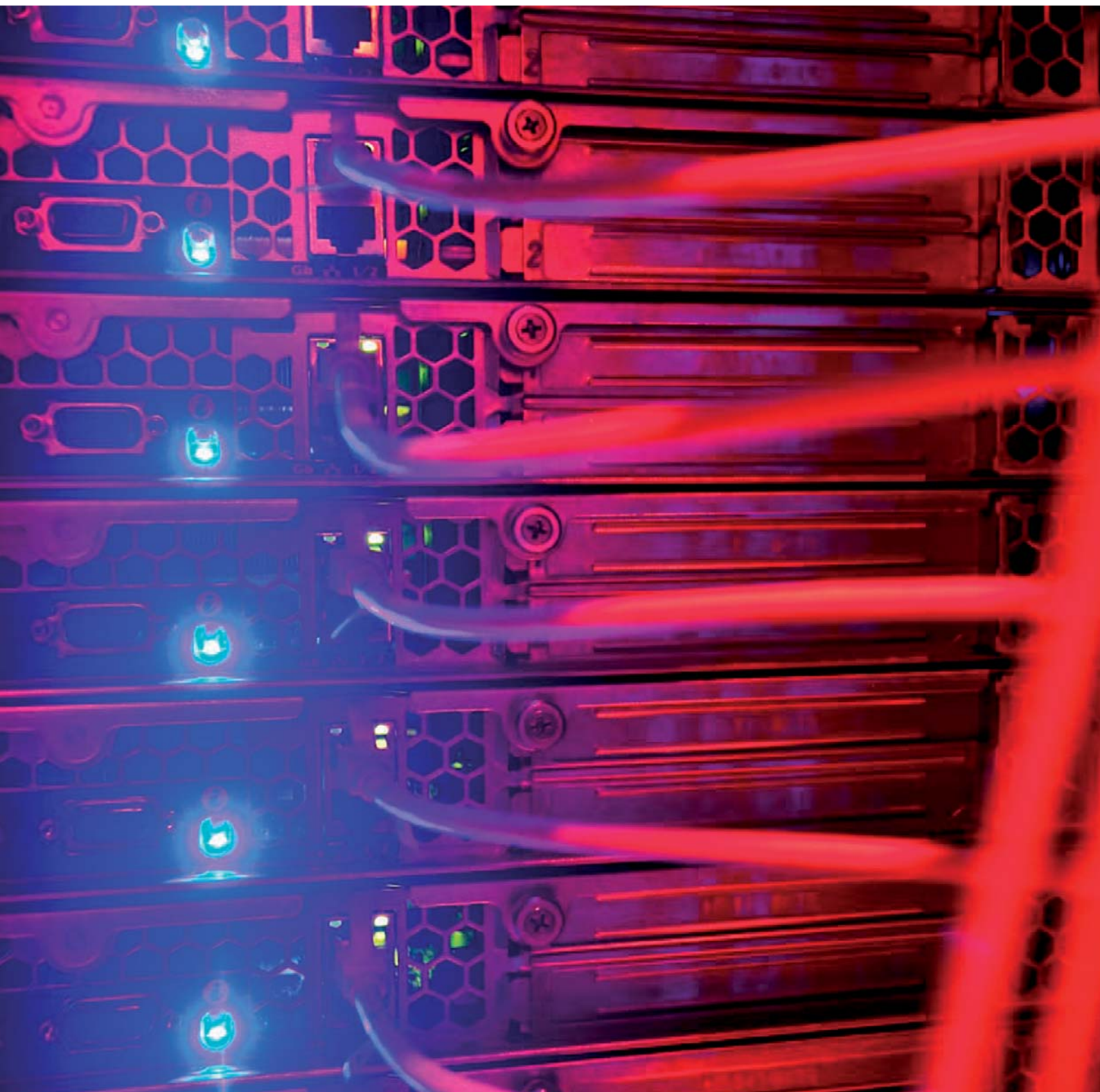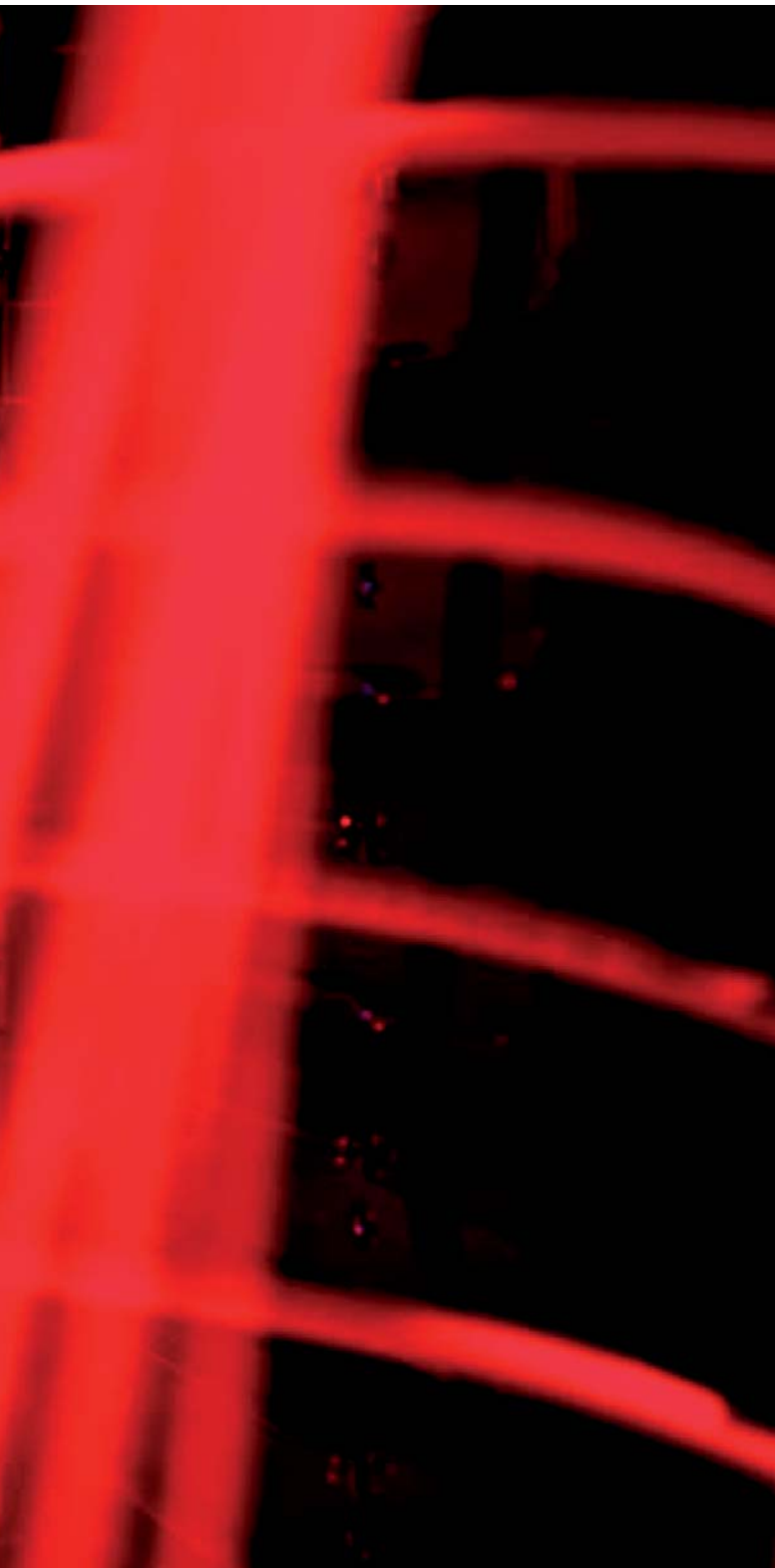
CESGA SUPPORT İNFRASTRUCTURES

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

EQUIPMENT	CHARACTERISTICS
ELECTRICAL SUPPLY	
General Circuit Breaker Board Remodeling	10 New circuit breaker boards (general distribution board, UPS distribution boards, 6 distribution boards in data centre)
Transformers	1-1.600 KVA 2-630 KVA
UPS	2 x 400 KVA 2 x 180 KVA
External Electrical Supply Line	1.5 Mw
Power Generator	1.100 KVA
COOLING	
Chilled Water Plants	2 x 580 Kw
CRAC	8 Units x 120 Kw
DATA CENTER ROOM	
Technical Flooring Surface Area	340 m^2
FIRE SUPPRESSION	
Fire Detection & Extinction System	Based on HFC227 Gas

Energy Savings and Efficiency Plan

Energy efficiency is increasingly more important for a supercomputing centre because electrical consumption (servers, storage, and the network) has skyrocketed. This is demonstrated by the fact that, today, a supercomputing centre such as CESGA has an average consumption greater than 600 KW which implies an elevated cost for electricity. Thus, it is very important to evaluate mechanisms to improve energy efficiency either by reducing usage or by taking better advantage of the required resources which would be of great benefit both economically as well as in terms of the environment.

The basic objective of the Energy Savings and Efficiency Plan is **the improvement of CESGA's energy efficiency to levels that are similar to those of the best supercomputing centres**. Logically, it is not possible to establish a reduction in electrical consumption in the short term with the technologies that now exist. That could imply a decrease in the capacity for technological growth as well as service to the clients of the Centre. For that reason, PUE (Power Usage Effectiveness) is now the agreed measure for energy efficiency for the majority of data processing centres. PUE is a measure of efficiency.

The PUE for the Centre was 1.9 for 2010. According to a recent study by the EPA[*] (U.S. Environmental Protection Agency), the average value for those centres that measure their PUE is 1.924, with a minimum of 1.362 and a maximum of 3.598. Actually, an optimum PUE value in our geographical area is approximately 1.5.

The reduction of our PUE to those values could mean significant savings. For example, with an average annual consumption of 700 KWh (6,132,000Kwh a year), a reduction of 0.1 would mean savings of approximately 45,000€ per year.

Nevertheless, these improvements also involve important investment and, for that reason, a continual multiyear PUE is proposed. Specifically, a 5% annual reduction in the PUE value of the CPD is determined for the 2010-2015 period, with the objective of arriving at values close to 1.5 at the end of 2015.

* http://www.energystar.gov/ia/business/evaluate_performance/ data_center_tech_desc.pdf

PUE Reductions mean Significant Savings

Actions Taken During the Year 2010

Next, some of the actions taken in 2010 related to the reduction of energy consumption are listed below.

The installation of glass panels to separate cold and hot aisles.

The reduction of the number of functioning acclimatisers from 8 to 5. In that manner, 3 are on stand-by and are activated only when necessary.

The development of an integrated management system for monitoring and tracking energy consumption and the support infrastructures, with instant measurement of the PUE as well as the generation of efficiency statistics.

The acquisition of efficient hardware from an energy use perspective.

The deactivation of obsolete hardware (for example, the Beowulf cluster).

The increase in the temperature of the cool aisles from 20º C to 25º C, following ASHRAE recommendations.

The increase of the set point of the water coolers from 10º C to 14º C in order to use free-cooling for a greater number of hours during the year.

Compliance with the norm concerning temperature conditions in public buildings, for example, heating temperatures (21º C in winter) and air conditioning (26º C in summer).

The completion of energy audits and the implementation of recommendations.

The maximum utilisation of free-cooling and heat recuperation technologies.

PROJECTS

Research Projects

The activity in the Projects Area was intense during 2010, with a total of 17 competitive RTD project grant applications submitted. Six were successful and some of them are still pending of approval. Remarkably, two European Commission proposals in the area of e-Infrastructures have been granted, one directly related to the new European infrastructure for distributed computing (EGI-Inspire) and another (EMI, European Middleware Initiative) focused on the new software for it. The Rural Schools proposals, a research project devoted to Cloud enabled e-learning, deserves special mention because it is the first funded by the HPLabs program.

It is also important to highlight the attainment of funding through the Spanish Science & Innovation Ministry's Scientific-Technological Infrastructures Programme (ICTS) which has open access to the FinisTerrae supercomputer to the entire European and Latin American scientific community. Additionally, ICTS funding has allowed CESGA to host 18 research fellow visits in 2010. Also significant is the geographic information systems department participation in an international research project (FAROS).

AREA	PROJECTS		
	2008	2009	2010
Computing	19	19	18
Network Communications	4	3	3
Collaboration Tools & e-Learning	3	9	5
Geographical Information Systems	4	3	3
Technology Transfer & e-Business	4	4	2
Other Grants for Research	4	6	6
TOTAL	**38**	**44**	**37**

GRANT SOURCE	PROJECTS		
	2008	2009	2010
European Commission	10	10	8
Spanish Goverment	7	13	9
Galician Regional Goverment	17	19	17
Industry	4	2	3
TOTAL	**38**	**44**	**37**

Thematic Networks, Tecnological Platforms	19	19	14

37
RTD & Innovation Projects Underway in 2010

COMPUTİNG

EGİ-İnspire

Partners: Over 50 European and international institutions including, for example: CSIC, CESNET, CSC, CNRS, GRNET, NORDUNET, TCD, CERN, LIP, Universiti Putra Malaysia,and the National University of Signapore.
Coordinator: Steven Newhouse, EGI.eu
Principal Researcher: C. Fernández, CESGA
Financing: European Commission: Information Society Technologies Programme
Project Code: INFSO-RI-261323
Budget: 1,352,784€
Period: 2010-14
Objective: The EGI-InSPIRE project will support the transition from a project-based system to a sustainable pan-European e-Infrastructure by supporting 'grids' of high-performance computing (HPC) and high-throughput computing (HTC) resources. EGI-InSPIRE will also be ideally placed to integrate new Distributed Computing Infrastructures (DCIs) such as Clouds, supercomputing networks, and desktop grids in order to benefit the user communities within the European Research Area.

EMİ, European Middleware İnitiative

Partners: Over 20 European and international institutions including, for example: CSIC, STFC, FZJ Juelich, DESY, GRNET, TCD, CERN, CESNET, and CINECA.
Coordinator: Alberto di Meglio, CERN
Principal Researcher: C. Fernández, CESGA
Financing: Avanza I+D
Project Code: INFSO-RI-261611
Budget: 90,000€
Period: 2010-13
Objective: The European Middleware Initiative is a collaboration of the three major middleware providers in Europe (ARC, gLite and UNICORE), and other consortia. EMI aims to deliver a consolidated set of middleware components for deployment in EGI, PRACE and other DCIs; to extend the interoperability between grids and other computing infrastructures; to streng then the reliability of the services; and to establish a sustainable model to maintain and evolve the middleware thereby fulfilling the requirements of the user communities.

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 and with 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.

Optimisation 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/optimise 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 about these hybrid architectures during the project 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: The project is dedicated to the creation of a Cloud based on the resources of the computer labs of Galician universities thereby 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 with the output files and following correct organisation, 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 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 optimisation and their parallelisation. We will use the Cloud Computing infrastructure as a remote computational resource and the platform will be validated by the hospital Radiophysics staff.

Access and improvement of FinisTerrae, a Unique Scientific Technological İnfrastructure (İCTS)

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 (ICTS).
Project Code: ICST-2009-40.
Budget: 434,732€
Period: 2009-2010
Objective: Project objectives include the provision of access to FinisTerrae in open calls such as Science and Technology Infrastructure (ICTS), to improve the FinisTerrae ICTS, and 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.

İmprovement 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: The goal is to improve the usability and productivity of UPC.

Hardware Counters Use to İmprove 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€
Período: 2008-2011
Objective: The goal 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.

MDCAD: A Supercomputing Infrastructure for Medical Imaging advanced services: CAD and Storage

Partners: CESGA, USC, Bahia Software
Coordinator: J.R. Varela, Bahia Software
Principal Researcher: C. Veiga (CESGA)
Financing: Directorate General for Research Development and Innovation (DXIDI), Galician Regional Government (Xunta de Galicia)
Project Code: 10SIN030E
Budget: 89.182,5€
Period: 2009 - 2012
Objective: The goal is to research technical requirements and implementation details of medical imaging advanced services on a supercomputing infrastructure such as Computerized Aided Diagnostics (CAD), storage, and visualisation.

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 across organisations.

İNGENİO MATHEMATİCA (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.

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.

e-LEARNİNG & COLLABORATİON TOOLS

ABC: Learning Based on Competences: İntermediation System Based on the 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 financed by the Director General for RTD of the Galician Government.

Standards-based İntermediation 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.

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: This project provides an intelligent tutor for the production of personalised learning contents adaptable to T-learning and M-learning on MHP and DVB-H.

Application of Pedagogical Competencies and Skills for Teachers – İCTeachers

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.

Rural Schools Virtual Communities for Education in the Cloud – Rural Schools

Partners: CRA Boqueixón-Vedra, Spain, CESGA, Spain
Coordinator: CESGA, Spain
Principal Researcher: M. J. Rodríguez Malmierca, CESGA
Financing: HP Labs
Project Code: None
Budget: 60,619.00€
Period: 2009-2010
Objectives: The aim of the project is to test a Cloud-based solution to provide rich media e-collaborative and learning services to disperse rural school networks.

GIS

TECHNOLOGY TRANSFER & E-BUSINESS

METEO-XIS: Geographical Information System for the 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 organisation, management, and dissemination of meteorological and oceanographic information in Galicia by implementing GIS-components and web services.

IDEPATRI: Design and Development of a Data Model for an Archaeological SDI of the Iron Age in Galicia

Partners: CESGA, Universidad Santiago de Compostela
Principal Researcher: F. Landeira Vega, CESGA
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 for the generation and supply of data from archaeological activities. The coordinated efforts of several research groups will design a platform for the exchange of archaeological geospatial information via the Internet.

FAROS: Integral Networking of Fishing Sector Actors to Organize a Responsible, Optimal, and Sustainable Exploitation of Marine Resources

Partners: IIM CSIC, CESGA, APV Puerto Vigo, CETMAR, IEO, INRB-IPIMAR
Coordinator: Luis Taboada, IIM CSIC
Principal Researcher: Antonio Álvarez Alonso, IIM CSIC
Financing: European Union LIFE+
Project Code: LIFE08 ENV/E/000119
Budget: 1.063.357€
Period: 2010-2012
Objectives: The main objective of the project is the development and implementation of an efficient and integral discard and by-catch management network, implying all actors present in the fishing sector (fleets, ports, auctions, industries, etc.), which aims at both the minimisation of discards/by-catch as well as their optimal evaluation in order to recover and to produce valuable chemicals of interest in the food and pharmaceutical industries.

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, recognised 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.

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 – 2010
Objectives: The project aim is to launch a national communications network for the testing of new services.

OTHER GRANTS FOR RESEARCH

unid-inv-10: Renewal contract for Consolidation and Structure of Competitive Research Units of the Galician İ+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 -30/12/2010
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.

İsabel 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: 2008-2011
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 in order to provide opportunities for the training and consolidation of researchers and technitians that may allow them to have a stable position in the Galician R+D+I system.

İsidro 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 in order to 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.

İsidro Parga Pondal Program 09, Human Resources Partners: CESGA

Partners: CESGA
Coordinator: Beatriz Fernández Domínguez , CESGA
Principal Researcher: Beatriz Fernández Domínguez
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 in order to provide chances for the training and consolidation of researchers and technicians that may allow them to have a stable position in the Galician R+D+I system.

RESEARCH NETWORKS & TECHNOLOGİCAL PLATFORMS IN WHİCH CESGA ACTİVELY PARTİCİPATED İN 2010

CAPAP-H
High Performance Computing Network on heterogeneous parallel architectures

Members: 13 research groups from Spanish Universities and CESGA

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

Financing: Ministerio de Ciencia e Innovacion

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

Objectives: The objectives include the facilitation of the exchange and transfer of knowledge and experiences among the different research groups interested in CAPAP-H in a way that will promote cooperation among them. Another is to assist with the consolidation and dissemination of existing knowledge concerning CAPAP-H. A third objective is to promote the development and use of new techniques and methodologies that make CAPAP-H possible, principally along those lines in which the Partners are researching. Another objective is to optimise and to organise individual efforts in order to identify and reach the most ambitious objectives such as consolidating the community that works in this environment in a way that will augment their specific weight at an international level, in order to later obtain its own identity in the European Research Space. Another goal is to tighten the relations between the participating groups in the network as well as other public and private organisations, national or international, that collaborate in the development of publications, projects, conferences, and seminars.

CyTED-Grid Grid Technology for the İberamerican Project of Science and Technology for Development

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

Coordinator: Francisco Tirado Fernández, Universidad Complutense de Madrid

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

URL: www.cytedgrid.org

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

eBSN
European e-Business Support Network

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

Coordinator: Iordana Eleftheriadou, European Commission

Financing: European Commission

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

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

More concrete objectives are listed below.

Organise meetings of managers in order to adopt decisions in the field of business with the objective of sharing information and discussing the orientation to enlighten strategic policies.

Provide a platform for the coordination of policies among European Union members.

Provide a "one-stop-shop" in order to obtain information about initiatives and regional, national, and European financing possibilities for SMEs.

Organise special meetings of governmental experts as a platform for sharing practical experience and to identify future challenges.

eMOV
Spanish Platform of Wireless Communications

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

Coordinator: Luis Jorge Romero, Telefonica

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

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

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

Red Española de e-Ciencia
Spanish e-Science Network

Members: ACUALSA/UAL, ADE/UJ, ARCO/UNEX, ARCOS/ UC3M, ArTeCS/UCM, ATC/UCBIFI/UNIZAR, BSC, CESCA, CESGA, CeSViMa, CETA-UAA/CIEMAT, CETA-USE/CIEMAT, CFM/CSIC-EHU, CGG/CEIT, CICA, CIEMAT, CNB/CSIC, CNDS/ UPC, DELi/DEUSTO, DIPC/UPV, DPCS/UOC, e-CA, EEC/ UNEX, ESAC-CSG/ESA, ETSF/UPV, Fi2cat, GAC/UDC, GAC/ UMA, GAC/USC, GACSO/UAB, GASDS/UCM, GB/CIPF, GB/ UPVLC, GCC/INTA, GCOC/UPVLC, GEA/UNEX, GFA/UGR, GFAE/USC, GFEAE/UB, GFTAE/UGR, GFTS/FATRONIK, GGC-IFIC/CSIC, GGE/UVEG, GGRID/UPNA, GHPC-CTI/CSIC, GIDS/UPM, GMA/UC, GMI/UPVLC, GMT/UPVLC, GQMA/ UPVLC, GQT/ UPV, GQTC/UVEG, GRTC/US, GRV/EUVE, GRyCAP/UPVLC, GTC/UPVLC, i2BASK, I3A/UNIZAR, IFAE/ UAB, IFCA-GRID/CSIC, IFISC/CSIC, IMDEA-Networks, IMDEA-Software, IRAM/UGR, ISG/UPV, LabGP/IBMCP, LMFC/UPM, LNF/CIEMAT, MICINN, MTC-LABSIS/USC, NEIKER, OEG/ UPM, PIC, PRHLTG/UPVLC, PURG/UVEG, QCyCAR/UCLM, RAAP/UCLM, REBIUN, RedIRIs, RETICS/UCLM, SAVIE/ UPVLC, SBG, SCompBio/CNIO, SDBG/ESI, SGI/IZO/EHU, SPAS/UAH, TIC/CIEMAT
Coordinator: Vicente Hernández García, Universidad Politecnica de Valencia
Financing: Spanish Ministry of Science and Innovation
URL: http://www.e-ciencia.es
Objective: The Spanish e-Science Network is designed to organise, coordinate, and move e-Science forward in Spain, as well as to constitute a tool that is complementary to projects, infrastructure programmes, and other resources within the e-Science environment.

The general objectives are listed below:

> to have an e-Science infrastructure coordinated among different institutions that facilitates user access from different areas of science to supercomputing and GRID infrastructure resources,

> to improve Spanish participation in European e-Science projects,

> to improve scientific excellence by means of access to e-Infrastructures,

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

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

GRİDCHEM
Grid Computing in Chemistry

Members: Research institutions from 18 Europan states.
Coordinator: Hans Peter Luthi, Physical Chemistry Laboratory - ETH Zurich
Financing: COST (European Cooperation in Science and Technology)
URL: http://w3.cost.esf.org/index.php?id=189&action_number=D37
Objectives: One objective is to facilitate the creation and utilisation of distributed computing infrastructures (Grid) in chemistry with the goal of taking chemical computational models and simulations to new frontiers of complexity and to a new time-to-solution regime. This will stimulate innovation in the creation and manipulation of chemical knowledge. The fields of application include traditional chemistry, material science, molecular biology, and environmental chemistry. The presence of chemistry in the network will also have an impact on the development of middleware and the creation and availability of network infrastructures. The final objective is to facilitate and accelerate the transition of researchers to the computational science infrastructure of the XXI century which should, in turn, make European Computational Chemistry much more competitive.

Mathematica Network -
Consulting and Computing of Galicia

Members: 14 research groups in applied mathematics and computing from Galician Universities and Technology Centres.
Coordinator: Wenceslao Gonzalez Manteiga, USC.
Financing: Galician Regional Ministry of Education, Xunta de Galicia
URL: http://mathematica.nodo.cesga.es/content/view/13/27
Objectives: The goal is to promote research and working relationships among members as well as to transfer of math and computing methods and technology to industry and administrations.

İNES
Spanish Technological Platform of Software and Services

Members: 136 Spanish Telecom Companies, Industries, Business Associations, Technology Centres, and Universities.
Coordinator: Santiago Ristol, Atos Origin
Financing: Spanish Ministry of Industry, Tourism, and Commerce
URL: www.ines.org.es
Objectives: The objective is to define a strategic research programme adapted to Spanish necessities and capacities including proposals for unique scientific and technological strategic projects, setting medium and long term goals.

İNSME
İnternational Small and Medium Enterprise Network

Members: Members from 5 continents: governmental bodies, international organisations, international non-profit organisations and representatives of 36 networks and their intermediaries that work in the field of innovation and the transfer of technology to PYMEs.
Coordinator: Paolo Anselmo, Italian Business Angels Network (IBAN)
Financing: OECD. UNIDO.
URL: http://www.insme.org
Objectives: The aim is to create a permanent forum for the promotion and strengthening of multilateral dialogue between stake holders, as follows:

to develop "North-South" interaction and cooperation,

to facilitate knowledge exchange and the arousal of synergies and economies of scale, and

to indirectly support the competitiveness of the SME at local, national, and international levels.

RGB
Galician Bioinformatics Network

Partners: Medicina Genomica-Universidad de Santiago de Compostela, Grupo de Poblaciones Geneticas y Cyto-Genetica-Universidad de Vigo, Grupo de investigacion de Sistemas Complejos-Universidad de Santiago de Compostela, Grupo de Bio-Farmacia- Universidad de Santiago de Compostela, Grupo de MathBioinfo-Universidad de Santiago de Compostela, Grupo de Red de Neuronas Artificiales y Sistemas Adaptativos- Centro de Informatica Medica y Diagnostico Radiologico-Universidad de A Coruna, CESGA.
Coordinator: A. Pazos Sierra, UDC
Financing: Galician Regional Ministry of Education, Xunta de Galicia
URL: http://rgb.cesga.es
Objectives: The RGB is an initiative that has the objective of structuring and integrating research and teaching activities in Bioinformatics that take place in Galicia.

RED-GHPC
Galician High Performance Computing Network

Members: Grupo de Antenas-Universidad de Vigo, Grupo de Arquitectura de Computadores-Universidad de A Coruna, Grupo de Arquitectura de Computadores - Universidad de Santiago de Compostela, Grupo de Fisica de la Atmosfera y el Oceano-Universidad de Vigo, Grupo de Fisica no Lineal- Universidad de Santiago de Compostela, Grupo Integrado de Ingenieria-Universidad de A Coruna, Grupo Laboratorio de Sistemas - Universidad de Santiago de Compostela, Grupo de Metodos Matematicos y Simulacion Numerica en Ingenieria y Ciencias Aplicadas-Universidad de A Coruna, Grupo de Quimica Teorica y Computacional-Universidad de Santiago de Compostela, Grupo de Resolucion Numerica de Ecuaciones en Derivadas Parciales-Universidad de Santiago de Compostela, Centro de Investigacion e Informacion Ambiental (CINAM), and Centro de Supercomputacion de Galicia (CESGA) Coordinator: Ramon Doallo, UDC.
Financing: Galician Regional Ministry of Education, Xunta de Galicia
URL: http://ghpc.udc.es
Objectives: The Galician Thematic Network of High Performance Computing (Red G-HPC) is designed to put in contact and to propitiate collaboration among groups and research centres of the University System of Galicia (USG) and users of HPC technologies (High Performance Computing).

The Red G-HPC network has two fundamental purposes:

1. to promote interdisciplinary research collaboration among groups integrated in the network as well as other research groups or companies that may be interested in research and/or in the development of technologies that require supercomputing or other HPC techniques, and

2. the organisation of training courses, conferences, seminars, or workshops that help to disseminate knowledge concerning HPC technologies.

RETGALİA
Galician Technological Centre Network

Members: 21 technological centres of Galicia
Coordinator: Javier García Tobío, CESGA
Financing: Galician Regional Government, Xunta de Galicia
URL: http://www.retgalia.org
Objective: The aim is to coordinate the Technological Centres that operate in Galicia in a way that all potentialities will be taken advantage of, thereby contributing to the achievement of total quality in the Galician system of innovation. The intention is to also support the development of specific actions for the dissemination of knowledge, information, and promotion of science and technology as well as the offering of services to businesses.

Elearningeuropa.info

Members: European Union e-Learning community and stake holders.
Coordinator: María José Rodríguez Malmierca (CESGA)
Financing: European Commission
URL: http://www.elearningeuropa.info
Objective: The aim is to promote innovation in e-learning throughout a person's lifetime.

İ+dea
Audiovisual İndustry Technology Platform

Members: The Galician Audiovisual Technological Plaform is composed of businesses that are active in strengthening RTD and innovation, universities, technology centres, and other entities committed to technological progress in the audiovisual industry of Galicia, managers of policies and grant programs, and the business associations related with the sector.
Coordinator: Xunta de Galicia / Galician Audiovisual Cluster
Financing: Xunta de Galicia
URL: http://www.idea.org.es/?q=gl/node/121
Objective: The Technological Platform i +dea is an open work forum for the Galician audiovisual industry and research entities and other organisations related to their scientific and technological progress.

The strategic objectives include:

to elaborate a consensual vision of the priorities of the RTD of the sector,

to develop a work program that will stimulate technological advancement in the sector and exploit new business opportunities,

to achieve better collaboration, coherence, and critical mass in RTD activities that are promoted for the sector, and

to insert the strategic objectives of the sector into the organisations and forums of influence regarding RTD material.

GIS

Legend

- Seaportts

Bathymetry GEBCO

DEPTH

— 100
— 101 - 200
— 201 - 500
— 501 - 1000
— 1001 - 2000

ICES_Areas_20051103

ICES

FAROS

Projection: World Mercator

0 100 200 300 400

Km
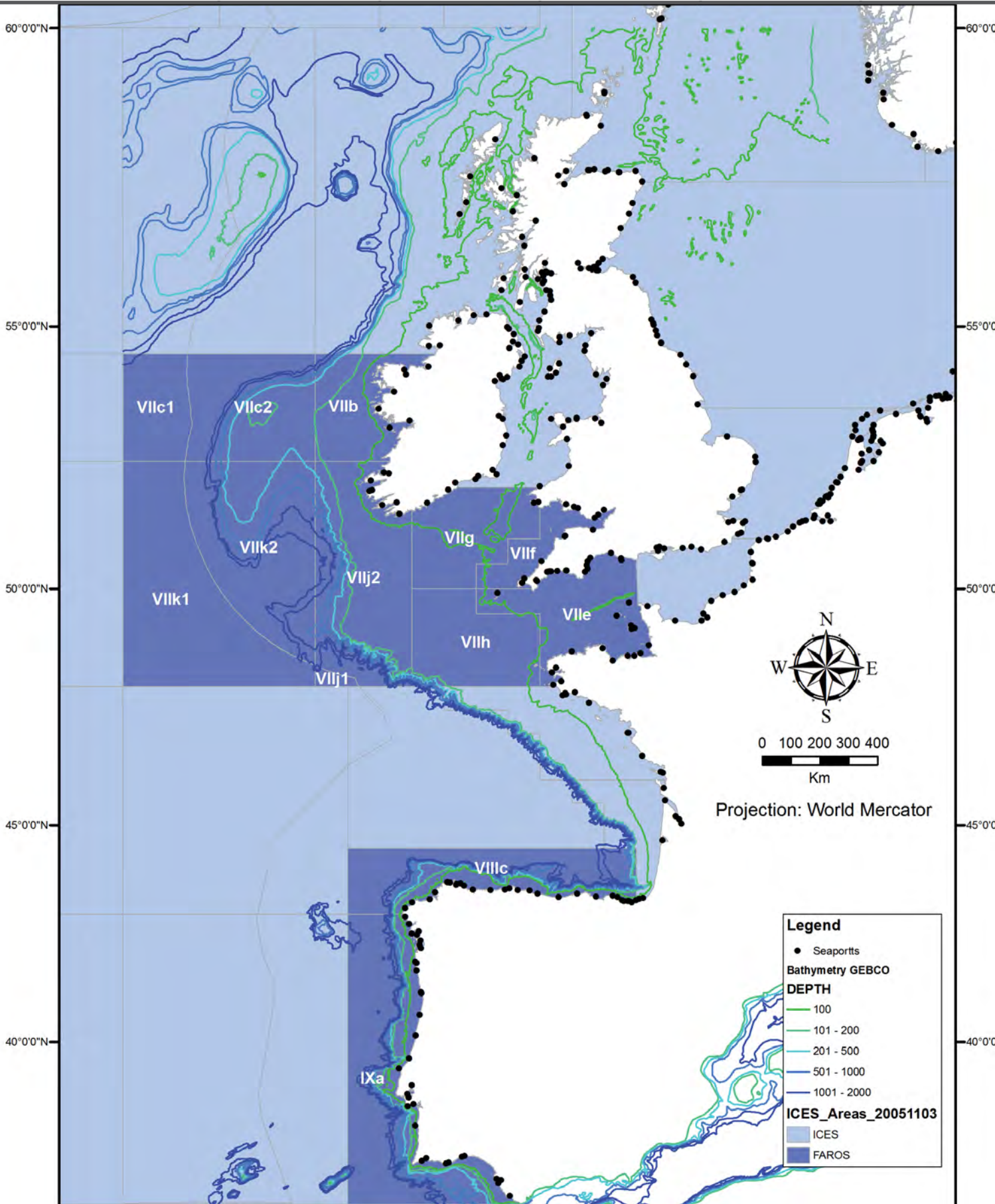
Geographic İnformation Systems

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

Noteworthy Activity in 2010

Projects

METEO-XİS: Geographical İnformation System for Management and Distribution of Meteorological and Oceanographic İnformation of Galicia

This project aims to provide adequate organisation, management, and dissemination of meteorological and oceanographic information in Galicia by implementing GIS-components and web services.

İDEPATRİ: Design and Development of a Date Model for an Archaeological İDE of İron Age in Galicia

This initiative aims to create an operational system for the generation and supply of data from archaeological activities. The coordinated efforts of several research groups will design a platform for the exchange of archaeological geospatial information via the Internet.

FAROS: İntegral Networking of Fishing Sector Actors to Organize a Responsible, Optimal, and Sustainable Exploitation of Marine Resources

The main objective of the project is the development and implementation of an efficient and integral discards and by-catch management network, implying all actors present in the fishing sector (fleets, ports, auctions, industries, etc.), which aims at both the minimisation of discards/by-catch as well as their optimal valorisation to recover and to produce valuable chemicals of interest in the food and pharmaceutical industry

Dissemination activities

Map Server of Surnames of Galicia

The map of Surnames that was developed by the University of Santiago Galician Language Institute (ILGA) on Internet remained operative.

Sueloempresarial.com

The web of industrial parks developed for the Consorcio Zona Franca of Vigo remained operative.

Map of Gas Stations

This web with the distribution of gas stations throughout Galicia was maintained and the gas prices updated weekly.

Training

Teacher Training course of the Regional Ministry of Education, "Possibilities of Networked Geographic Information Systems".

e-LEARNİNG & COLLABORATİON TOOLS

Objectives

Research in the area of e-learning and collaborative applications in different environments, promotion and dissemination of the use of ICT applied to learning and collaboration processes, and

promotion of 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 live collaboration platform (Multiconference webminar).

Hardware for mobile learning and T-learning.

Web 2.0 tools for e-learning information and management.

2010 Activity Highlights

Collaboration in the planning, development, and evaluation of training activities for CESGA personnel and HPC users.

First training course for HPC researchers on e-collaboration tools and Web 2.0 resources.

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 high-level work group concerning Ethics and ICT, organised by the European Commission.

Collaboration with the State 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 Galician universities, primary, and secondary education centres.

Publication of 2 articles in international proceedings.

Participation in three University master courses.

Presentations at 2 international conferences in the ICT and Education sectors.

Participation in **5 e-learning projects** during 2010

Rural Schools Virtual Communities for Education in the Cloud

This is an international research project financed by HP Labs in California along the "Cloud computing and education" line. We are designing, implementing, and evaluating the use of Cloud computing as a means of sharing, learning, and getting the most out of tight IT resources located in a small rural school network.

ICTeacher

There is a pilot course for the European Computer Driving License 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

This is an intelligent tutor that provides and serves perso-nalised training content for television learning experien-ces (t-Learning). This project is financed by the Direc-torate 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 Go-vernment of Galicia.

ABC

The ABC project aims to expand on e-Procura project findings. It targets learning based on competencies and is an intermediation system based on semantic web te-chnologies. It is financed by the Directorate General for RTD&I of the Government of Galicia.

TECHNOLOGY TRANSFER & e-BUSİNESS

During 2010, the e-Business & Transfer area has accomplished the strategic objective of shifting its focus from previous project-based activities to become the CESGA Foundation Transfer Department. While the previous activities of the Department were focused on promoting regional development by means of ITC-based innovation projects for Galician enterprises, now the area has the goal of channeling knowledge transfer of CESGA computational science research as well as encouraging the Centre's relations with industry in these research fields. The Department is also responsible for the quality management related to ISO 9001 activities at CESGA.

As a result of the previous commitment of the Department with international innovation projects in the field of ICT and SMEs, and due to the acquired experience in collaboration with many international institutions, the Department has participated in networks such as the European e-Business Support Network for SMEs (eBSN), the International Network for Small and Medium Sized Enterprises (INSME), and the Forum Euro-Latinoamericano di Torino.

Some of the outputs of the e-Business Department for leveraging regional e-Business in the past years were selected as best practices for capitalisation of EU regional projects in two European Interreg IVC Projects. Some of the activities of these projects were supported by the collaboration of other Galician public authorities including the Regional Government (Xunta de Galicia), the Galician Institute for Economic Promotion (IGAPE), and BIC Galicia, as well as a representation of Galician municipalities.

Highlights

Participation in European innovation projects:

İnterreg İVC - Regional İnitiative Project

Title: Exchange, Valorisation and Transfer of regional best policy measures for SME support on IT and e-business Adoption (EVITA)

Priority: Innovation and the knowledge economy

Theme: Information Society

Type of intervention: Regional Initiative Project

Nine partner regions

İnterreg İVC - Capitalisation Project

Title: Innovation and Change: Network of One Stop Shops Plus (ICHNOS Plus)

Six partner regions

The Department organised an interregional event and seminar for the transfer of results of ICHNOS Plus and EVITA projects. This included presentation of the projects and a seminar on Digital Marketing Techniques for Enttrepreneurs and Businesses. A Coruña, June, 2010.

The e-Business area also organized the following panels within

İCHNOS Plus

activities.

Interregional Experts Transfer Panel on Entrepreneurship and support to SMEs (Vigo, June 2010) with the participation of experts from public authorities and private institutions of Galicia and Portugal.

Interregional Experts Transfer Panel on Entrepreneurship and support to SMEs for Municipalities and Local Authorities (A Coruña, June, 2010) with the participation of experts from Galician municipalities as well as Portuguese institutions.

Participation in the International Conference, "New Ways to Competitiveness 2010 - from European Cooperation to Local Actions" held on May 10-12 in Tartu, Estonia.

Other activities

Evita:

e-Tutor Seminar, Malta, March 2010

Steering committee meeting, Riga, June 2010

Project meeting in Moravske Toplice, October 2010

İCHNOS Plus:

Steering committee May 2010

Final Conference of the project May 2010

Samos interregional seminar June 2010

Developments in the

EVİTA Project

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 recognised 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 training and collaborative techniques and methodologies for reaching SME in remote areas.

In some countries, successful regional policy measures in the field have contributed to the faster improvement of SME access to the Information Society whereas in other regions, especially from the "new" European countries, IT and e-business penetration encounters obstacles related to its growth.

The e-Business and Transfer Department also developed some software pilots for their use by SMEs and other partners of the EVITA Project. A software implementation of Alfresco was developed. This is an OSS content management system which is used as management software for documents, web pages, records, pictures, and collaborative development of content.

The Department Team also provided a software solution for indexing training multimedia content such as videos, carrying out the task of indexing the videos of a seminar held in Malta. The Team linked the main subjects in the Table Of Contents with the corresponding part in the seminar videos (about 12 GB).

The Team also received training from the e-Learning Department and implemented and tested the OpenMeeting platform in other software solutions for collaborative work in order to provide it to other EVITA partners.

EVİTA Project

TRAİNİNG ACTİVİTİES

62
Training Activities in 2010

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 benefited from training activities carried out in 2010. The Annual Training Plan is the keystone around which the organisation of these activities is structured.

During 2010, the Centre participated in the organisation of a total of 62 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.

In 2010, we highlighted the celebration of the second 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	2010
COURSES	16	21	22	16	49	39	42
SESSIONS AND SEMINARS	8	7	8	11	7	16	19
CONFERENCES	1	3	2	1	2	0	1
	25	31	32	28	58	55	62

TRAINING FOR USERS

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
Virtualisation - Cloud - Opennebula	Course	CESGA	18/01/10	26/06/09	13
Publish to impact New forms of scientific publication	Course	CESGA	11/02/10	11/02/10	4
CESGA Computational Science Summer School 2010	Course	CESGA	21/06/10	15/09/10	140
Fortran Programming	Course	CESGA	22/06/10	25/06/10	20
C Programming	Course	CESGA	28/06/10	02/07/10	20
Computational Mathematics: compilation, implementation, and optimization of programs	Course	CESGA	05/07/10	09/07/10	20
Introduction to algorithms for solving scientific applications	Course	CESGA	12/07/10	16/07/10	20
Parallel programming using OpenMP directives	Course	CESGA	20/07/10	23/07/10	20
Introduction to MPI Programming	Course	CESGA	26/07/10	29/07/10	20
Development tools parallel applications: Debugging and performance analysis	Course	CESGA	02/08/10	05/08/10	20
E-collaboration tools for researchers (second edition)	Course	CESGA	09/11/10	10/11/10	5
CESGA HPCN 2010 WORKSHOP	Workshop	CESGA	25/11/10	25/11/10	8
E-Science Courses 2010	Course	E-Ciencia Centres	09/11/10	10/11/10	5

TRAİNİNG FOR CESGA STAFF

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
English Course	Course	Picadilly Academia	01/01/10	31/12/10	56
Strategic Management	Course	Javier Montes	02/01/10	30/12/10	32
Introduction to CISCO Network Technologies	Course	Training Channel	11/01/10	26/01/10	20
Email and Internet	Course	Training Channel	18/01/10	21/01/10	8
Intermediate - Level 1	Course	Training Channel	01/02/10	16/02/10	20
Electronic ID	Course	CESGA	26/03/10	26/03/10	2
Linux Administration I	Course	Training Channel	12/04/10	23/04/10	20
CSS 2.1 Web pages design	Course	Training Channel	03/05/10	18/05/10	20
Linux Administration II	Course	Training Channel	03/05/10	19/05/10	20
Projects Management: Basic Level	Course	CESGA	04/05/10	07/05/10	15
Using the telephone	Course	Training Channel	07/05/10	07/05/10	2
SOA/WOA Course	Course	CESGA	10/05/10	20/05/10	24
Introduction to Apache configuration	Course	Training Channel	11/05/10	11/05/10	2

TRAİNİNG FOR CESGA STAFF

Activity	Type	Responsible Organisation	Start Date	End Date	Hours
Webservices OCG XIS	Course	CESGA	24/05/10	28/05/10	20
Adobe Dreamweaver: web pages design, creation, and maintenance	Course	Training Channel	07/06/10	22/06/10	20
Configuring, managing, and troubleshooting VMware vSphere	Course	Training Channel	27/09/10	08/10/10	20
Office 2007: Dynamic Excel Charts	Course	Training Channel	28/09/10	28/09/10	2
Office 2007: Excel functions	Course	Training Channel	08/10/10	08/10/10	2
e-collaboration tools for researchers	Course	CESGA	03/11/10	04/11/10	5
Advanced workshop in digital video editing with Adobe After Effects CS5	Course	CNTG	22/11/10	03/12/10	40
Photoshop CS5 Course: creation of Animated Gifts	Course	Training Channel	29/11/10	29/11/10	2
Illustrator CS5 3D Objects creation	Course	Training Channel	02/12/10	02/12/10	2
Indesign CS5: Brochure creation	Course	Training Channel	13/12/10	13/12/10	2
Power Point 2007: Presentations	Course	Training Channel	16/12/10	16/12/10	2

Mathematica.nodo.cesga.es Outreach Activities in 2010

Activity	Type	Responsible Organisation	Date
Curso avanzado en Regresión Spline Penalizada y Regresión Geoaditiva utilizando BayesX	Course	USC	08/02/10-12/02/10
Short course on Numerical Simulation in Electromagnetism and Industrial Applications	Course	USC	22/02/10-25/02/10
3rd i-MATH Free/Open Software for Science and Engineering Intensive Course	Course	UDC, UCA, USC, UVIGO, CESGA	12/07/10-23/09/10
Summer School on Mathematical Modelling and Numerical Simulation of the Cardiovascular System	Course	UDC	07/07/10-09/07/10
Mathematical Transfer Course	Course	USC, UDC, UVIGO	13/09/10-04/11/10
i-MATH Consulting for Industry and Public Administration	Industrial Days	USC	08/11/10-10/11/10
VII Applied Math and Industry Interaction Day	Forum	USC	11/06/10
VI Forum of Public Statistics	Forum	UDC	16-09-10
Forum of Statistics in Sports: ED 2010	Forum	UVIGO	15-10-10
Radiotherapy & Mathematics Workshop	Workshop	USC	20/05/10
i-MATH Consulting Workshop: present and future	Workshop	USC	26/05/10-27/05/10
Strategic Data Analysis Workshop	Workshop	USC	29/06/10
V International Workshop on Spatio-Temporal Modelling (METMAV)	Workshop	USC	30/06/10-02/07/10
Numerical Simulation of Building Fires Workshop	Workshop	USC	02/12/10
CESGA Computational Science Summer School 2010	Course	CESGA	21/06/10-15/09/10

İCTS SEMİNARS

Activity	Type	Responsible Organisation
Analysing the application robustness against transient faults	ICTS Seminar	CESGA
Parallel Application Signature for Performance Prediction	ICTS Seminar	CESGA
Dinámica Molecular nos Fosfatos de Zirconio	ICTS Seminar	CESGA
Estudio de la separación de fases cuánticas para transiciones metal-aislante combinando técnicas ab-initio, analíticas y experimento	ICTS Seminar	CESGA
Modelación in silico de Receptores Acoplados a Proteínas G	ICTS Seminar	CESGA
Next Generation Sequencing Analysis on Next Generation computing infrastructure of CESGA	ICTS Seminar	CESGA
CFD para Aerogeneradores	ICTS Seminar	CESGA
Ideales monomiales: algoritmos básicos y descomposiciones	ICTS Seminar	CESGA
Hybrid Method for Optimisation in the Radiotherapy	ICTS Seminar	CESGA
Characterising predictability of extreme convective events through HPC and HydroMeteorology	ICTS Seminar	CESGA

D**I**SSEMINATION

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 publications.

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

Organisation of conferences, workshops, and seminars.

2010 Highlights

Publication of the periodical magazine, "díxitos".

Publication of the 2009 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.

Organisation of the 2010 CESGA High Performance Computing and Networking Workshop.

Participation in the organisation and dissemination of courses, workshops, and seminars for CESGA users.
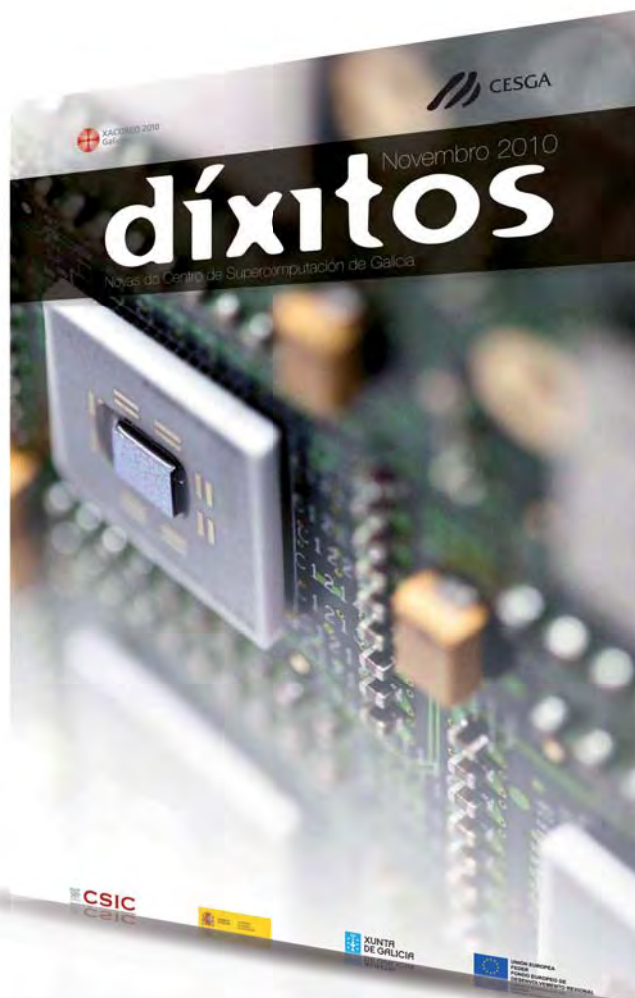
Implementation of CESGA's Communication Plan.

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: EGI-Inspire, EMI, NUBA, RENDER, Formiga-Cloud, EIMRT-II, Gis-Océano, EGEE-III, Smart-LM, i-MATH, Rural Schools, FAROS, and IDEPATRI.

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 and participation with CSIC officials in the Exper-i-Ciencia dissemination activity in 2010.

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

Compilation of users' scientific production data from 2009 and preparation for the collection campaign of the same type of data for 2010.

Support to the Spanish Royal Society of Mathematics (RSME), the International Mathematics Olympics (IMO), the Society of Statistics and Operative Research (SEIO), and the European Courses in Advanced Statistics (ECAS) concerning the hosting of their websites on CESGA servers.

Collaboration regarding the maintenance of CESGA's on-demand video repository for training and dissemination activities, tv.cesga.es.

Production of user training videos for www.cesga.es

Organisation and attention to the 968 visitors from 38 different educational and technological institutions.
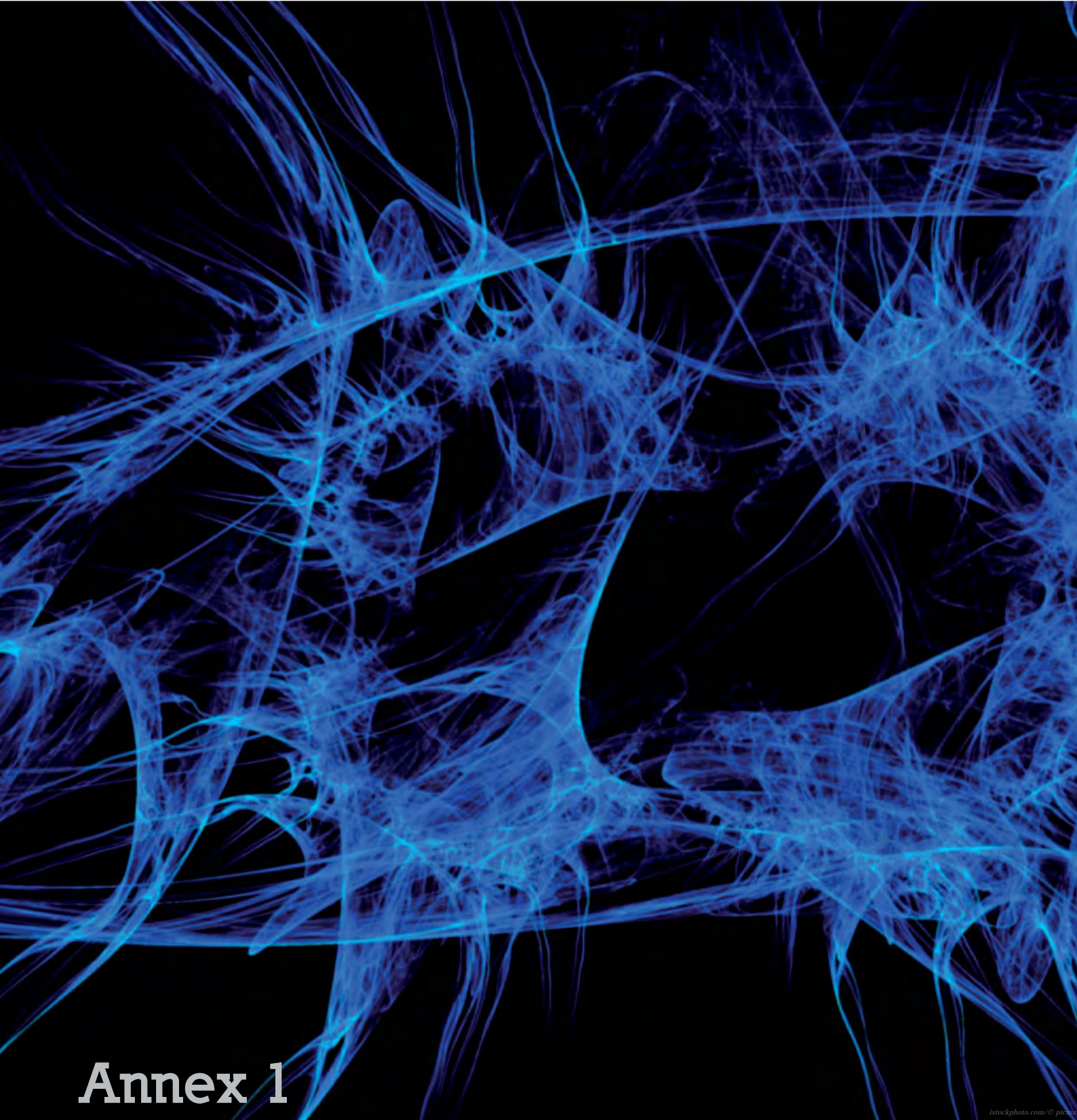
Annex 1

SCiENTiFiC PRODUCTiON

reported by CESGA Users in 2010

CSIC
Consejo Superior de Investigaciones Científicas

SPANİSH NATİONAL RESEARCH COUNCİL (CSİC)

SCİENTİFİC ARTİCLES PUBLİSHED

FOURY-LEYLEKIAN, PASCALE AND POUGET, JEAN-PAUL AND LEE, YOUNG-JOO AND NIEMINEN, RISTO M. AND ORDEJON, PABLO AND CANADELL, ENRIC
Density-wave Instability in alpha-(BEDT-TTF)_2KHg(SCN)_4 Studied by x-ray Diffuse Scattering and by First-principles Calculations
Phys. Rev. B 82 13 134116 Oct 2010 10.1103/PhysRevB.82.134116

MARÍA PILAR DE LARA CASTELLS, PABLO VILLARREAL, GERARDO DELGAD, ALEXANDER O. MITRUSHCHENKOV
Microscopic Description of Small Doped 3He Clusters Through the Full-Configuration-Interaction Nuclear Orbital Approach: The (3He)(N)-Br2(X) Case Revisited
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 2.

H. MANZANO, J. S. DOLADO AND A. AYUELA
Structural, Mechanical and Reactivity Properties of Tricalcium Aluminate Using First-principles Calculations
JOURNAL OF AMERICAN CERAMIC SOCIETY. 4 2009.

H. MANZANO, J. S. DOLADO AND A. AYUELA
Aluminun incorporation to Dreierketten Silicate Chains
JOURNAL OF PHYSICAL CHEMISTRY B 9 2009.

PORRO A, DOLADO JS, GAITERO JJ, ET AL.
"Nanotechnology and Concrete Concepts and Approach"
TRANSPORTATION RESEARCH RECORD 2142 2010.

NOVAES, FREDERICO D. AND RURALI, RICCARDO AND ORDEJÓN, PABLO
Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes
ACS Nano 4 12 7596-7602 2010 10.1021/nn102206n.

H. MANZANO, J. S. DOLADO, A. AYUELA
Elastic properties of the main phases present in Portland cement pastes
ACTA MATERIALIA 5 2009.

ANDRIGHETTO, GIULIA AND VILLATORO, DANIEL AND CONTE, ROSARIA
Norm Internalization in Artificial Societies
AI Communications 23 325-339 2010.

ORTEGA-CASTRO, J. AND HERNANDEZ-HARO, N. AND DOVE, M.T. AND HERNANDEZ-LAGUNA, A. AND SAINZ-DIAZ, C.I.
Density functional theory and Monte Carlo study of octahedral cation ordering of Al/Fe/Mg cations in dioctahedral 2:1 phyllosilicates
American Mineralogist 95 2-3 209-220 2010 10.2138/am.2010.3273.

ORTEGA-CASTRO, J. AND HERNANDEZ-HARO, N. AND TIMON, V. AND SAINZ-DIAZ, C.I. AND HERNANDEZ-LAGUNA, A.
High-pressure Behavior of 2M1 Muscovite
American Mineralogist 95 2-3 249-259 2010 10.2138/am.2010.3035.

ÁLVAREZ, ELEUTERIO AND HERNÁNDEZ, YOHAR A. AND LÓPEZ-SERRANO, JOAQUÍN AND MAYA, CELIA AND PANEQUE, MARGARITA AND PETRONILHO, ANA AND POVEDA, MANUEL L. AND SALAZAR, VERÓNICA AND VATTIER, FLORENCIA AND CARMONA, ERNESTO
Metallacyclic Pyridylidene Structures from Reactions of Terminal Pyridylidenes with Alkenes and Acetylene.
Angewandte Chemie International Edition 49 20 3496-3499 2010 10.1002/anie.201000608.

JORDI FARAUDO, CARLES CALERO AND MARCEL AGUILELLA-ARZO
Ionic Partition and Transport in Multi-Ionic Channels: A Molecular Dynamics Simulation Study of the OmpF Bacterial Porin.
Biophysical Journal 99 7 2107-2115 October 2010 10.1016/j.bpj.2010.07.058.

M.L.SENENT, R. RUIZ, M.VILLA, AND R.DOMÍNGUEZ-GÓMEZ CCSD(T)
Study of the Far-Infrared Spectrum of Ethyl-Methyl-Ether Isotopic Varieties
Chem.Phys.

M.L.SENENT, R.DOMINGUEZ-GOMEZ
Ab initio Characterization of the C_4Si
Chem.Phys.Lett.

DÍAZ, M. DOLORES AND PALOMINO-SCHÄTZLEIN, MARTINA AND CORZANA, FRANCISCO AND ANDREU, CECILIA AND CARBAJO, RODRIGO J. AND DEL OLMO, MARCELLÍ AND CANALES-MAYORDOMO, ANGELES AND PINEDA-LUCENA, ANTONIO AND ASENSIO, GREGORIO AND JIMÉNEZ-BARBERO, JESÚS
Antimicrobial Peptides and Their Superior Fluorinated Analogues: Structure-Activity Relationships as Revealed by NMR Spectroscopy and MD Calculations
ChemBioChem 11 17 2424-2432 2010 10.1002/cbic.201000424

REVUELTA, JULIA AND CORZANA, FRANCISCO AND BASTIDA, AGATHA AND ASENSIO, JUAN LUIS;
The Unusual Nucleotide Recognition Properties of the Resistance Enzyme ANT(4'): Inorganic Tri/Polyphosphate as a Substrate for Aminoglycoside Inactivation
Chemistry - A European Journal 16 29 8635-8640 2010 10.1002/chem.201000641

REVUELTA, JULIA AND VACAS, TATIANA AND CORZANA, FRANCISCO AND GONZALEZ, CARLOS AND BASTIDA, AGATHA AND ASENSIO, JUAN LUIS
Structure-Based Design of Highly Crowded Ribostamycin/Kanamycin Hybrids as a New Family of Antibiotics
Chemistry - A European Journal 16 10 2986-2991 2010 10.1002/chem.200903003

STOUFFER, DANIEL B. AND BASCOMPTE, JORDI
Understanding food-web persistence from local to global scales.
Ecology Letters 13 2 154-161 2010 10.1111/j.1461-0248.2009.01407.x.

BEGOÑA MARTÍNEZ-CRUZ, RENAUD VITALIS, LAURE SÉGUREL, FRÉDÉRIC AUSTERLITZ, MYRIAM GEORGES, SYLVAIN THÉRY, LLUIS QUINTANA-MURCI, TATYANA HEGAY, ALMAZ ALDASHEV, FIRUZA NASYROVA AND EVELYNE HEYER
In the heartland of Eurasia: the multilocus genetic landscape of Central Asian populations
European Journal of Human Genetics 19 216-223 February 2011 doi:10.1038/ejhg.2010.153.

JORDANO, PEDRO
Coevolution in Multispecific Interactions among Free-Living Species.
Evolution: Education and Outreach 3 40-46 2010 10.1007/s12052-009-0197-1

BERENGUER, JESÚS R. AND FERNÁNDEZ, JULIO AND GIL, BELÉN AND LALINDE, ELENA AND SÁNCHEZ, SERGIO
Rhomboidal Heterometallic Alkynyl Based Pt2Cd2 Clusters: Structural, Photophysical, and Theoretical Studies
Inorganic Chemistry 49 9 4232-4244 2010 10.1021/ic100072a

DÍEZ, ALVARO AND FERNÁNDEZ, JULIO AND LALINDE, ELENA AND MORENO, M. TERESA AND SÁNCHEZ, SERGIO;
High-Nuclearity Pt-Tl-Fe Complexes: Structural, Electrochemistry, and Spectroelectrochemistry Studies
Inorganic Chemistry 49 24 11606-11618 2010 10.1021/ic102000s

ADROVER, MIQUEL AND FRAU, JUAN AND CALDÉS, CATALINA AND VILANOVA, BARTOLOMÉ AND DONOSO, JOSEFA AND MUÑOZ, FRANCISCO
Impact of the ionic forms on the UV-Vis spectra 2-hydroxybenzylamine. A TD-DFT study
International Journal of Quantum Chemistry 110 12 2179-2191 2010 10.1002/qua.22696

CASASNOVAS, RODRIGO AND FRAU, JUAN AND ORTEGA-CASTRO, JOAQUÍN AND SALVÀ, ANTONI AND DONOSO, JOSEFA AND MUÑOZ, FRANCISCO
Simplification of the CBS-QB3 method for predicting gas-phase deprotonation free energies
International Journal of Quantum Chemistry 110 2 323-330 2010 10.1002/qua.22170

K. LENGYEL, V. TIMÓN, A. HERNÁNDEZ-LAGUNA, V. SZALAY, L. KOVÁCS
Structure of OH- defects in $LiNbO_3$
IOP Conference Series: Materials Science and Engineering, 012015 1 - 5 2010

A. AGUADO, P. BARRAGÁN, R. PROSMITI, G. DELGADO-BARRIO, P. VILLARREAL AND O. RONCERO
A new accurate and full dimensional potential energy surface of H5+ based on a triatomics-in-molecules analytic functional form.
J. Chem. Phys, 2010

CRISTINA SANZ-SANZ, OCTAVIO RONCERO, RAMON HERNANDEZ-LAMONEDA, JORDAN M. PIO, MOLLY A. TAYLOR AND KENNETH C. JANDA
Communications: A model study on the electronic predissociation of the NeBr_2 van der Waals complex.
J. Chem. Phys. 2010

PATRICIA BARRAGÁN, RITA PROSMITI, OCTAVIO RONCERO, ALFREDO AGUADO, PABLO VILLARREAL AND GERARDO DELGADO-BARRIO
Toward a realisting density functional theory potnetial energy surface for the H5+ cluster.
J. Chem. Phys, 2010

R. PÉREZ DE TDELA, M. MÁRQUEZ-MIJARES, T. GONZÁLEZ-LEZANA, O. RONCERO, S. MIRET-ARTÉS, G. DELGADO-BARRIO AND P. VILLARREAL
A path-integral Monte Carlo study of a small cluster: the Ar trimer
J. Chem. Phys, 2010

ALEZANDRE ZANCHET, TOMÁS GONZÁLEZ-LEZANA, ALFREDO AGUADO, SUSANA GÓMEZ-CARRASCO AND OCTAVIO RONCERO
Non-adiabatic state-to-state reactive collisions among open shell reactants with conical intersections: the OH(^2\Pi) + F(^2P) example
J. Phys. Chem, **A** 2010

ALEXANDRE ZANCHET, ANAÍS DORTA-URRA, ALFREDO AGUADO AND OCTAVIO RONCERO
Uncderstanding Structure, Size and charge effects for the H2 dissociation mechanism on planar gold clusters
J. Phys. Chem, C 2011

N.INOSTROZA AND M.L.SENENT
Ab initio Characterization of the C_3SiH- anion
J.Chem.Phys.

N. INOSTROZA, R.LETELIER AND M.L.SENENT,), (1-3), 40-44 (2010)
On the numerical determination of Dunham's coefficients. An application to $X1\Sigma+HCl$ isotopomers
J.Mol.Struct (TEOCHEM), 1-3

H.MASSÓ AND M.L.SENENT
Ab Initio Characterization of C6
J.Phys.Chem, A

FORTUNA, MIGUEL A. AND STOUFFER, DANIEL B. AND OLESEN, JENS M. AND JORDANO, PEDRO AND MOUILLOT, DAVID AND KRASNOV, BORIS R. AND POULIN, ROBERT AND BASCOMPTE, JORDI
Nestedness versus modularity in ecological networks: two sides of the same coin?
Journal of Animal Ecology, 79 4 811-817 2010 10.1111/j.1365-2656.2010.01688.x

A. AGUADO, P. BARRAG\'AN, R. PROSMITI,G. DELGADO-BARRIO, P. VILLARREAL, AND O. RONCERO
A new accurate and full dimensional potential energy surface of H$_5^+$ based on a triatomics-in-molecules analytical functional form
Journal of Chemical Physics, 024306 1-15 2010

MARÍA PILAR DE LARA-CASTELLS, NÉSTOR F.AGUIRRE, PABLO VILLARREAL, GERARDO DELGADO BARRIO, ALEXANDER MITRUSHCHENKOV
Quantum solvent states and rovibrational spectra of small doped 3He clusters through the full-configuration-interaction nuclear orbital approach: The (3He)(N)-Cl2(X) case (N <-4)
Journal of Chemical Physics, 19

P. BARRAG\'AN, R. PROSMITI, O. RONCERO, A. AGUADO, P. VILLARREAL, AND G. DELGADO-BARRIO
Toward a Realistic DFT Potential Energy Surface for the H$_5^+$ Cluster
Journal of Chemical Physics, 054303 1-10 2010

ALONSO, MERCEDES AND HERRADÓN, BERNARDO
A universal scale of aromaticity for Π-organic compounds
Journal of Computational Chemistry, 31 5 917-928 2010 10.1002/jcc.21377

HENDRICKX, PIETER M. S. AND CORZANA, FRANCISCO AND DEPRAETERE, STEFAAN AND TOURWÉ, DIRK A. AND AUGUSTYNS, KOEN AND MARTINS, JOSÉ C.
The use of time-averaged 3JHH restrained molecular dynamics (tar-MD) simulations for the conformational analysis of five-membered ring systems: Methodology and applications
Journal of Computational Chemistry, 31 3 561-572 2010 10.1002/jcc.21345

D. MUÑOZ-SANTIBURCIO, J. ORTEGA-CASTRO, C. I. SAINZ-DÍAZ, F. J. HUERTAS-PUERTA Y A. HERNÁNDEZ-LAGUNA.
Theoretical estudy of the adsorption of 2-nitro-1-propanol on smectite surface models
Journal of Molecular Structure, (Theochem) 95 - 104 2009

J. ORTEGA-CASTRO, N. HERNÁNDEZ-HARO, D. MUÑOZ-SANTIBURCIO, A. HERNÁNDEZ-LAGUNA Y C. I. SAINZ-DÍAZ
Crystal structure and hydroxyl group vibrational frequencies of phyllosilicates by DFT methods
Journal of Molecular Structure, (Theochem) 82 -87 2009

A. J. MOTA, L. ÁLVAREZ DE CIENFUEGOS, R. ROBLES, E. COLACIO, J. E. PEREA-BUCETA,V. TIMÓN, AND A. HERNÁNDEZ-LAGUNA
Organic catalysis on nucleosidation reactions: A DFT mechanism trough molecular complex models
Journal of Molecular Structure, (Theochem), 43 - 52 2010

E. MOLINA-MONTES, D. DONADIO, A. HERNÁNDEZ-LAGUNA1 , C. I. SAINZ-DÍAZ
Exploring the Rehydroxylation Reaction of Pyrophyllite by means of ab initio Molecular Dynamics
Journal of Physical Chemistry, B 7593 - 7601   2010

ROBERTA POLONI AND JORGE ÍÑIGUEZ AND ALBERTO GARCÍA AND ENRIC CANADELL
An efficient computational method for use in structural studies of crystals with substitutional disorder
Journal of Physics: Condensed Matter, 22 41 415401 2010 10.1088/0953-8984/22/41/415401

LARS ARNSKOV OLSEN AND JAVIER LÓPEZ-SOLANO AND ALBERTO GARCÍA AND TONCI BALIC-ZUNIC AND EMIL MAKOVICKY
Dependence of the lone pair of bismuth on coordination environment and pressure: An ab initio study on Cu4Bi5S10 and Bi_2S_3
Journal of Solid State Chemistry. 183 9 2133 - 2143 2010 10.1016/j.jssc.2010.07.022

CAMPOS, JESÚS AND ESQUEDA, ANA C. AND LÓPEZ-SERRANO, JOAQUÍN AND SÁNCHEZ, LUIS AND COSSIO, FERNANDO P. AND DE COZAR, ABEL AND ALVAREZ, ELEUTERIO AND MAYA, CELIA AND CARMONA, ERNESTO
A Cationic Rh(III) Complex That Efficiently Catalyzes Hydrogen Isotope Exchange in Hydrosilanes
Journal of the American Chemical Society, 132 47 16765-16767 2010 10.1021/ja108521b

VACAS, TATIANA AND CORZANA, FRANCISCO AND JIMÉNEZ-OSÉS, GONZALO AND GONZÁLEZ, CARLOS AND GÓMEZ, ANA M. AND BASTIDA, AGATHA AND REVUELTA, JULIA AND ASENSIO, JUAN LUIS
Role of Aromatic Rings in the Molecular Recognition of Aminoglycoside Antibiotics: Implications for Drug Design
Journal of the American Chemical Society. 132 34 12074-12090 2010 10.1021/ja1046439

SACRISTAN, JAVIER
Investigation of the Crossover From Simple Liquid-Like to a Polymer-Like Behavior of Polyisoprene by Means of MD Simulations
Macromolecular Theory and Simulations 19 7 407-413 2010 10.1002/mats.201000014

J. SACRISTÁN, C. MIJANGOS
Free Volume Analysis and Transport Mechanisms of PVC Modified with Fluorothiophenol Compounds
A Molecular Simulation Study Macromolecules, 17 7357-7367 2010
http://pubs.acs.org/doi/abs/10.1021/ma1011045?prevSearch=%2528sacristan%2529%2BNOT%2B%255Batype%253A%2Bad%255D%2BNOT%2B%255Batype%253A%2Bacs-toc%255D&searchHistoryKey=

M.HOCHLAF, G.CHAMBAUD AND M.L.SENENT
H_2NSi Radical: Structures, Isomerisation Pathways and Electronic States Characterisation
Mol.Phys, 10

JOAN PONS AND IGNACIO RIBERA AND JAUME BERTRAN-PETIT AND MICHAEL BALKE
Nucleotide Substitution Rates for the Full Set of Mitochondrial Protein-Coding Genes in Coleoptera
Molecular Phylogenetics and Evolution. 56 2 796 - 807 2010 10.1016/j.ympev.2010.02.007

A.M. MANCHO, S. WIGGINS, A. TURIEL, E. HERNÁNDEZ-GARCÍA, C. LÓPEZ, E. GARCÍA LADONA
Nonlinear Processes in Oceanic and Atmospheric Flows
Nonlinear Processes in Geophysics, 3 283-285 2010

C. MENDOZA, A.M. MANCHO, M.H. RIO
The Turnstile Mechanism Across the Kuroshio Current: Analysis of Dynamics in Altimeter Velocity Fields
Nonlinear Processes in Geophysics, 2 103-111 2010

CRISTÓBAL, CRISPÍN AND GARCÍA-RUBÍN, SILVIA AND HERNÁNDEZ, YOHAR A. AND LÓPEZ-SERRANO, JOAQUÍN AND PANEQUE, MARGARITA AND POSADAS, CRISTINA M. AND POVEDA, MANUEL L. AND RENDÓN, NURIA AND ALVAREZ, ELEUTERIO
Iridafurans by Coupling of Alkynes and Aldehydes on a $Tp^{Me2I}r$ System. Facile Demethoxycarbonylation of a ß-CO_2Me Substituent
Organometallics, 29 22 5744-5747 2010 10.1021/om1006853

ALONSO, MERCEDES AND HERRADON, BERNARDO
Substituent effects on the aromaticity of carbocyclic five-membered rings
Phys. Chem. Chem. Phys, 12 1305-1317 2010 10.1039/B917343A

GARCIA-VELA, A. AND BANARES, L.
Wave packet calculations on the effect of the femtosecond pulse width in the time-resolved photodissociation of CH_3I in the A-band
Phys. Chem. Chem. Phys. 13 2228-2236 2011 10.1039/c0cp01508c

RAMOS, JAVIER AND CRUZ, VICTOR L. AND MARTINEZ-SALAZAR, JAVIER AND CAMPILLO, NURIA E. AND PAEZ, JUAN A.
Dissimilar interaction of CB1/CB2 with lipid bilayers as revealed by molecular dynamics simulation
Phys. Chem. Chem. Phys. 13 3660-3668 2011 10.1039/C0CP01456G

SCHULLER, A. AND WINTER, H. AND GRAVIELLE, M. S. AND PRUNEDA, J. M. AND MIRAGLIA, J. E.
He-LiF surface interaction potential from fast atom diffraction
Phys. Rev.A, 80 6 062903 Dec 2009 10.1103/ **Phys.Rev. A,** 80.062903

DAUMONT, C. J. M. AND FAROKHIPOOR, S. AND FERRI, A. AND WOJDEL, J. C. AND ÍNIGUEZ, JORGE AND KOOI, B. J. AND NOHEDA, B.
Tuning the atomic and domain structure of epitaxial films of multiferroic BiFeO$_3$
Phys. Rev. B, 81 14 144115 Apr 2010 10.1103/PhysRevB.81.144115.

GAUYACQ, JEAN-PIERRE AND NOVAES, FREDERICO D. AND LORENTE, NICOLAS
Magnetic transitions induced by tunneling electrons in individual adsorbed M-phthalocyanine molecules (M=Fe and Co)
Phys. Rev. B, 81 16 165423 Apr 2010 10.1103/PhysRevB.81.165423, Article-Number = 165423

NOVAES, FREDERICO D. AND LORENTE, NICOLÁS AND GAUYACQ, JEAN-PIERRE
Quenching of magnetic excitations in single adsorbates at surfaces: Mn on CuN/Cu(100)
Phys. Rev. B, 82 15 155401 Oct 2010 10.1103/PhysRevB.82.155401, Article-Number = 155401

WITEK, HELVI AND CARDOSO, VITOR AND HERDEIRO, CARLOS AND NEROZZI, ANDREA AND SPERHAKE, ULRICH AND ZILHAO, MIGUEL
Black holes in a box: Toward the numerical evolution of black holes in AdS space-times
Phys. Rev. D, 82 10 104037 Nov 2010 10.1103/PhysRevD.82.104037

WITEK, HELVI AND ZILH~AO, MIGUEL AND GUALTIERI, LEONARDO AND CARDOSO, VITOR AND HERDEIRO, CARLOS AND NEROZZI, ANDREA AND SPERHAKE, ULRICH
Numerical relativity for D dimensional space-times: Head-on collisions of black holes and gravitational wave extraction
Phys. Rev. D, 82 10 104014 Nov 2010 10.1103/PhysRevD.82.104014

DELIA FERNÁNDEZ-TORRE, TRISTAN ALBARET, ALESSANDRO DE VITA
Role of Surface Reconstructions in (111) Silicon Fracture
Phys. Rev. Lett. 185502 2010

WOJDEL, JACEK C. AND ÍÑIGUEZ, JORGE
Ab Initio Indications for Giant Magnetoelectric Effects Driven by Structural Softness
Phys. Rev. Lett, 105 3 037208 Jul 2010 10.1103/PhysRevLett, 105.037208

NADIA SANCHEZ, SILVIA GALLEGO, J. CERDÁ, M.CARMEN MUÑOZ
Tuning Surface Metallicity and Ferromagnetism by H Adsorption in the Polar ZnO(0001) Surface
Physical Review B, 115301 2010

SILVIA GALLEGO, NADIA SANCHEZ, SOFIA MARTIN, M. CARMEN MUÑOZ, LASZLO SZUNYOGH
Reversible Enhancement of the Magnetism of Ultrathin Co Films by H Adsorption
Physical Review B, 085414 2010.

WITEK, HELVI AND CARDOSO, VITOR AND GUALTIERI, LEONARDO AND HERDEIRO, CARLOS AND SPERHAKE, ULRICH, AND OTHERS
Head-on Collisions of Unequal Mass Black Holes in D=5 Dimensions
Physical Review D

C. MENDOZA, A.M. MANCHO
Hidden Geometry of Ocean Flows
Physical Review Letters, 3 038501 2010

JOMAA, AHMAD AND STEWART, GEORDIE AND MARTÍN-BENITO, JAIME AND ZIELKE, RYSZARD AND CAMPBELL, TRACEY L. AND MADDOCK, JANINE R. AND BROWN, ERIC D. AND ORTEGA, JOAQUIN
Understanding Ribosome Assembly: The Structure of in Vivo Assembled Immature 30S Subunits Revealed by Cryo-Electron Microscopy
RNA, 10.1261/rna.2509811

AGUILELLA-ARZO, MARCEL AND CALERO, CARLES AND FARAUDO, JORDI
Simulation of Electrokinetics at the Nanoscale: Inversion of Selectivity in a Bio-nanochannel
Soft Matter, 6 6079-6082 2010 10.1039/c0sm00904k

CARLES CALERO AND JORDI FARAUDO
The Interaction Between Electrolyte and Surfaces Decorated with Charged Groups: A Molecular Dynamics Simulation Study
The Journal of Chemical Physics, 132 2 024704 2010 10.1063/1.3289726

MARÍA PILAR DE LARA-CASTELLS, NÉSTOR F. AGUIRRE, PABLO VILLARREAL, GERARDO DELGADO BARRIO AND ALEXANDER O. MITRUSHCHENKOV
Quantum Solvent States And Rovibrational Spectra of Small Doped 3He Clusters Through the Full-Configuration-Interaction Nuclear Orbital Approach: The (3He)N-Cl2(X) Case (N<=4)
The Journal of Chemical Physics, 2010

MARÍA PILAR DE LARA-CASTELLS,,A NÉSTOR F. AGUIRRE, PABLO VILLARREAL, GERARDO DELGADO BARRIO, AND ALEXANDER O. MITRUSHCHENKOV
Quantum Solvent States and Rovibrational Spectra of Small Doped 3He Clusters Through the Full-Configuration-Interaction Nuclear Orbital Approach: The (3He)N-Cl2(X) Case (N<= 4)
THE JOURNAL OF CHEMICAL PHYSICS, 132, 194313 2010

A. AGUADO, P. BARRAGÁN, R. PROSMITI, G. DELGADO-BARRIO, P. VILLARREAL AND O. RONCERO
A New Accurate and Full Dimensional Potential Energy Surface of H5+ Based on a Triatomics-in-Molecules Analytic Functional Form
THE JOURNAL OF CHEMICAL PHYSICS, 132, 244303 2010

R. PÉREZ DE TUDELA, M. MÁRQUEZ-MIJARES, T. GONZÁLEZ-LEZANA, O. RONCERO, S. MIRET-ARTÉS, G. DELGADO-BARRIO, AND P. VILLARREAL
A Path-Integral Monte Carlo Study of a Small Cluster: The Ar Trimer
THE JOURNAL OF CHEMICAL PHYSICS, 132, 244303 2010

PATRICIA BARRAGÁN, RITA PROSMITI, OCTAVIO RONCERO, ALFREDO AGUADO, PABLO VILLARREAL, AND GERARDO DELGADO-BARRIO
Toward a Realistic Density Functional Theory Potential Energy Surface for the H5+ Cluster
THE JOURNAL OF CHEMICAL PHYSICS, 133, 054303 2010

ALONSO, MERCEDES AND CHICHARRO, ROBERTO AND MIRANDA, CARLOS AND ARÁN, VICENTE J. AND MAESTRO, MIGUEL A. AND HERRADÓN, BERNARDO
X-ray Diffraction, Solution Structure, and Computational Studies on Derivatives of (3-sec-Butyl-2,3-dihydro-1H-iso-quinolin-4-ylidene)acetic Acid: Compounds with Activity as Calpain Inhibitors
The Journal of Organic Chemistry, 75 2 342-352 2010 10.1021/jo902091u

OTÓN, FRANCISCO AND PFATTNER, RAPHAEL AND OXTOBY, NEIL S. AND MAS-TORRENT, MARTA AND WURST, KLAUS AND FONTRODONA, XAVIER AND OL-IVIER, YOANN AND CORNIL, JÉROME AND VECIANA, JAUME AND ROVIRA, CONCEPCIÓ
Benzodicarbomethoxytetrathiafulvalene Derivatives as Soluble Organic Semiconductors
The Journal of Organic Chemistry, 76 1 154-163 2011 10.1021/jo101817j

WANG, HAO AND MICHALAK, KAROL AND MICHALAK, MICHALAK, K. AND JIMÉnEZ-OSÉS, GONZALO AND WICHA, J. AND HOUK, K. N.
Steric Control of α- and β-Alkylation of Azulenone Interme-diates in a Guanacastepene A Synthesis
The Journal of Organic Chemistry, 75 3 762-766 2010 10.1021/jo902283a

GONZALEZ, JAVIER AND ANGLADA, JOSEP M.
Gas Phase Reaction of Nitric Acid with Hydroxyl Radical without and with Water. A Theoretical Investigation
The Journal of Physical Chemistry A, 114 34 9151-9162 2010 10.1021/jp102935d

ZOPPI, LAURA AND GARCIA, ALBERTO AND BALD-RIDGE, KIM K.
Theoretical Investigation of the Binding Process of Coran-nulene on a Cu(111) Surface+
The Journal of Physical Chemistry A, 114 33 8864-8872 2010 10.1021/jp102662t

SOLÍS-CALERO, CHRISTIAN AND ORTEGA-CASTRO, JOAQUÍN AND MUÑOZ, FRANCISCO
Reactivity of a Phospholipid Monolayer Model under Pe-riodic Boundary Conditions: A Density Functional Theory Study of the Schiff Base Formation between Phosphati-dylethanolamine and Acetaldehyde
The Journal of Physical Chemistry B, 114 48 15879-15885 2010 10.1021/jp1088367

ROMERO-GÓMEZ, P. AND HAMAD, SAID AND GONZÁLEZ, J. C. AND BARRANCO, A. AND ESPINÓS, J. P. AND COTRINO, J. AND GONZÁLEZ-ELIPE, A. R.
Band Gap Narrowing versus Formation of Electronic States in the Gap in N-TiO$_2$ Thin Films
The Journal of Physical Chemistry C, 114 51 22546-22557 2010 10.1021/jp104634j

SANZ-NAVARRO, CARLOS AND GRIMA, ROGELI AND GARCÍA, ALBERTO AND BEA, EDGAR AND SOBA, ALE-JANDRO AND CELA, JOSÉ AND ORDEJÓN, PABLO
An Efficient Implementation of a Qm-Mm Method in Siesta Theoretical Chemistry Accounts: Theory
Computation, and Modeling (Theoretica Chimica Acta), 1-9 2010 10.1007/s00214-010-0816-5

SCİENTİFİC ARTİCLES İN-PRESS

M. P. DE LARA-CASTELLS1, N. F. AGUIRRE, G. DEL-GADO-BARRIO, P. VILLARREAL AND A. O. MITRUSH-CHENKOV
A Full-Configuration-Interaction Nuclear Orbital approach and application for small doped He clusters
AIP (American Institute of Physics) Conference Proceedings, 2011

R. PÉREZ DE TUDELA, D. LÓPEZ-DURÁN, M.P. DE LARA-CASTELLS, R. PROSMITI, O. RONCERO, G. DEL-GADO-BARRIO, F.A. GIANTURCO, J. JELLINEK AND P. VILLARREAL
A Quantum Chemistry Approach to Energies, Structures, and Spectroscopy of Doped Helium Clusters
American Institute of Physics, Advances in Computational Science, Lectures presented at the International Conference on Computational Methods in Sciences and Engineering 2009 (ICCMSE 2009) 2010

J.CERNICHARO, A.SPIEFIELDEL, C.BALANÇA, F.DAYOU, M.L.SENENT, N.FEAUTRIER, A.FAURE, L.CRESSIOT-VINCENT AND L.WIESENFELD AND J.R.PARDO
Collisional Excitation of So_2 in Cold Molecular Clouds
Astron&Astrophys

VIRGINIA ROLDÓS, JAVIER CAÑADA, JESÚS JIMÉNEZ-BARBERO
Carbohydrate-Protein Interactions. A 3D view by NMR
ChemBioChem, 2011

VICENÇ TORRA, GUILLERMO NAVARRO-ARRIBAS AND DANIEL ABRIL
Supervised Learning for Record Linkage through Weighted Means and OWA Operators
Control and Cybernetics, 4 2010

EDUARDO J. FERNÁNDEZ, ANTONIO LAGUNA, JOSÉ M. LÓPEZ-DE-LUZURIAGA, MIGUEL MONGE* EVA SÁNCHEZ-FORCADA
Different Phosphorescent Excited States of Tetra- and Octanuclear Dendritic-Like Phosphine Gold(I) Thiolate Complexes: Photophysical and Theoretical Studies
Dalton Trans, 2011

MARIA A. MORANDO,+[A] ALESSANDRA NURISSO,+[B] NATHALIE GRENOUILLAT,[C] BORIS VAUZEILLES,[C] JEAN-MARIE BEAU,[C] F. JAVIER CAÑADA,[A] JESUS JIMÉNEZ-BARBERO,*[A] AND ANNE IMBERTY*[B]
NMR and Molecular Modelling Reveal Key Structural Features of Synthetic Nodulation Factors
Glycobiology, 2011

M. CARMEN MUÑOZ, SILVIA GALLEGO, NADIA SANCHEZ
Surface Ferromagnetism in Non-Magnetic and Dilute Magnetic Oxides
J. Phys.: Conference Series, 2011

JORGE S. DOLADO, FREDERIK HEBER, JAN HAMAEK-ERS AND MICHAEL GRIEBEL
The Nano-branched structure of Cementitious C-S-H gel
JOURNAL OF MATERIALS CHEMISTRY, DOI:10.1039/C0JM04185H, 2011

J.RAMOS, J. MARTÍNEZ-SALAZAR
Computer Modeling of the Crystallization Process of Single-Chain Ethylene/1-Hexene Copolymers from Dilute Solutions
Journal of Polymer Science: Part B: Polymer Physics, 2011

CARLES CALERO, JORDI FARAUDO, MARCEL AGUILELLA-ARZO
Molecular Dynamics Simulations of Concentrated Aqueous Electrolyte Solutions
Molecular Simulation, 2011
http://arxiv.org/abs/1005.2857

LUIS P. CALLE, F. J. CAÑADA, J. JIMÉNEZ-BARBERO
Application of Nmr Methods to the Study of the Interaction of Natural Products with Biomolecular Receptors
Natural Products Reports

L. RUBIO-LAGO, J.D. RODRÍGUEZ, A. GARCÍA-VELA, M.G. GONZÁLEZ Y L. BAÑARES
A Slice Imaging and Multisurface Wave Packet Study of the Photodissociation of Ch_3i At 304 nm
Phys. Chem. Chem. Phys, 2011

DAVID LÓPEZ-DURÁN, RICARDO PÉREZ DE TUDELA, ROCÍO RODRÍGUEZ-CANTANO, TOMÁS GONZÁLEZ-LEZANA, MARÍA PILAR DE LARA-CASTELLS, GERARDO DELGADO-BARRIO Y PABLO VILLARREAL
Diffusion Monte Carlo Energies and Geometric Properties of Cs_2-($_4He$)N Clusters: An Example of Weak Dopant-Helium Interaction
PHYSICA SCRIPTA, 2011

SPERHAKE, ULRICH AND BERTI, EMANUELE AND CARDOSO, VITOR AND PRETORIUS, FRANS AND YUNES, NICOLAS
Superkicks in Ultrarelativistic Encounters of Spinning Black Holes
Physical Review D, 2011

CARLES CALERO, JORDI FARAUDO, MARCEL AGUILELLA-ARZO
A First Passage Time Analysis of Atomic-Resolution Simulations of the Ionic Transport in a Bacterial Porin
Physical Review E, 2011
http://arxiv.org/abs/1011.3952

JORDI S. ANDREU, JUAN CAMACHO AND JORDI FARAUDO
Aggregation Of Superparamagnetic Colloids in Magnetic Fields: The Quest for the Equilibrium State
Soft Matter, 2010

AYALA, REGLA AND SPEZIA, RICCARDO AND VUIL-LEUMIER, RODOLPHE AND MARTÍNEZ, JOSÉ MANUEL AND PAPPALARDO, RAFAEL R. AND SÁNCHEZ MARCOS, ENRIQUE
An Ab Initio Molecular Dynamics Study on the Hydrolysis of the Po(IV) Aquaion in Water
The Journal of Physical Chemistry B, 114 40 12866-12874 2010 10.1021/jp1010956

PRESENTARÍONS AT CONGRESSES / CONFERENCES

A. GARCÍA-VELA
Full Dimensional Wave Packet Study of the Cl_2-He_2 Vibrational Predissociation Dynamics
ECAMP X, European Conference on Atoms, Molecules, and Photons, Salamanca (Spain), July 4-9, 2010

A. GARCÍA-VELA
Full Dimensional Wave Packet Study of the Cl_2-He_2 Vibrational Predissociation Dynamics
MOLEC XVIII, European Conference on Dynamics of Molecular Collisions, Curia (Portugal), September 5-10, 2010

A. GARCÍA-VELA AND L. BAÑARES
Wave Packet Calculations on the Effect of the Femtosecond Pulse width in the Time-Resolved Photodissociation of Ch_3i in the A-band
MOLEC XVIII, European Conference on Dynamics of Molecular Collisions, Curia (Portugal), September 5-10, 2010

CANIZARES, PRISCILLA AND SOPUERTA, CARLOS F.
An Efficient Time-Domain Method to Model Extreme-Mass-Ratio Inspirals
8th International LISA Symposium, Stanford, June 28 - July 2, 2010

DANIEL VILLATORO AND GIULIA ANDRIGHETTO AND ROSARIA CONTE AND JORDI SABATER-MIR
Simulating the Relative Effects of Punishment and Sanction in the Achievement of Cooperation
Eighth European Workshop on Multi-Agent Systems (EUMAS08), 2010

E. ESCAMILLA ROA, V. TIMÓN Y A. HERNÁNDEZ-LAGUNA
Absorción de Ni sobre la superficie (001) de Anatasa
Chitel 2010. **Anglet,** France 9, 2010

F. CORZANA, J. H. BUSTO, M. GARCÍA DE LUIS, F. MARCELO, J. L. ASENSIO, J. JIMÉNEZ-BARBERO, A. AVENOZA, J. M. PEREGRINA
Mucin-like Glycopeptides: Effect of the Peptide Backbone Conformation on Molecular Recognition
The 25th International Carbohydarte Simposium, (ICS 2010).

J. DURÁ, R. DE NALDA, A. GARCÍA-VELA, AND L. BAÑARES
Femtosecond Velocity Map Imaging Experiments and Wave Packet Calculations of CH_3I Photodissociation in the A band
I International Meeting on Atomic and Molecular Physics and Chemistry, IMAMPC IMadrid (Spain), June 29-July 2, 2010

J. DURÁ, R. DE NALDA, A. GARCÍA-VELA, AND L. BAÑARES
Femtosecond Velocity Map Imaging Experiments and Wave Packet Calculations of CH_3I Photodissociation in the A band
ECAMP X, European Conference on Atoms, Molecules, and Photons, Salamanca (Spain), July 4-9, 2010

J. DURÁ, R. DE NALDA, A. GARCÍA-VELA, AND L. BAÑARES
Femtosecond Velocity Map Imaging Experiments and Wave Packet Calculations of CH_3I Photodissociation in the A band
MOLEC XVIII, European Conference on Dynamics of Molecular Collisions, Curia (Portugal), September 5-10, 2010

J. SACRISTÁN, C. MACIAS, F. AGUADO, G. RASINES, C. MIJANGOS
Modelization of Resorcinol/formaldehyde Xerogels and Aerogels
Soft Matter Conference, 2010
http://ismc2010.ugr.es

JOAQUÍN LÓPEZ-SERRANO, ELEUTERIO ÁLVAREZ, JESÚS CAMPOS, ERNESTO CARMONA, FERNANDO P. COSSÍO, ABEL DE COZAR Y ANA CRISTINA ESQUEDA
The (η5-C_5Me_5)Rh Fragment and PXyl2Me. Electronic structure and reactivity with H_2 of a Novel Cationic Complex
III ESCUELA DE QUÍMICA ORGANOMETÁLICA MARCIAL MORENO MAÑAS

JOAQUÍN LÓPEZ-SERRANO, ERNESTO CARMONA, MANUEL L. POVEDA
Irtp Pyridylidenes as Hydrogen Shuttle. A Mechanistic Insight
XXVIII Reunión de Grupo Especializado de Química Organometálica de la RSEQ

JORDI S. ANDREU, JUAN CAMACHO, JORDI FARAUDO
Equilibrium and non-Equilibrium Aggregation of SuperparaMagnetic Colloids
8th International Conference on the Scientific and Clinical Applications of Magnetic Carriers, May 25-29, 2010, Rostock, Germany 5 2010
http://www.magneticmicrosphere.com/meetings/meet2010/index.php

M. AGUILELLA-ARZO, C. CALERO, J. FARAUDO
Elecrokinetics at the Nanoscale: Selectivity Inversion by Multivalent Ions in a Biological Nanochannel
IInd International Soft Matter Conference, Granada, Spain July 5-9, 2010
http://ismc2010.ugr.es

M. CARMEN MUÑOZ
Novel magnetism in non-magnetic oxides Joint
European Magnetic Symposia (JEMS), 2010

M. L. FERNÁNDEZ-CRUZ, A. VALDEHITA, M. ALONSO, E. MANN, B. HERRADÓN, J. M. NAVAS
Aryl hydrocarbon receptor induction by alpha- and ss-pifithrin
XII International Congress of Toxicology (IUTOX), July 19-23, 2010. Barcelona. **Toxicology Letters,** 2010, 196S, Abstract P302-030, page S258 Barcelona, Spain 7 2010
http://www.sciencedirect.com/science/article/B6TCR-501F18P-10C/2/9dbcf6e167f057fa355cf27a84a6c8b2

M.L.SENENT
Ro-Vibrational Inelastic Collisions of Small Astrophysical Species with He And H_2
Collisions Moléculaires Inélastiques, Tunisie-Hammamet : March 18-20, 2010

M.L.SENENT
Ro-Vibrational Inelastic Collisions of Small Astrophysical Species with He And H_2
Workshop on Molecular Complexes in our Atmosphere and Beyond, Brussels, April 20 - 23, 2010

M.L.SENENT CCSD(T)
Study of the Far-Infrared Spectrum of Complex Molecules: Dimethyl-Ether and Ethyl-Methyl-Ether
4th Meeting on High Performance Computing in Molecular Simulation, (Madrid, September 2010)

M.L.SENENT CCSD(T)
Stuffy of the Far-Infrared Spectrum of Complex Molecules: Dme and Eme
Cost Action: The Chemical Cosmos: Annual conference (Grenoble 2010)

C. MENDOZA, A.M. MANCHO
Hidden Geometry of Ocean Flows
Physical Review Letters, 3 038501 2010

M.L.SENENT, R.DOMINGUEZ-GOMEZ
Ab Initio studies of the Far-Infrared Spectrum of Non-Rigid Molecules of Astrophysical Interest
Sixth International Meeting Mathematical Methods for Ab Initio Quantum Chemistry, (Niza, November, 2010)

M.L.SENENT, V.BRITES AND M.HOCHLAF
Characterization and Formation Processes of C_4^-, C_4H and C_4H
Molecular Spectroscopy Conference (Ohio State University, 2010)

M.VILLA AND M.L.SENENT
Dimethyl Ether Three Dimentional
Spectra Molecular Spectroscopy Conference, (Ohio State University, 2010)

MAIN OKDEH, DELFINA BASTOS-GONZÁLEZ, JORDI FARAUDO AND CARLES CALERO
Understanding Ionic Specificity on Charge Inversion
2nd International Soft Matter Conference, Granada, Spain 7 2010
http://ismc2010.ugr.es

MARCEL AGUILELLA-ARZO, CARLES CALERO AND JORDI FARAUDO
Electrokinetics at the Nanoscale: Selectivity inversion by multivalent Ions in a Biological Nanochannel
ELKIN 9th International Conference, Turku, Finland, June 6-10, 2010.
http://www.elkin2010.fi/index.html

MARCEL AGUILELLA-ARZO, CARLES CALERO, JORDI FARAUDO
Molecular Simulation of Ompf Channel in Salts of Divalent Cations: Molecular Insight on Charge Inversion Biophysical Society
54th Annual Meeting, (ISSN:0006-3495), San Francisco (USA) February 20-24, 2010, 2 2010
http://www.biophysics.org/Default.aspx?alias=www.bio-physics.org/2010meeting

MARCEL AGUILELLA-ARZO, CARLES CALERO, JORDI FARAUDO
Electrokinetics at the Nanoscale: Selectivity Inversion by Multivalent Ions in a Biological Nanochannel
IV Spanish Portuguese Biophysical Congress, Zaragoza, Spain 7 2010
http://bifi.es/events/biophysics2010

MARÍA PILAR DE LARA CASTELLS
An Optimized Full-Configuration-Interaction Nuclear Orbital Approach to a Microscopic Description of Small Doped He Clusters
The 3rd milliKelvin Day, Universidad de Barcelona 6 2010
http://www.ecm.ub.es/millikelvin

MARÍA PILAR DE LARA CASTELLS
An Optimized Full-Configuration-Interaction Nuclear Orbital Approach to a Microscopic Description of Small Doped He Clusters
Eigth International Conference of Computational Methods in Sciences and Engineering, (ICCMSE 2010) Kos, Greek 9 2010
http://www.iccmse.org/ICCMSE2010/index.htm

N. HERNÁNDEZ HARO, J. ORTEGA CASTRO, C. PÉREZ DEL VALLE, C.I. SAINZ DÍAZ Y A. HERNÁNDEZ-LAGUNA DFT
Study of the Elastic Properties of Muscovite-Paragonite Series
Chitel2010**,** 9 2010

N. INOSTROZA Y M.L.SENENT
Characterization of C_3SiH-
Molecular Spectroscopy Conference, (Ohio State University, 2010)

N. L. JORGE, J. M. ROMERO, A. GRAND, Y A. HERNÁNDEZ LAGUNA
La reacción de termólisis en fase gas del diperóxido de formaldehido
Estudio Cinético Y Mecanismo Teórico, Chitel2010 Anglet, Francia 9 2010

N. SANCHEZ, S. GALLEGO, M.C. MUÑOZ
Ferromagnetism at Wurtzite-like CoO Surfaces
Joint European Magnetic Symposia, (JEMS) 2010

N. SANCHEZ, S. GALLEGO, M.CARMEN MUÑOZ
Magnetism at Cu/ZnO Structures: Towards a True
DMO Psi-k Conference, 2010

NÉSTOR F. AGUIRRE, ALEXANDER MITRUSHCHENKOV, AND MARÍA PILAR DE LARA CASTELLS
Interaction of He with a Rutile TiO_2 Surface as a Prototype Case to Include Dynamical Correlation in Extended Systems
First International Meeting on Atomic and Molecular Physics, IMAMPC, 2010 6 2010
http://www.iff.csic.es/fama/con/imampc-2010/index.html

NÉSTOR F. AGUIRRE, ALEXANDER O. MITRUSHCHENKOV AND M. PILAR DE LARA-CASTELLS
Interaction of He with a Rutile TiO2(110) Surface as a Prototype Case to Include Dynamical Correlation in Extended Systems
IMAMPC, 2010

O.ALVAREZ-BAJO, M.CARVAJAL, R.DOMÍNGUEZ-GÓMEZ, M.VILLA Y M.L.SENENT. M.CARVAJAL
Theoretical Spectra Analysis for the Torsional and COC Bending Degrees of Freedom of Dimethyl Ether (CH_3OCH_3)
New experimental and theoretical developments in molecular spectroscopy: atmospheric and astrophysical applications, (Soleil, Saint Aubin, November 2010).

R. PROSMITI
Theoretical Study of Small H$\_{2n+1}^+$ clusters:} Potential Energy Surfaces for Studying SpectrosCopy and Dynamics.
MOLEC, 2010

ROSARIA CONTE AND GIULIA ANDRIGHETTO AND DANIEL VILLATORO
From Norm Adoption to Norm Internalization
DEON, 1 2010

S. GALLEGO
Co Nanostructures at ZnO Surfaces
4th Meeting on High Performance COmputing in Molecular Simulations (HPC IV), 10 2010

S. GALLEGO, M.CARMEN MUÑOZ
Manipulating the Magnetic Anisotropy by H Adsorption: the Case of Co/Ru(0001)
Psi-k Conference, 2010

S. GALLEGO, M.CARMEN MUÑOZ
Ferromagnetism at Wurtzite-like CoO Surface
Psi-k Conference, 2010

Ph.D. DISSERTATION (DEFENDED)

DANIEL ABRIL CASTELLANO
Supervised Learning Methods on Distance Based Record Linkage. 7 2010

H. MANZANO
A Atomistic Simulation Studies of the Basque Country. 2009

GRADUATE THESIS AND FINAL PROJECTS

NÉSTOR FABIÁN AGUIRRE CASTIBLANCO. DIRECTOR: MARÍA PILAR DE LARA CASTELLS
He@TiO_2(110) como prototipo para incluir la correlación electrónica en sistemas extendidos

BOOKS AND BOOK CHAPTERS

NÉSTOR F. AGUIRRE CASTIBLANCO, ALEXANDER O. MITRUSHCHENKOV, AND MARÍA PILAR DE LARA CASTELLS
Wave-Function-Based Correlation Methods for Extended Systems: Application to the interaction of a He atom with a rutile TiO_2 (110) surface. Molecular photoreactivity on metal-oxide surfaces from first-principles: photocathalysis and photovoltaics
78-81 2010
http://digital.csic.es/handle/10261/23106

UNIVERSIDADE DE SANTIAGO DE COMPOSTELA (USC)

SCIENTIFIC ARTICLES PUBLISHED

PEÓN, A; OTERO, JM; TIZÓN, L; PRAZERES, VF; LLAMAS-SAIZ, AL; FOX, GC; VAN RAAIJ, MJ; LAMB, H; HAWKINS, AR; GAGO, F; CASTEDO, L; GONZÁLEZ-BELLO, C.
Understanding the Key Factors that Control the iInhibition of TypeII Dehydroquinase by (2R)-2-benzyl-3-dehydroquinic Acids
ChemMedChem, 1726-33. 2010

I. VALIÑO AND J. ALVAREZ-MUÑIZ AND M. ROTH AND R.A. VAZQUEZ AND E. ZAS
Characterisation of the Electromagnetic Component in Ultra-high Energy IInclined Air Showers
Astroparticle Physics, 32 6 304 - 317   2010 10.1016/j.astropartphys.2009.09.008

P.M. HANSEN, J. ALVAREZ-MUÑIZ, R.A. VÁZQUEZ
A comprehensive study of shower to shower fluctuations
Astroparticle Physics, 6 503-512 2011

DOMÍNGUEZ, JOSÉ L. AND CHRISTOPEIT, TONY AND VILLAVERDE, M. CARMEN AND GOSSAS, THOMAS AND OTERO, JOSÉ M. AND NYSTROM, SUSANNE AND BARAZNENOK, VERA AND LINDSTROM, ERIK AND DANIELSON, U. HELENA AND SUSSMAN, FREDY
Effect of the Protonation State of the Titratable Residues on the Inhibitor Affinity to BACE-1
Biochemistry, 49 34 7255-7263 2010 10.1021/bi100637n

WILLEM SIEBRAND AND ZORKA SMEDARCHINA AND ANTONIO FERNÁNDEZ-RAMOS
Tunneling splitting and level ordering in a CO-stretch fundamental of the formic acid dimer
Chemical Physics Letters, 459 1-6 22 - 26 2008 10.1016/j.cplett.2008.04.131

DAVID SERANTES, MARINA SPASOVA, DANIEL BALDOMIR, MICHAEL FARLE AND VERONICA SALGUEIRIÑO
Magnetic Hardness of Fe_60Pt_40 Nanoparticles Controlled by Surface Chemistry
CHEMISTRY OF MATERIALS, 7

CRIADO, ALEJANDRO AND PEÑA, DIEGO AND COBAS, AGUSTÍN AND GUITIÁN, ENRIQUE
Domino Diels-Alder Cycloadditions of Arynes: New Approach to Elusive Perylene Derivatives
Chemistry - A European Journal, 16 32 9736-9740 2010 10.1002/chem.201001057

KAPOERCHAN, VARSHA V. AND KNIJNENBURG, ANNE-MIEK D. AND NIAMAT, MIQUEL AND SPALBURG, EMILE AND DE NEELING, ALBERT J. AND NIBBERING, PETER H. AND MARS-GROENENDIJK, ROOS H. AND NOORT, DAAN AND OTERO, JOSÉ M. AND LLAMAS-SAIZ, ANTONIO L. AND VAN RAAIJ, MARK J.
An Adamantyl Amino Acid Containing Gramicidin S Analogue with Broad Spectrum Antibacterial Activity and Reduced Hemolytic Activity
Chemistry - A European Journal, 16 40 12174-12181 2010 10.1002/chem.201001686

KAPOERCHAN, VARSHA V. AND SPALBURG, EMILE AND DE NEELING, ALBERT. J. AND MARS-GROENENDIJK, ROOS H. AND NOORT, DAAN AND OTERO, JOSÉ M. AND FERRACES-CASAIS, PATRICIA AND LLAMAS-SAIZ, ANTONIO L. AND VAN RAAIJ, MARK J. AND VAN-DOORN, JOOP AND VAN DER MAREL, G
Gramicidin S Derivatives Containing cis-and trans-Morpholine Amino Acids (MAAs) as Turn Mimetics
Chemistry - A European Journal, 16 14 4259-4265 2010 10.1002/chem.200902984

FAN, YING AND MIGUEZ-MACHO, GONZALO
A simple hydrologic framework for simulating wetlands in climate and earth system models
Climate Dynamics nono, 1-26 2010 10.1007/s00382-010-0829-8

FAN, Y. AND MIGUEZ-MACHO, G.
Potential groundwater contribution to Amazon evapotranspiration
Hydrology and Earth System Sciences, 14 10 2039-2056 2010 10.5194/hess-14-2039-2010

D. SERANTES, D. BALDOMIR, C. MARTINEZ-BOUBETA, K. SIMEONIDIS, M. ANGELAKERIS, E. NATIVIDAD, M. CASTRO, A. MEDIANO, D.-X. CHEN, A. SANCHEZ, LI. BALCELLS, AND B. MARTÍNEZ
Influence of dipolar interactions on hyperthermia properties of ferromagnetic particles
Journal of Applied Physics, 7 4

MEANA-PANÉDA, RUBÉN AND TRUHLAR, DONALD G. AND FERNÁNDEZ-RAMOS, ANTONIO
Least-Action Tunneling Transmission Coefficient for Polyatomic Reactions
Journal of Chemical Theory and Computation, 6 1 6-17 2010 10.1021/ct900420e

MEANA-PANÉDA, RUBÉN AND TRUHLAR, DONALD G. AND FERNÁNDEZ-RAMOS, ANTONIO
Direct Dynamics Implementation of the Least-Action Tunneling Transmission Coefficient. Application to the $CH_4/CD_3H/CD_4 + CF_3$ Abstraction Reactions.
Journal of Chemical Theory and Computation, 6 10 3015-3025 2010 10.1021/ct100285a

A. PIÑEIRO, V. PARDO, D. BALDOMIR, S. BLANCO-CANOSA, F. RIVADULLA, J.E. ARIAS AND J. RIVAS
Study of the pressure effects in TiOCl by ab initio calculations.
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, 9-12 3 0304-8853

S. BLANCO-CANOSA, F. RIVADULLA, A. PIÑEIRO, V. PARDO, D. BALDOMIR, M.A. LÓPEZ-QUINTELA AND J. RIVAS
High-pressure magnetic and structural properties of TiOX (X=Cl, Br)
JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS, 9-12 3

SONIA GOY-LÓPEZ, JOSUÉ JUÁREZ, ADRIANA CAMBÓN, JORGE BOTANA, MANUEL PEREIRO, DANIEL BALDOMIR, PABLO TABOADA, AND VÍCTOR MOSQUERA
Block copolymer-regulated synthesis of gold nanocrystals with sharp tips and edges
J. Mater. Chem., 20, 6808-6814, 2010, 10.1039/C0JM00731E

ERASTOVA, VALENTINA AND RODRÍGUEZ-OTERO, JESÚS AND CABALEIRO-LAGO, ENRIQUE AND PEÑA-GALLEGO, ÁNGELES
A computational study of the mechanism of the unimolecular elimination of α,β-unsaturated aldehydes in the gas phase
Journal of Molecular Modeling, 17 21-26 2011 10.1007/s00894-010-0700-1

JOSA, DANIELA AND PEÑA-GALLEGO, ANGELES AND RODRÍGUEZ-OTERO, JESÚS AND CABALEIRO-LAGO, ENRIQUE
A MP2 and DFT study of the aromatic character of polyphosphaphospholes. Is the pyramidality the only factor to take into consideration?
Journal of Molecular Modeling nono 1-6 2010 10.1007/s00894-010-0827-0

D. BALDOMIR, D. SERANTES, M. PEREIRO, J. BOTANA, J. E. ARIAS, S. H. MASUNAGA, AND J. RIVAS
Role of the Dipolar Interaction on the Macroscopic State of Magnetic Nanoparticle Systems: A Monte Carlo Study
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, 2717-2721 2010

D. SERANTES, D. BALDOMIR, M. PEREIRO, J. BOTANA, V. M. PRIDA, B. HERNANDO, J. E. ARIAS, E J. RIVAS
Magnetocaloric Effect in Magnetic Nanoparticle Systems: How to Choose the Best Magnetic Material?
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, 2512 2512-2517

M. PEREIRO, J. BOTANA, D. BALDOMIR, D. SERANTES, AND J. E. ARIAS
Density Functional Study of the Oxidation of Small Neutral and Charged Silver Clusters.
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, 2595-2599

PILAR BROCOS, XAVIER BANQUY, NORMA DÍAZ-VERGARA, SILVIA PÉREZ-CASAS, MIGUEL COSTAS, ÁNGEL PIÑEIRO
Similarities and differences between Cyclodextrin-Sodium Dodecyl Sulfate Host-Guest Complexes of Different Stoichiometries: Molecular Dynamics Simulations at Several Temperatures
Journal of Physical Chemistry B, 12455-12467 2010
http://pubs.acs.org/doi/pdf/10.1021/jp103223u

PINEIRO A, BOTANA AS, PARDO V , BALDOMIR D
Fermiology and magnetism in weak itinerant ferromagnet CoS$_2$: an ab initio study
JOURNAL OF PHYSICS-CONDENSED MATTER, 5056026

HASSAN, NATALIA AND GÁRATE, M. PILAR AND SAN-DOVAL, TANIA AND ESPINOZA, LUIS AND PIÑEIRO, AN-GEL AND RUSO, JUAN M.
On the Self-Assembly of a Highly Selective Benzothiazole-Based TIM Inhibitor in Aqueous Solution
Langmuir, 26 22 16681-16689 2010 10.1021/la102916x

ELENA BLANCO, ÁNGEL PIÑEIRO, REINHARD MILLER, JUAN M. RUSO, GERARDO PRIETO, FÉLIX SARMIENTO
Langmuir monolayers of a hydrogenated/fluorinated catanionic surfactant: from the macroscopic to the nanoscopic size-scale.
Langmuir, 25 8075-8082 2009 10.1021/la900593c

FRANCISCO RIVADULLA, MANUEL BAÑOBRE-LÓPEZ, CAMILO X. QUINTELA, ALBERTO PIÑEIRO, VICTOR PARDO, DANIEL BALDOMIR, MANUEL ARTURO LÓPEZ-QUINTELA, JOSÉ RIVAS, CARLOS A. RAMOS, HORACIO SALVA, JIAN-SHI ZHOU AND JOHN B. GOODENOUGH
Questionable collapse of the bulk modulus in CrN reply nature materials
4 1

JAIME ALVAREZ-MUÑIZ AND WASHINGTON R. CAR-VALHO JR. AND ENRIQUE ZAS AND ANDRÉS ROMERO-WOLF AND MATÍAS TUEROS
Radio pulses from electromagnetic, hadronic and neutrino-induced showers up to EeV energies
Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment In Press, Corrected Proof - 2010, doi:10.1016/j.nima.2010.11.043

LÇCZKOWSKI, KRZYSZTOF Z. AND GARCÍA, DIEGO AND PEÑA, DIEGO AND COBAS, AGUSTÍN AND PÉREZ, DO-LORES AND GUITIÁN, ENRIQUE
Highly Selective Insertion of Arynes into a C(sp)-O(sp3)σBond
Organic Letters, 0 0 2011 10.1021/ol103001k

LONGO, R. C. AND CARRETE, J. AND FERRER, J. AND GALLEGO, L. J.
Structural, magnetic, and electronic properties of Nin and Fen nanostructures (n=1-4) adsorbed on zigzag graphene nanoribbons
Phys. Rev. B, 81 11 115418 Mar 2010 1 0.1103/ PhysRevB, 81.115418.

ALVAREZ-MUÑIZ, JAIME AND ROMERO-WOLF, ANDRÉS AND ZAS, ENRIQUE
Čerenkov radio pulses from electromagnetic showers in the time domain
Phys. Rev. D, 81 12 123009 Jun 2010 10.1103/**PhysRevD,** 81.123009

D. SERANTES, D. BALDOMIR, M. PEREIRO, C. E. HOPPE, F. RIVADULLA AND J. RIVAS
Nonmonotonic evolution of the blocking temperature in dispersions of superparamagnetic nanoparticles
Physical Review B, 13 5

J. SOUTO, M.M.G. ALEMANY, L.J. GALLEGO, L.E. GONZÁLEZ, AND D.J. GONZÁLEZ
Ab initio molecular dynamics study of the static, dynamic, and electronic properties of liquid Bi near melting using re-alspace pseudopotentials
Physical Review B, 134201 2010
http://prb.aps.org/abstract/PRB/v81/i13/e134201

J. SOUTO, M.M.G. ALEMANY, R. C. LONGO, L.J. GAL-LEGO, L.E. GONZÁLEZ, AND D.J. GONZÁLEZ
Investigation of fivefold symmetry at the liquid Pb/Si(001) interface: An ab initio molecular dynamics study
Physical Review B, 134118 2010
http://prb.aps.org/abstract/PRB/v82/i13/e134118

LUCAS V. BESTEIRO, LUIS TORTAJADA, MURILO L. TIAGO, L.J. GALLEGO, JAMES R. CHELIKOWSKY, AND M.M.G. ALEMANY
n-type doping via avoiding the stabilization of DX centers in InP quantum dots
Physical Review B, (Rapid Communications) 121307 2010
http://prb.aps.org/abstract/PRB/v81/i12/e121307

SALAS, ANTONIO AND AMIGO, JORGE
A Reduced Number of mtSNPs Saturates Mitochondrial DNA Haplotype Diversity of Worldwide Population Groups
PLoS ONE 5 5 e10218 05 2010 10.1371/journal.pone.0010218

R. C. LONGO AND J. CARRETE AND L. J. GALLEGO
Magnetism of substitutional Fe impurities in graphene nanoribbons
The Journal of Chemical Physics, 134 2 024704 2011 10.1063/1.3520149

BROCOS, PILAR AND DÍAZ-VERGARA, NORMA AND BANQUY, XAVIER AND PÉREZ-CASAS, SILVIA AND COS-TAS, MIGUEL AND PIÑEIRO, ANGEL
Similarities and Differences Between Cyclodextrin-Sodium *Do-decyl Sulfate Host-Guest Complexes of Different Stoichiometries: Molecular Dynamics Simulations at Several Temperatures*
The Journal of Physical Chemistry B, 114 39 12455-12467 2010 10.1021/jp103223u

GARCÍA-FANDIÑO, REBECA AND CASTEDO, LUIS AND GRANJA, JUAN R. AND VÁZQUEZ, SAULO A.
Interaction and Dimerization Energies in Methyl-Blocked α,γ-Peptide Nanotube Segments
The Journal of Physical Chemistry B, 114 15 4973-4983 2010 10.1021/jp910919k

CABALEIRO-LAGO, ENRIQUE AND RODRÍGUEZ-OTERO, JESÚS AND PEÑA-GALLEGO, ÁNGELES
Study of the interaction between aniline and CH_3CN, CH_3Cl and CH_3F
Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) nono, 1-9 2010 10.1007/s00214-010-0789-4

SMEDARCHINA, ZORKAM, SIEBRAND, WILLEM, FERN-ANDEZ-RAMOS, ANTONIO, MEANA-PANEDA, RUBEN
Mechanisms of Double Proton Transfer. Theory and Applications
Read More: http://www.oldenbourg-link.com/doi/abs/10.1524/zpch.2008.5389
Zeitschrift für Physikalische Chemie, 222 8-9 1291-1309 nana 10.1524/zpch.2008.5389

SCIENTIFIC ARTICLES IN-PRESS

ÁNGEL PIÑEIRO, PETER J. BOND AND SYMA KHALID
Exploring the conformational dynamics and membrane interactions of PorB from C. glutamicum: a multi-scale molecular dynamics simulation study
BBA-Biomembranes, 2011

PRESENTATIONS AT CONCRESSES/ CONFERENCES

A. GARCÍA-LOUREIRO, M. ALDEGUNDE, N. SEOANE, K. KALNA AND A. ASENOV
Impact of Random Dopant Fluctuations on a Tri-Gate MOSFET
International Conference on Ultimate Integration on Silicon, 3 2010

A. MARTINEZ DE LA TORRE, A. RIOS ENTENZA, L GESTAL SOUTO, G. MIGUEZ MACHO
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
10th EMS Annual Meeting 8th European Conference on Applied Climatology, Zürich, Switzerland, September 13-17, 2010
http://meetings.copernicus.org/ems2010

A. MARTÍNEZ DE LA TORRE, A. RIOS ENTENZA, L. GESTAL SOUTO, G. MIGUEZ MACHO
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
10th EMS Annual Meeting 8th European Conference on Applied Climatology, (Zürich) 9 2010

A. MARTÍNEZ DE LA TORRE, A. RIOS ENTENZA, L. GESTAL SOUTO, AND G. MIGUEZ MACHO
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
DAMES'2010 Data Analysis and Modelling in Earth Sciences, University of Lisbon, Portugal
http://sites.google.com/site/dames2010org/home

A. MARTÍNEZ DE LA TORRE, A. RIOS ENTENZA, L. GESTAL SOUTO, G. MIGUEZ MACHO
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
DAMES'2010 Data Analysis and Modelling en Earth Sciences, September 22-24, 2010 University of Lisbon, Portugal
http://sites.google.com/site/dames2010org

ALBA CAMPO-CACHARRÓN, ENRIQUE M. CABALEIRO-LAGO, JESÚS RODRÍGUEZ-OTERO
Interaction between anions and naphthalendiimides
I4th International electronic conference on synthetic organic chemistry, (ECSOC-14) 23 11 2010

ALBERTO MARTINEZ DE LA TORRE, ALEXANDRE RÍOS ENTENZA, LUCÍA GESTAL SOUTO Y GONZALO MIGUEZ
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
10th EMS (European Meteorological Society) Annual Meeting. (Zurich, Switzerland)

ALBERTO MARTINEZ DE LA TORRE, ALEXANDRE RÍOS EN-TENZA, LUCÍA GESTAL SOUTO Y GONZALO MIGUEZ MACHO
Coupling WRF with LEAFHYDRO: introducing groundwater and a fully dynamic water table in regional climate simulations
2nd International Conference on Data Analysis and Modelling in Earth Sciences, (University of Lisbon, Portugal)

ALEXANDRE RIOS-ENTENZA AND GONZALO MIGUEZ-MACHO
Moisture recycling and the maximum of precipitation in the spring in the Iberian Peninsula European Geophysical Union (EGU)
General Assembly, Vienna, 2010
http://meetings.copernicus.org/egu2010

ANTONIO PEÓN, EMILIO LENCE, LUIS CASTEDO AND CONCEPCIÓN GONZÁLEZ-BELLO
Towards Understanding the Catalytic Mechanism of Type II Dehydroquinase by Molecular Dynamic Simulations
7th ERA-CHEMISTRY Flash Conference, 10 2010

C. FONG PADRÓN, E CABALEIRO LAGO AND J RO-DRÍGUEZ OTEROL
Estimatedc BS ccsD(T) limit of the interaction energy between water and some ionic liquids
ESPA2010, 6-2010

D. JOSA, J. RODRÍGUEZ-OTERO, AND E CABALEIRO-LAGO DFT
Study of Corannulene Dimers
ESPA2010,6 2010

ENRIQUE M. CABALEIRO-LAGO, JESÚS RODRÍGUEZ-OTERO, AND ANGELES PEÑA-GALLEGO
Computational Study of the Hydration Effect upon the Interaction Between Pyrrolidinium Cation and Aromatic Systems.
ESPA2010, 6 2010

FAN, Y., LI H. AND G. MIGUEZ-MACHO
Global water table depth from observations and a model synthesis
American Geophysical Union Fall Meeting,12 2010

FREDY SUSSMAN, JOSÉ L. DOMÍNGUEZ, TONY CHRISTOPEIT, M. CARMEN VILLAVERDE, JOSÉ M. OTERO, U. HELENA DANIELSON
Search for cell active bio-available BACE-1 inhibitors as drugs leads against Alzheimer disease
7th ERA-Chemistry Flash Conference Bioinspired Chemistry, 2010

GERARDO CASAL, JOSE ANTONIO ÁLVEREZ DIOS, JOSE CARLOS CABALEIRO
A generalization of s-teps variants of Gradient methods
International Conference on Computational and Mathematical Methods in Science and Engineering 2010, 96-107 Almería, Spain 7 2010
http://gsii.usal.es/~CMMSE

J. L. DOMÍNGUEZ, T. CHRISTOPEIT, T. GOSSAS, S. NYSTRÖM, V. BARAZNENOK, E. LINDSTRÖM, M. C. VILLAVERDE, U. H. DANIELSON Y F. SUSSMAN
Effect of the protonation state of the titrable residues on the inhibitor affinity to BACE-1
Segundo Simposio Iberoamericano de Química Orgánica (SIBEAQO-II), 2010

J. RODRÍGUEZ-OTEROT,E . M. CABALEIRO-LAGO AND A. PEÑA-GALLEGO
Ab Initio and DFT Studv of the Structure. Bowl-to-Bowl Inversion Barrier. and aromaticity of óorannulen
ESPA2010, 6 2010

J. SOUTO, M.M.G. ALEMANY, L.J. GALLEGO, L.E. GONZÁLEZ, AND D.J. GONZÁLEZ
Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of liquid Bi
March Meeting of the American Physical Society,
Portland, EE.UU. 3 2010
http://meetings.aps.org/Meeting/MAR10/Content/1812

JORGE A. CARRAZANA GARCÍA, ENRIQUE M. CABALEIRO LAGO, JESÚS RODRÍGUEZ OTERO DFT
Study of the complex formation between alkaline cations and curved π systems derived from fullerene
7th ERA-Chemistry Flash Conference . Bioinspired Chemistry, 10 2010

JORGE A. CARRAZANA-GARCÍA, ENRIQUE M. CABALEIRO-LAGO AND JESÚS RODRÍGUEZ-OTERO
Cation - p complexes between alkaline cations and molecular bowls related with fullerene: a DFT study
I4[th] nInternational electronic conference on synthetic organic chemistry (ECSOC-14), 10 10

LUCAS V. BESTEIRO, LUIS TORTAJADA, MURILO L. TIAGO, L.J. GALLEGO, JAMES R. CHELIKOWSKY, AND M.M.G. ALEMANY
Efficient n-type doping of zinc-blende III-V semiconductor quantum dots
March Meeting of the American Physical Society , Portland, EE.UU. 3 2010
http://meetings.aps.org/Meeting/MAR10/Content/1812

LUCÍA GESTAL SOUTO, GONZALO MÍGUEZ MACHO Y YING FAN
Water table depth and potential capillary flux to the land surface in the Iberian Peninsula EGU (European Geosciences Union)
General Assembly, 2010 (Vienna, Austria)

LUCÍA GESTAL SOUTO, GONZALO MÍGUEZ MACHO Y YING FAN
Calculation of the equilibrium water table depth in the Iberian Peninsula. Is the groundwater reservoir important in climate simulations?
2nd International Conference on Data Analysis and Modelling in Earth Sciences, (University of Lisbon, Portugal)

LUIS TORTAJADA, M.M.G. ALEMANY, MURILO L. TIAGO, L.J. GALLEGO, AND JAMES R. CHELIKOWSKY
The role of quantum confinement in p-type semiconductor InP nanocrystals
March Meeting of the American Physical Society, Portland, EE.UU. 3 2010
http://meetings.aps.org/Meeting/MAR10/Content/1812

MIGUEZ-MACHO G. AND Y. FAN
Potential contribution of groundwater to dry-season ET in the Amazon European Geosciences
Union General Assembly, 5 2010

MIGUEZ-MACHO, G AND FAN, Y.
Groundwater as a Source of Evapotranspiration in the Dry Season in Amazonia: Simulations with the LEAFHYDRO LSM.
American Geophysical Union Fall Meeting, 12 2010

MIGUEZ-MACHO, G AND YING FAN
A simple hydrologic framework for simulating continental and global wetlands European Geosciences
Union General Assembly, 5 2010

PEÓN, A.; LENCE, E.; CASTEDO, L.; GONZÁLEZ-BELLO, C.
Towards Understanding the Catalytic Mechanism of Type II Dehydroquinase by Molecular Dynamic Simulations
SISOC7: 7th ERA-Chemistry Flash Conference, 10 2010

PEÓN, A.; TIZÓN L., PRAZERES, V. F. V.; CASTEDO, L.; GONZÁLEZ-BELLO, C.
Steady-State Fluorescence and Molecular Dynamic Studies on the Inhibition of Type II Dehydroquinase by (2R)-3-Benzyl-3-Dehydroquinic Acids
XXIst International Symposium on Medicinal Chemistry, 9 2010

VALIN, R AND SEOANE, N. AND GARCIA-LOUREIRO, A. AND ALDEGUNDE, M AND LOPEZ CACHEIRO, J.
SMNanoS: Submitting and Monitoring Nanoelectronic Simulations in the VO-MOSFET 4th
Iberian Grid Infrastructure, 2010

X. PAREDES, A.S. PENSADO, P. MALFREYT, A.A.H. PÁDUA, J. FERNÁNDEZ
How molecular simulation can help to understand the structure of the liquid-vacuum interfaces of ionic liquids based in the alkylsufate anion?
ICCT2010.

GRADUATE THESIS AND FINAL PROJECTS

OSCAR GARCÍA LORENZO FRANCISCO FERNÁNDEZ RIVERA JUAN ÁNGEL LORENZO DEL CASTILLO
Description of Memory Acceses Using Hardware Counters Caracterización de Accesos a Memoria Usando Contadores Hardware

ALBA CAMPO CACHARRÓN
Proyecto fin carreira estudo computacional da interacción anión-p nunha canle iónica sintética
7 2010

Ph.D. DISSERTATION (DEFENDED)

BRAIS PARADELO NUÑEZ
Estudo computacional de complexos formados por catión pirrolidinio hidratado e benceno
9 2010

MANUEL PEREIRO LÓPEZ
Quantum Mechanical Study of Electronic Structure of Low-Dimensional Systems at the Nanoscale
11 2010

Universida~de~Vigo

UNİVERSİDADE DE VİGO (UVİGO)

SCİENTİFİC ARTİCLES PUBLİSHED

GARCÍA J, FRANCI G, PEREIRA R, BENEDETTI R, NEB-BIOSO A, RODRÍGUEZ-BARRIOS F, GRONEMEYER H, ALTUCCI L, LERA AR.
Epigenetic profiling of the antitumor natural product psammaplin A and its analogues
Bioorganic & Medicinal Chemistry, 2010

GAYATHRI, CHAKICHERLA AND DE LA FUENTE, M. CARMEN AND LUY, BURKHARD AND GIL, ROBERTO R. AND NAVARRO-VÁZQUEZ, ARMANDO
Probing heterocycle conformation with residual dipolar couplings
Chem. Commun, 46 5879-5881 2010 10.1039/c0cc01271

ROBERTO SANZ, DELIA MIGUEL, MUKUT GOHAIN, PATRICIA GARCÍA-GARCÍA, MANUEL A. FERNÁNDEZ-RODRÍGUEZ, ADÁN GONZÁLEZ-PÉREZ, OLALLA NIE-TO-FAZA, ANGEL R. DE LERA, AND FÉLIX RODRÍGUEZ
Synthesis of Diverse Indole-Containing Scaffolds by Gold(I)-Catalyzed Tandem Reactions of 3-Propargylindoles Initiated by 1,2-Indole Migrations: Scope and Computational Studies
Chem. Eur. J. 9818 2010

SONIA ÁLVAREZ-BARCIA AND JESÚS R. FLORES
How H2 can be formed by the interaction of Al atoms with a few water molecules: A theoretical study
Chemical Physics, 374 1-3 131 - 137 2010 10.1016/j.chemphys.2010.07.013

ANTONIO VILA AND RICARDO A. MOSQUERA
On the non-planarity of 1,3-dioxole and 1,3-dioxolane
Chemical Physics Letters, 488 1-3 17 - 21 2010 10.1016/j.cplett.2010.02.001

RIVERA-FUENTES, PABLO AND ALONSO-GÓMEZ, JOSÉ LORENZO AND PETROVIC, ANA G. AND SEILER, PAUL AND SANTORO, FABRIZIO AND HARADA, NOBUYUKI AND BEROVA, NINA AND RZEPA, HENRY S. AND DIED-ERICH, FRANÇOIS
Enantiomerically Pure Alleno-Acetylenic Macrocycles: Synthesis, Solid-State Structures, Chiroptical Properties, and Electron Localization Function Analysis
Chemistry - A European Journal, 16 32 9796-9807 2010 10.1002/chem.201001087

SANZ, ROBERTO AND MIGUEL, DELIA AND GOHAIN, MUKUT AND GARCÍA-GARCÍA, PATRICIA AND FERNÁN-DEZ-RODRÍGUEZ, MANUEL A. AND GONZÁLEZ-PÉREZ, ADÁN AND NIETO-FAZA, OLALLA AND DE LERA, ÁNGEL L . AND RODRÍGUEZ, FÉLIX
Synthesis of Diverse Indole-Containing Scaffolds by Gold(I)-Catalyzed Tandem Reactions of 3-Propargylindoles Initiated by 1,2-Indole Migrations: Scope and Computational Studies
Chemistry - A European Journal, 16 32 9818-9828 2010 10.1002/chem.201001162

ERDÉLYI, MÁTÉ AND NAVARRO-VÁZQUEZ, ARMANDO AND PFEIFFER, BERNHARD AND KUZNIEWSKI, CHRIS-TIAN N. AND FELSER, ANDREA AND WIDMER, TONI AND GERTSCH, JÜRG AND PERA, BENET AND DÍAZ, JOSÉ FERNANDO AND ALTMANN, KARL-HEINZ AND CARLOMAGNO, TERESA
The Binding Mode of Side Chain- and C3-Modified Epothilones to Tubulin
ChemMedChem, 5 6 911-920 2010 10.1002/cmdc.201000050

GEIST, JULIE G. AND LAUW, SUSAN AND ILLARIONO-VA, VICTORIA AND ILLARIONOV, BORIS AND FISCHER, MARKUS AND GRÄWERT, TOBIAS AND ROHDICH, FELIX AND EISENREICH, WOLFGANG AND KAISER, JOHANNES AND GROLL, MICHAEL AND SCHEURER, CHRISTIAN AND WITTLIN, SERGIO AND ALO
Thiazolopyrimidine Inhibitors of 2-Methylerythritol 2,4-Cyclodiphosphate Synthase (IspF) from Mycobacterium tuberculosis and Plasmodium falciparum
ChemMedChem, 5 7 1092-1101 2010 10.1002/cmdc.201000083

ABALDE-CELA, SARA AND HERMIDA-RAMÓN, JOSÉ M. AND CONTRERAS-CARBALLADA, PABLO AND DE?COLA, LUISA AND GUERRERO-MARTÍNEZ, ANDRÉS AND ALVA-REZ-PUEBLA, RAMÓN A. AND LIZ-MARZÁN, LUIS M. SERS
Chiral Recognition and Quantification of Enantiomers through Cyclodextrin Supramolecular Complexation
ChemPhysChem, n/a-n/a 2010 10.1002/cphc.201000800

ANA DOPAZO-PAZ, PAULA GÓMEZ-ÁLVAREZ AND DIEGO GONZÁLEZ-SALGADO
Thermodynamics and structure of the water + methanol system viewed from three simple additive pair-wise intermolecular potentials based on the rigid molecule approximation
Collect. Czech. Chem. Commun, 75 617-635 May 2010 doi:10.1135/cccc2009097

NIETO FAZA, OLALLA AND S FELDMAN, KEN AND SILVA LOPEZ, CARLOS
Cyclization Cascade of Allenyl Azides: Synergy Between Theory and Experiment
Current Organic Chemistry, 14 1646-1657(12) September 2010 10.2174/138527210793563305.

PETROVIC, A.G.A , NAVARRO-VÃZQUEZ, A.B , ALONSO-GÃMEZ, J.L.B
From relative to absolute configuration of complex natural products: Interplay between NMR, ECD, VCD, and ORD assisted by ab initio calculations
Current Organic Chemistry, 14 15 1612-1628 2010
http://www.scopus.com/inward/record.url?eid=2-s2.0-77956415052&partnerID=40&md5=0f81da440b0737e3afcdaf53ecf70c97

BUSCHHAUS, BORIS AND CONVERTINO, VITO AND RIVERA-FUENTES, PABLO AND ALONSO-GÓMEZ, JOSÉ LORENZO AND PETROVIC, ANA G. AND DIEDERICH, FRANÇOIS
Optically Active Trialkynyl(phenyl)methane: Synthesis and Determination of Its Absolute Configuration by Vibrational Circular Dichroism (VCD) and Optical Rotatory Dispersion (ORD).
European Journal of Organic Chemistry, 2010 13 2452-2456
http://dx.doi.org/10.1002/ejoc.20100007610.1002/ejoc.201000076

KRASZEWSKA, AGNIESZKA AND RIVERA-FUENTES, PABLO AND RAPENNE, GWÉNAËL AND CRASSOUS, JEANNE AND PETROVIC, ANA G. AND ALONSO-GÓMEZ, JOSÉ LORENZO AND HUERTA, ELISA AND DIEDERICH, FRANÇOIS AND THILGEN, CARLO
Regioselectivity in Tether-Directed Remote Functionalization - The Addition of a Cyclotriveratrylene-Based Trimalonate to C60 Revisited
European Journal of Organic Chemistry, 2010 23 4402-4411
http://dx.doi.org/10.1002/ejoc.20100039610.1002/ejoc.201000396

VIJANDE, JAVIER AND PIÑEIRO, MANUEL M. AND LEGIDO, JOSÉ C. MARTINS L. AND BESSIÉRES, DAVID
Group-Contribution Method for the Molecular Parameters of the PC-SAFT Equation of State Taking into Account the Proximity Effect. Application to Nonassociated Compounds
Industrial & Engineering Chemistry Research, 49 19 9394-9406 2010 10.1021/ie1002813

MAMELI, MARTA AND LIPPOLIS, VITO AND CALTAGIRONE, CLAUDIA AND CAPELO, JOSÉ LUIS AND FAZA, OLALLA NIETO AND LODEIRO, CARLOS
Hg_2+ Detection by New Anthracene Pendant-Arm Derivatives of Mixed N/S- and N/S/O-Donor Macrocycles: Fluorescence, Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry and Density Functional Theory Studies
Inorganic Chemistry, 49 18 8276-8286 2010 10.1021/ic1007439

ELISABETE OLIVEIRA AND S.P.G. COSTA AND M.M.M. RAPOSO AND OLALLA NIETO FAZA AND CARLOS LODEIRO
Synthesis, characterization, fluorescence and computational studies of new Cu_2+, Ni_2+ and Hg_2+ complexes with emissive thienylbenzoxazolyl-alanine ligands
Inorganica Chimica Acta, 366 1 154 - 160 2011 10.1016/j.ica.2010.10.025
http://www.sciencedirect.com/science/article/B6TG5-51CJ3CD-1/2/fd83f4c1dc1a3d959257e2aa291a64c1

RINCÓN, DAVID A. AND CORDEIRO, M. NATÁLIA D. S. AND MOSQUERA, RICARDO A.
Theoretical study of morphine and heroin: Conformational study in gas phase and aqueous solution and electron distribution analysis
International Journal of Quantum Chemistry, 110 13 2472-2482 2010 10.1002/qua.22851

M. HEGGLIN ET AL. (INCLUDING , J. A. AÑEL)
Multimodel assessment of the upper troposphere and lower stratosphere: Extra-tropics
J. Geophys. Res. D009M09 2010
http://www.agu.org/journals/ABS/2010/2010JD013884.shtml

ESTÉVEZ, L.; OTERO, N.; MOSQUERA, R. A.
A Computational Study on the Acidity Dependence of Rad*ical-Scavenging Mechanisms of Anthocyanidins*
J.Phys.Chem.B, 114 9706-9712 2010

JOSÉ A. SOUTO, MARTÍN PÉREZ, CARLOS SILVA LÓPEZ, ROSANA ALVAREZ, ALICIA TORRADO AND ANGEL R. DE LERA
Competing Thermal Electrocyclic Ring-Closure Reactions of (2Z)-Hexa-2,4,5-trienals and Their Schiff Bases
Structural, Kinetic, and Computational Studies, JOC 4453 2010

MANDADO, MARCOS AND CORDEIRO, M. NATÁLIA D. S.
On the stability of metal-aminoacid complexes in water based on water-ligand exchange reactions and electronic properties: Detailed study on iron-glycine hexacoordinated complexes
Journal of Computational Chemistry 31 15 2735-2745 2010 10.1002/jcc.21567
http://dx.doi.org/10.1002/jcc.21567

PATRICIA GARCÍA, MANUEL MARTÍN-PASTOR, ANGEL R. DE LERA AND ROSANA ALVAREZ
Determination of the geometry of acetoxyendiynes and acetoxyenynes by NMR heteronuclear 13C-1H scalar couplings and 13C NMR chemical shifts. Structural assignment of the oxylipin natural products peyssonenynes A and B
Magn. Reson. Chem. 543

LAHOZ, INMA R. AND SICRE, CRISTINA AND NAVARRO-VÁZQUEZ, ARMANDO AND LÓPEZ, CARLOS SILVA AND CID, MARÍA-MAGDALENA
Mechanistic Investigation on the Formation of Indolizines from 2-Enynylpyridines
Organic Letters 11 21 4802-4805 2009 10.1021/ol901760a
http://pubs.acs.org/doi/abs/10.1021/ol901760a

MARTÍN PÉREZ-RODRÍGUEZ, ATAUALPA A. C. BRAGA, ANGEL R. DE LERA, FELIU MASERAS, ROSANA ALVA-REZ, AND PABLO ESPINET
A DFT Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes
Organometallics 4983 D. BES

PÉREZ-RODRÍGUEZ, MARTÍN AND BRAGA, ATAUALPA A. C. AND DE LERA, ANGEL R. AND MASERAS, FELIU AND ÁLVAREZ, ROSANA AND ESPINET, PABLO A DFT
Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes+
Organometallics 29 21 4983-4991 2010 10.1021/om1001974
http://pubs.acs.org/doi/abs/10.1021/om1001974

HERMIDA-RAMÓN, JOSE M. AND MANDADO, MARCOS AND SÁNCHEZ-LOZANO, MARTA AND ESTÉVEZ, CARLOS M.
Enhancing the interactions between neutral molecular tweezers and anions
Phys. Chem. Chem. Phys. 12 164-169 2010 10.1039/b915483c
http://dx.doi.org/10.1039/B915483C

ARMANDO NAVARRO-VÁZQUEZ AND JOSÉ-LORENZO ALONSO-GÓMEZ AND JOHAN LUGTENBURG AND MARÍA-MAGDALENA CID
Mechanistic elucidation of ketenimine-butynoate cycloaddition reaction: role of biradical intermediates in isotopomeric purity of benzyl (1,1a,6,6a-13C4)-6-methyl anthranilic ester
Tetrahedron 66 21 3855 - 3860 2010 10.1016/j.tet.2010.03.035
http://www.sciencedirect.com/science/article/B6THR-4YM-7FDD-3/2/30a856a5abfd1a3213d51d2f6022f4a3

D. BESSIERES AND M. M. PINEIRO AND G. DE FERRON AND F. PLANTIER
Analysis of the orientational order effect on n-alkanes: Evidences on experimental response functions and description using Monte Carlo molecular simulation
The Journal of Chemical Physics, 133 7 074507 2010 10.1063/1.3472283

J. M. MIGUEZ AND D. GONZALEZ-SALGADO AND J. L. LEGIDO AND M. M. PINEIRO
Calculation of interfacial properties using molecular simulation with the reaction field method: Results for different water models
The Journal of Chemical Physics, 132 18 184102 2010. 10.1063/1.3422528

GONZÁLEZ PÉREZ, ADÁN AND SILVA LÓPEZ, CARLOS AND MARCO-CONTELLES, JOSÉ AND NIETO FAZA, OLALLA AND SORIANO, ELENA AND DE LERA, ANGEL R.
Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl)oxiranes: A Dual Role of the Catalyst
The Journal of Organic Chemistry, 74 8 2982-2991 2009 10.1021/jo802516k

SOUTO, JOSÉ C. MARTINS A. AND PÉREZ, MARTÍN AND SILVA LÓPEZ, CARLOS AND ÁLVAREZ, ROSANA AND TORRADO, ALICIA AND DE LERA, ANGEL R.
Competing Thermal Electrocyclic Ring-Closure Reactions of (2Z)-Hexa-2,4,5-trienals and Their Schiff Bases. Structural, Kinetic, and Computational Studies+
The Journal of Organic Chemistry, 75 13 4453-4462 2010 10.1021/jo100558p

TRIGO-MOURIÑO, PABLO AND SANTAMARÍA-FERNÁNDEZ, RAQUEL AND SÁNCHEZ-PEDREGAL, VÍCTOR M. AND NAVARRO-VÁZQUEZ, ARMANDO
Conformational Analysis of an Isoquinolinium Hydrochloride in Water Using Residual Dipolar Couplings
The Journal of Organic Chemistry, 75 9 3101-3104 2010 10.1021/jo902502h

LAFITTE, THOMAS AND MENDIBOURE, BRUNO AND PIÑEIRO, MANUEL M. AND BESSIÈRES, DAVID AND MIQUEU, CHRISTELLE
Interfacial Properties of Water/CO2: A Comprehensive Description through a Gradient Theory-SAFT-VR Mie Approach
T**he Journal of Physical Chemistry B,** 114 34 11110-11116 2010 10.1021/jp103292e

NI, WEIHAI AND MOSQUERA, RICARDO A. AND PÉREZ-JUSTE, JORGE AND LIZ-MARZÁN, LUIS M.
Evidence for Hydrogen-Bonding-Directed Assembly of Gold Nanorods in Aqueous Solution
The Journal of Physical Chemistry Letters, 1 8 1181-1185 2010 10.1021/jz1002154

FAZA, OLALLA AND RODRÍGUEZ, ROI AND LÓPEZ, CARLOS
Performance of density functional theory on homogeneous gold catalysis
Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) nono, 1-15   2010 10.1007/s00214-010-0843-2

SCIENTIFIC ARTICLES IN PRESS

NICOLÁS OTERO, STIJN FIAS, SLAVKO RADENKOVIC, PATRICK BULTINCK, ANA M. GRAÑA AND MARCOS MANDADO
How Does Aromaticity Rule the Thermodynamic Stability of Hydroporphyrins?
Chemistry A European Journal, 2011

MARTA SÁNCHEZ-LOZANO, NICOLÁS OTERO, JOSE M. HERMIDA-RAMÓN, CARLOS M. ESTÉVEZ AND MARCOS MANDADO
Anion-π; Aromatic Neutral Tweezers Complexes. Are They Stable In Polar Solvents?
Journal of Physical Chemistry, 2011

MARTA SÁNCHEZ-LOZANO, NICOLÁS OTERO, JOSE M. HERMIDA-RAMÓN, CARLOS M. ESTÉVEZ, AND MARCOS MANDADO
Anion-π; Aromatic Neutral Tweezers Complexes: Are They Stable in Polar Solvents?
Journal of Physical Chemistry A, 2011

PRESENTATIONS AT CONGRESSES / CONFERENCES

A. NAVARRO-VÁZQUEZ, M. J. RIVEIRA, M. MISCHNE, C. GAYATHRI, R. R. GIL
Characterizations of cyclopentahydrobenzofuranes through NMR in aligned media and ab initio chemical shift computation
Segundo Simposio Iberoamericano de Química Orgánica (SIBEAQO-II)

J. DE ROO, R. A. MOSQUERA, A. GRAÑA, P. BULTINCK, N. OTERO QTAIM
Study of the Reversed Anomeric Effect
ESPA-2010

J. M. MÍGUEZ, D. GONZÁLEZ-SALGADO, J. L. LEGIDO, M. M. PIÑEIRO
Determination of interfacial properties of the water + methane mixture under slab confinement using Monte-Carlo simulation
8th Liblice Conference on the Statistical Mechanics of Liquids, 1 6 2010

J. M. MÍGUEZ, D. GONZÁLEZ-SALGADO, J. L. LEGIDO, M. M. PIÑEIRO
Calculation of interfacial properties of water using Monte-Carlo simulation with the reaction field method
21st IUPAC International Conference on Chemical Thermodynamics, Tsukuba, Japón 6 2010

J. M. MÍGUEZ, F. J. BLAS, C. DOS RAMOS, D. GONZÁLEZ-SALGADO, J. L. LEGIDO, M. M. PIÑEIRO
Propiedades interfaciales de agua, metano y CO_2: interfases fluidas y confinamiento
XII Encuentro Inter-Bienal del Grupo Especializado de Termodinámica, Las Palmas 2 9 2010

L. ESTÉVEZ, N. OTERO, R.A. MOSQUERA
Electron density reorganization upon copigmentation of cyanidin by apigenin
ESPA-2010

M. DE DIOS, A. B. DAVILA-IBÁÑEZ, V. SALGUEIRIÑO, M. M. PIÑEIRO
Synthesis of Co_2B nanoparticles
A Simulation Study E-MRS (European Materials Research Society) Spring Meeting, 1 6 2010

M. DE DIOS, A. B. DAVILA-IBÁÑEZ, V. SALGUEIRIÑO, M. M. PIÑEIRO
Síntesis de nanopartículas de Co$_2$B, Estudio computacional
XII Encuentro Inter-Bienal del Grupo Especializado de Termodinámica, Las Palmas 2 9 2010

M. M. PIÑEIRO, D. BESSIÈRES Y T. LAFITTE
A comparison of SAFT and Molecular Simulation techniques in the calculation of response functions and interfacial properties of fluids
Symposium: 20 years of the SAFT Equation: Recent Advances and Challenges, 1 9 2010

N. OTERO, L. ESTÉVEZ, M. MANDADO, R.A. MOSQUERA
Topological and energetic study of pyrrole dimers using QTAIM atomic space
Comparing CC vs. M06-2X approaches, ESPA-2010

OLALLA NIETO FAZA, CARLOS SILVA LÓPEZ
Estudio computacional del mecanismo de formación de β;-lactamas a partir de O-propargil arilaldoximas
II Encontro Galego de Cinética e Catálise (EGC2), Portomarín 1 2010

OLALLA NIETO FAZA, ROI ÁLVAREZ RODRÍGUEZ, CARLOS SILVA LÓPEZ
Computational studies in homogeneous gold catalysis
Segundo Simposio Iberoamericano de Química Orgánica, 176 Santiago de Compostela 9 2010
http://www.usc.es/sibeaqo2/index.php

ROI ALVAREZ RODRÍGUEZ, INMA R. LAHOZ, OLALLA NIETO FAZA, MARÍA-MAGDALENA CID, CARLOS SILVA LÓPEZ
Theoretical and Experimental Study of Resveratrol Photoisomerization: characterization of 2,4,6-trihydroxyphenanthrene as a photoproduct
XXIII Reunión Bienal del Grupo Especializado de Química Orgánica de la RSEQ, Murcia 6 2010
http://www.um.es/23rbqo/index.php

BOOKS AND BOOK CHAPTERS (IN PRESS)

M. DE DIOS, ANA B. DAVILA-IBAÑEZ, VERONICA SALGUEIRIÑO, MANUEL M. PIÑEIRO
Síntesis de nanopartículas de Co$_2$B. Estudio computacional
La investigación del Grupo Especializado de Termodinámica de las Reales Sociedades Españolas de Física y Química, 2011

BOOKS AND BOOK CHAPTERS PUBLISHED

R.A. MOSQUERA, M. MANDADO, L. ESTÉVEZ, N. OTERO
Electron density distributions of heterocycles: a shortcoming of the resonance model
Quantum Frontiers of Atoms and Molecules, 359-383 2010

RICARDO A. MOSQUERA, MARÍA J. GONZÁLEZ MOA, LAURA ESTÉVEZ, MARCOS MANDADO AND ANA M. GRAÑA
An Electron Density-Based Approach to the Origin of Stacking Interactions
Quantum Biochemistry, 365-387 2010

Ph.D. DISSERTATION (DEFENDED)

ISABEL IGLESIAS FERNÁNDEZ
Interacción Océano-Atmósfera. Influencia de la SST y de la circulación termohalina
12-2010

ADÁN GONZÁLEZ PÉREZ
Propuestas Computacionales, Basadas en DFT, para reordenamientos de Sistemas Propargílicos Catalizados por Au y Pt y para la Reacción de Negishi
1 -2011

REPORT PUBLISHED

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.
http://www.atmosp.physics.utoronto.ca/SPARC/ccmval_final/index.php

UNIVERSIDADE DA CORUÑA

UNIVERSIDADE DA CORUÑA (UDC)

SCIENTIFIC ARTICLES PUBLISHED

J. KUMAR RAY, G. BARMAN, M. CANLE L., M.I. FERNÁN-DEZ P. J. A. SANTABALLA
Diethyl1-(4-methylphenyl)-3-(phenylyl)-5-oxopyrrolidine-2,2-dicarboxylate
Acta Crystallographica E, 2010.

J. KUMAR RAY, P. HALDAR, M. CANLE L., M.I. FERNÁN-DEZ, J. A. SANTABALLA
1-(3-Chloro-4-fluro-phenyl)-5-(2-diazo-acetyl)-4-phenyl-pyrrolidin-2-one
Acta Crystallographica E, 2103

JOSEP M. OLIVA, ANTONIO FERNÁNDEZ-BARBERO, LUIS SERRANO-ANDRÉS, MOISÉS CANLE-L., J. ARTURO SANTABALLA, M. ISABEL FERNÁNDEZ
Energy Landscapes in Diexo and Exo/Endo Isomers Derived from $Li_2B1_2H_{12}$
Chemical Physics Letters, 2010
http://www.elsevier.com/wps/find/journaldescription.cws_home/505707/description#description

M.I. FERNÁNDEZ, M. CANLE L., M.V. GARCÍA, J.A. SANTABALLA
A theoretical analysis of the acid-base equilibria of hydroxylamine in aqueous solution
Chemical Physics Letters, 159-164 2010
http://www.elsevier.com/wps/find/journaldescription.cws_home/505707/description#description

FERREIRÓS-MARTÍNEZ, RAQUEL AND PLATAS-IGLE-SIAS, CARLOS AND DE BLAS, ANDRÉS AND ESTEBAN-GÓMEZ, DAVID AND RODRÍGUEZ-BLAS, TERESA
Macrocyclic Receptor Showing Improved PbII/ZnII and PbII/CaII Selectivities
European Journal of Inorganic Chemistry, 2010 17 2495-2503
http://dx.doi.org/10.1002/ejic.20090121910.1002/ejic.200901219

REGUEIRO-FIGUEROA, MARTÍN AND ESTEBAN-GÓMEZ, DAVID AND DE BLAS, ANDRÉS AND RODRÍGUEZ-BLAS, TERESA AND PLATAS-IGLESIAS, CARLOS
Structure and Dynamics of Lanthanide(III) Complexes with an N-Alkylated do3a Ligand (H3do3a = 1,4,7,10-Tetraazacyclododecane-1,4,7-triacetic Acid): A Combined Experimental and DFT Study
European Journal of Inorganic Chemistry, 2010 23 3586-3595
http://dx.doi.org/10.1002/ejic.20100033410.1002/ejic.201000334

TRIPIER, RAPHAËL AND PLATAS-IGLESIAS, CARLOS AND BOOS, ANNE AND MORFIN, JEAN-FRANÇOIS AND CHARBONNIÈRE, LOÏC
Towards Fluoride Sensing with Positively Charged Lanthanide Complexes
European Journal of Inorganic Chemistry, 2010 18 2735-2745
http://dx.doi.org/10.1002/ejic.20090104510.1002/ejic.200901045

REGUEIRO-FIGUEROA, MARTÍN AND DJANASHVILI, KRISTINA AND ESTEBAN-GÓMEZ, DAVID AND DE BLAS, ANDRÉS AND PLATAS-IGLESIAS, CARLOS AND RODRÍGUEZ-BLAS, TERESA
Towards Selective Recognition of Sialic Acid Through Simultaneous Binding to Its cis-Diol and Carboxylate Functions
European Journal of Organic Chemistry, 2010 17 3237-3248
http://dx.doi.org/10.1002/ejoc.20100018610.1002/ejoc.201000186

GONZÁLEZ, C.H.; FRAGUELA, B.B.
A Generic Algorithm Template for Divide-and-Conquer in Multicore Systems
High Performance Computing and Communications (HPCC), 2010 12th IEEE International Conference on nono 79-88 September 2010 10.1109/HPCC.2010.24

FRAGUELA, B.B. ANDRADE, D. DOALLO, R.
Address-Independent Estimation of the Worst-Case Memory Performance
Industrial Informatics, IEEE Transactions 6 4 664 - 677 November 2010 10.1109/TII.2010.2064172

PURGEL, MIHÁLY AND BARANYAI, ZSOLT AND DE BLAS, ANDRÉS AND RODRÍGUEZ-BLAS, TERESA AND BÁNYAI, ISTVÁN AND PLATAS-IGLESIAS, CARLOS AND TÓTH, IMRE An NMR and DFT
Investigation on the Conformational Properties of Lanthanide(III) 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetate Analogues Containing Methylenephosphonate Pendant Arms
Inorganic Chemistry, 49 9 4370-4382 2010 10.1021/ic100177n

REGUEIRO-FIGUEROA, MARTÍN AND DJANASHVILI, KRISTINA AND ESTEBAN-GÓMEZ, DAVID AND CHAUVIN, THOMAS AND TÓTH, EVA AND DE BLAS, ANDRÉS AND RODRÍGUEZ-BLAS, TERESA AND PLATAS-IGLESIAS, CARLOS
Molecular Recognition of Sialic Acid by Lanthanide(III) Complexes through Cooperative Two-Site Binding
Inorganic Chemistry, 49 9 4212-4223 2010 10.1021/ic902461g

TABOADA, G. L. AND TOURI~NO, J. AND DOALLO, R.
Performance Analysis of Message-Passing Libraries on High-Speed Clusters
Intl. Journal of Computer Systems Science & Engineering; 25 1 63-78   2010

DANIEL RIVERO AND JULIAN DORADO AND JUAN RABUÑAL AND ALEJANDRO PAZOS
Generation and simplification of Artificial Neural Networks by means of Genetic Programming
Neurocomputing, 73 16-18 3200 - 3223   2010 10.1016/j.neucom.2010.05.010

DANIEL R. RAMOS, RAQUEL CASTILLO, MOISÉS CANLE L., M. VICTORIA GARCÍA, JUÁN ANDRÉS, J. ARTURO SANTABALLA.
A Theoretical Study on the Mechanism of the Base-promoted Decomposition of (N-Cl),N-methylethanolamine
Organic & Biomolecular Chemistry, 1807 -1814 2009
http://pubs.rsc.org/en/Journals/JournalIssues/OB

GRADUATE THESIS AND FINAL PROJECTS

ÓSCAR GARCÍA LÓPEZ
Diseño e Implementación de una Biblioteca de Computación Matricial Dispersa para el Lenguaje de Programación Paralela UPC

DIEGO FUSTES, DIEGO ORDOÑEZ, BERNARDINO ARCAY AND MINIA MANTEIGA

Ph.D. DISSERTATION DEFENDED

ÓSCAR IBÁÑEZ
Forensic Identification by Craniofacial Superimposition Using Soft Computing
9 2010

SONIA VILARIÑO PATIÑO
Fotodegradación de compuestos con actividad antibiótica (-lactamas) y fibratos
12 2009

SCIENTIFIC ARTICLES (IN PRESS)

D. MARTÍNEZ-REGO, O. FONTENLA-ROMERO, A. ALONSO-BETANZOS
Efficiency of local models ensembles for time series prediction
Expert Systems with Applications, (ESWA) 2011

PRESENTATIONS AT CONGRESSES / CONFERENCES

ANNE GOSSET, VICENTE DÍAZ CÁSAS & FERNANDO LÓPEZ PEÑA
Evaluation of the cavitatingFoam solver for low Mach number flow around a 2D hydrofoil
5th OpenFoam Workshop, 6 2010

ANNE GOSSET, VICENTE DÍAZ CÁSAS & FERNANDO LÓPEZ PEÑA
A method to speed up the prediction of cavitation extent on hydrofoils using Artificial Neural Networks
8th Euromech Fluid Mechanics Conference, 9 2010

ANNE GOSSET, VICENTE DÍAZ CASÁS, RICHARD J. DURO & FERNANDO LÓPEZ PEÑA
Improving the analysis of hydrofoils undergoing cavitation by using artificial neural networks
17th International Conference on Neural Information Processing, 11 2010

CARLOS H. GONZALEZ AND BASILIO B. FRAGUELA
A Generic Algorithm Template for Divide-and-Conquer in Multicore Systems
HPCC, 79-88 2010

CARLOS H. GONZALEZ Y BASILIO B. FRAGUELA
Una plantilla genérica para el patrón de paralelismo de divide-y-vencerás en sistemas multinúcleo
XXI Jornadas de Paralelismo, 19-26 9 2010

CARLOS TEIJEIRO, GUILLERMO L. TABOADA, JUAN TOURIÑO, RAMÓN DOALLO
Diseño e Implementación de MapReduce en el Modelo de Programación PGAS
XXI Jornadas de Paralelismo JP2010 (SARTECO) - CEDI, 2010

DIEGO ORDOÑEZ, CARLOS DAFONTE, BERNARDINO ARCAY AND MINIA MANTEIGA
A Combination of Connectionist Systems and Evolutionary Computation Techniques to Achieve the Optimal Domain for Stellar Spectra Signal Processing
International Joint Conference on Computational Intelligence, 2009 323-330 Funchal-Madeira, Portugal 10 2009

J. GONZÁLEZ-DOMÍNGUEZ AND G.L. TABOADA AND B.B. FRAGUELA AND M.J. MARTÍN AND J. TOURIÑO
Servet: A Benchmark Suite for Autotuning on Multicore Clusters
24th IEEE International Parallel and Distributed Processing Symposium, IPDPS'10, 9 pages 2010

JORGE GONZÁLEZ-DOMÍNGUEZ, GUILLERMO L. TABOADA, BASILIO B. FRAGUELA, MARÍA J. MARTÍN, JUAN TOURIÑO
Servet: una suite de benchmarks para el soporte del autotuning en clusters de sistemas multinúcleo
XXI Jornadas de Paralelismo, 467-474 9 2010

UNİVERSİTAT DE LES İLLES BALEARS (UİB)

SCİENTİFİC ARTİCLES PUBLİSHED

ADROVER M., FRAU J., CALDÉS C., VILANOVA B., DONOSO J. AND MUÑOZ F.
Impact of the ionic forms on the UV-Vis Spectra 2-hydroxy-benzylamine
A TD-DFT study Int. J. of Quant. Chem. 2179-2191 2010

ADROVER, M.; FRAU, J.; CALDÉS, C.; VILANOVA, B.; DONOSO, J.; MUÑOZ, F.
Theoretical and experimental study of the vertical excitation energies in the ionic and tautomeric forms of 4-aminomethylpyridine
Journal of Photochemistry and Photobiology A-Chemistry, 2010

ORTEGA-CASTRO, J.; ADROVER, M.; FRAU, J.; SALVÀ, A.; DONOSO, J.; MUÑOZ, F.
DFT Studies on Schiff Base Formation on Vitamin B6 analogues. Reaction between a pyridoxamine-analogue and carbonyl compounds
Journal of Physical Chemistry A, 4634-4640 2010

SCİENTİFİC ARTİCLES İN-PRESS

PINEDA F.P., ORTEGA CASTRO J. , ALVAREZ-IDABOY J.R., FRAU J., CABRERA B.M., RAMÍREZ J.C., DONOSO J., MUÑOZ, F.
The hydrolysis of a chlorambucil analogue. A DFT study
Journal of Physical Chemistry A, 2011

İNSTİTUTO ESPAÑOL DE OCEANOGRAFÍA (İEO)

PRESENTATİON AT CONGRESSES / CONFERENCES

COBAS GARCÍA, M., RUIZ VILLARREAL, M., GARCÍA GARCÍA, L.M. AND OTERO, P.
Sensibilidades en el modelo hidrodinámico con batimetrías realistas
I Encuentro Oceanografia Física Española, Barcelona 10 2010
http://www.locea.org/index.php/encuentro-oceanografia-fisica-espanola

COBAS-GARCÍA, M., RUIZ-VILLARREAL, M., GARCÍA-GARCÍA, L. AND P. OTERO.
Constraining model setup in a narrow shelf simulation using different data sources
42nd International Liège Colloquium on Ocean Dynamics, Liège, Belgium 4 2010
http://modb.oce.ulg.ac.be/colloquium/2010/

COBAS-GARCÍA, M., RUIZ-VILLARREAL, M., VÁZQUEZ-CENDÓN, E., GARCÍA-GARCÍA, L. AND P. OTERO
Circulation during a harmful algal Bloom in north-west Iberia: realistic simulation and sensitivity study
First European IAHR Congress, Edinburgh, UK

GARCÍA GARCÍA, LUZ MARÍA, RUÍZ VILLARREAL, MANUEL, OTERO TRANCHERO, PABLO, COBAS GARCÍA, MARCOS, MARTA ALMEIDA, MARTINHO
The Iberian-Biscay coastal forecasting system: IEO improvements during ECOOP
Ecoop Final Meeting/Workshop/Summer School, Estambul (Turkey) 3 2010

GARCÍA-GARCÍA, L.M.; RUIZ-VILLARREAL, M.; COBAS-GARCÍA, M.; OTERO-TRANCHERO, P.
Comparing Altimetry with Model Results off North and Northwest Iberia
3rd Coastal Altimetry Workshop, Frascati (Italy) 9 2009
http://www.congrex.nl/09C32

RUIZ VILLARREAL, M., GARCÍA, LUZ, OTERO, P., CO-BAS, M., SÁNCHEZ, R., GONZÁLEZ-POLA, C., CABANAS, JM, DÍAZ DEL RÍO, G., LAVÍN, A.
Variabilidad de mesoescala en el sistema de afloramiento del no de la península ibérica: observaciones y modelado
I Encuentro de la Oceanografía física española, Barcelona 10 2010.
http://www.locea.org/index.php/encuentro-oceanografia-fisica-espanola

RUIZ-VILLARREAL, M., GARCÍA-GARCÍA, L., OTERO, P., COBAS, M. AND M. BERNAL
Modelling oceanographic conditions influencing early stages of small pelagic fish MARIFISH-ICES
Joint Workshop on Integrated ecosystem modelling; building our capacity to understand and manage marine ecosystems in a changing world, 11 2010
http://vds1719.sivit.org/eoc/?q=node/22390

METEOGALICIA

PRESENTATIONS AT CONGRESSES / CONFERENCES

COSTA, PEDRO; CARRACEDO, PABLO; PÉREZ, EVA; VENÂNCIO, ANABELA; VILASA, LUIS
RAIA PROJECT.Operational Iberian Margin Hydrodynamical Model
I Encuentro de la Oceanografía Física Española (EOF1)

KAZIMIERZ WIELKI UNIVERSITY

SCIENTIFIC ARTICLES PUBLISHED

BARANOWSKA, ANGELIKA AND CAPELO, SILVIA BOUZÁN AND FERNÁNDEZ, BERTA
New basis sets for the evaluation of interaction energies: an ab initio study of the Hea[euro sign]He, Nea[euro sign]Ne, Ara[euro sign]Ar, Hea[euro sign]Ne, Hea[euro sign]Ar and Nea[euro sign]Ar van der Waals complex internuclear potentials and ro-v
Phys. Chem. Chem. Phys. 12 13586-13596 2010 10.1039/c0cp00535e

BARANOWSKA, ANGELIKA AND FERNÁNDEZ, BERTA AND SADLEJ, ANDRZEJ
Importance of electron correlation effects and basis set superposition error in calculations of interaction energies and interaction-induced electric properties in hydrogen-bonded complexes: a model study
Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) nono, 1-7 2010 10.1007/s00214-010-0817-4

Annex 2

SCİENTİFİC PRODUCTİON

CESGA Staff 2010

Work on projects has been intense during the year 2010. There were a number of requests (22) of which 6 were accepted (46% of total resolved this year) and 6 were also accepted of those submitted the previous year (75% of total yet to resolve this year). Although the number of applications was lower than the previous year, the number of successful applications was very similar, which means that the quality of the proposals was maintained. Among the proposals that have not yet been resolved include 3 European proposals in the area of e-infrastructure.

The scientific production of CESGA researchers and technicians which increased markedly in recent years, exploded in 2009 due to collaboration in large computing challenges. This year, as a result of project implementation and of the consolidation of the Research subunit, dependent on the Applications and Projects Area, the number of journal publications (a total of 9, most of the ISI Catalog) remained virtually unchanged. The number of conference contributions decreased because of the budget cuts imposed due the economic crisis.

CESGA

CESGA STAFF SCIENTIFIC PRODUCTION

SCIENTIFIC ARTICLES IN SCI JOURNALS

PIÑEIRO, V. PARDO, D. BALDOMIR, F. RIVADULLA, A. RODRÍGUEZ, A. GÓMEZ, J. E. ARIAS, J. RIVAS
Influence of the Ca_2+ inhomogeneity distribution in the physical properties of La0.625Ca0.375MnO$_3$
PHYSICA STATUS SOLIDI C - CURRENT TOPICS IN SOLID STATE PHYSICS, 2010, Vol. 7(11-12), pp. 2620-2623

ALESSANDRO COSTANTINI, EDUARDO GUTIÉRREZ, JAVIER LÓPEZ CACHEIRO, AURELIO RODRÍGUEZ, OSVALDO GERVASI, ANTONIO LAGANA
Porting of GROMACS Package into the Grid Environment Testing of a New Distribution Strategy, **Lecture Notes in Computer Science,** 2010, Vol. 6019/2010, pp. 41-52

ALESSANDRO COSTANTINI, EDUARDO GUTIÉRREZ, JAVIER LÓPEZ CACHEIRO, AURELIO RODRÍGUEZ, OSVALDO GERVASI, ANTONIO LAGANA
On the extension of the grid-empowered molecular science simulator: MD and visualisation tools, **International Journal of Web and Grid Services,** 2010, Vol 6(2), pp. 141-159.

COTELO, C.; GOMEZ, A.; LOPEZ, J. I.; MERA, D.; COTOS, J. M.; MARRERO, J. P. & VAZQUEZ, C.,
Retelab. A geospatial grid web laboratory for the oceanographic research community, **Future Generation Computer Systems,** 2010, Vol. 26(8), pp. 1157 - 1164

HASTINGS, M. B.; GONZÁLEZ, I.; KALLIN, A. B. & MELKO, R. G.,
Measuring Renyi Entanglement Entropy in Quantum Monte Carlo Simulations, **Phys. Rev. Lett.,** 2010, Vol. 104(15), pp. 157201

HEIDRICH-MEISNER, F.; GONZÁLEZ, I.; AL-HASSANIEH, K. A.; FEIGUIN, A. E.; ROZENBERG, M. J. & DAGOTTO, E.
Nonequilibrium electronic transport in a one-dimensional Mott insulator, **Phys. Rev. B,** 2010, Vol. 82(20), pp. 205110

MARTA LOUREIRO, MIGUEL PAN, MANUEL RODRÍGUEZ-PASCUAL, DAVID POSADA, RAFAEL MAYO
Grid selection of models of nucleotide substitution, **Studies in Health Technology and Informatics,** 2010, Vol. 159, pp. 244-248

SIMÓN, A.; LÓPEZ, J.; FREIRE, E.; FERNÁNDEZ, C. & DÍAZ, S.,
Providing Grid Services Based on Virtualization and Cloud. Euro-Par 2009, **Parallel Processing Workshops,** 2010, Vol. 6043/2010, pp. 444-453

REBECA DÍAZ REDONDO, ANA FERNÁNDEZ VILAS, MARÍA JOSÉ RODRÍGUEZ MALMIERCA, JOSÉ J. PAZOS ARIAS, SILVIA BASTOS MOLARES
Experiencia piloto para la provisión de formación personalizada en televisión sobre la plataforma T-Maestro, IEEE-RITA-P2010-084. (to be published)

BOOKS

MARÍA MARTÍN SEIJO, ALDARA RICO REY, ANDRÉS TEIRA BRIÓN, ISRAEL PICÓN PLATAS, IGNACIO GARCÍA GONZÁLEZ, EMILIO ABAD VIDAL
Guide of Archaeobotany, **Xunta de Galicia. Consellería de Cultura e Turismo. Dirección Xeral de Patrimonio Cultural (ed.),** 2010, pp. 122

TECHNICAL REPORTS

PICHEL, J.C.
Memoria xerárquica e mapping do FinisTerrae, 2010.

GÓMEZ, F.; LÓPEZ, J.
Instalación y evaluación de OpenNebula, 2010

R. MALMIERCA, M.; RUBIO, B.; ABUÍN, J.M.
Análisis de utilización del Sistema de Gestión de Cursos Aula Cesga, 2010

PARTICIPATION IN NATIONAL CONFERENCES

MARÍA JOSÉ RODRÍGUEZ MALMIERCA, BRUNO RUBIO GAYO, REBECA P. DÍAZ REDONDO, ANA FERNÁNDEZ VILAS
Producción y provisión de contenidos formativos individualizados para Televisión Digital Interactiva
EDUTEC 2010 Elearning 2.0: enseñar y aprender en la Sociedad del Conocimiento, 2010

AWARDS

Rural Schools & Cloud Computing Project
Finalists EGANET "Escola Dixital"
Santiago de Compostela (Spain), December 23, 2010.

SCIENTIFIC DISSEMINATION

CESGA HPCN High Performance Computing and Networking WORKSHOP.
Santiago de Compostela (Spain), November 25, 2010
Speaker - Carmen Cotelo Queijo
Cesga's ICTS Experience. Oral Presentation

4th Meeting on High Performance Computing in Molecular Simulation
Madrid (Spain), September 30 & October 1st, 2010.
Speaker - Andrés Gómez Tato
Computational challenges at CESGA-FinisTerrae Supercomputer in Molecular Simulations. Oral Presentation

Jornada "Colaboración en Proyectos de Innovación"
Santiago de Compostela (Spain), Nobember 17, 2010
Speaker - Andrés Gómez Tato
Caso de éxito 3: CESGA. Oral Presentation

Master de Ingeniería Matemática
Santiago de Compostela (Spain), September 8, 2010
Speaker - Andrés Gómez Tato
IMRT y la ecuación de transporte. Oral Presentation

CloudComputing 2010
Barcelona (Spain), October 26, 2010
Panel 1: Clouds for HPC: myth or reality
Moderator - Andrés Gómez Tato

HEPiX Spring 2010 Workshop
Lisbon (Portugal) April 26, 2010
CESGA Experience with the Grid Engine batch system
Speaker - Esteban Freire. Oral Presentation

5th EGEE User Forum Uppsala, April 12, 2010
Uppsala, 40280
Application Domain Accounting for EGI
Speaker - Javier Lopez. Oral Presentation

Ibergrid 2010
Braga (Portugal), May 24-27
The Metrics Portal: A tool to get statistics about EGEE operations
Speaker - Sergio Díaz. Oral Presentation

Ibergrid 2010
Braga (Portugal), May 24-27, 2010
The Road to Production: SGE Integration Process with CREAM-CE
Speaker - Javier López. Oral Presentation

Ibergrid 2010
Braga (Portugal), May 24-27, 2010
Ibergrid Transition to EGI
Speaker - Javier López. Oral Presentation

HPCN
Santiago de Compostela (Spain), November 25, 2010
Gestión de FinisTerrae como ICTS en IBERGRID 2010
Speaker - Carlos Fernández. Oral Presentation

Red Española de e-Ciencia
Barcelona (Spain), 40514
Cloud Distribuido para "High Performance Computing"
Speaker - Ruben Díez. Oral Presentation

II Iberian Supercomputing Workshops
Braga (Portugal), May 27, 2010
Speaker - Aurelio Rodríguez
Computarional Challenges on FinisTerrae
Oral Presentation

CESGA HPCN 2010 WORKSHOP
Santiago de Compostela (Spain), November 25, 2010
Speaker - Aurelio Rodríguez
Cesga's Aim For Excellence In Services – Response To User Demands. Oral Presentation

The 25th International Supercomputing Conference
Hamburg (Germany), May 30, 2010
UPC Operations Microbenchmarking Suite
Oral Presentation

IBERGIRD'2010
Braga (Portugal), May 27, 2010
II Jornadas Ibericas de Supercomputaçao
Workshop Organiser - José Carlos Mouriño Gallego

HP-CAST 2010 León (Spain), *UPC Libraries to Enhance Performance and Programmability in Multicore Systems*
Speaker - José Carlos Mouriño Gallego
Oral Presentation

TEACHING

Course - *Grid y e-Ciencia*
Andrés Gómez Tato, IFIC, July 6, 2010

Course - *The European Grid Initiative, IBERGRID and the Spanish NGI*
C. Fernandez, IFIC, 40360

Course - *Herramientas colaborativas para investigadores*
M. J. R. Malmierca
CESGA, November 2010.

Master - *Curso experto de e-learning. Experiencia de e-learning de un centro tecnológico*
M. J. R. Malmierca
USAL, October 2010

Master língua e usos profesionais. Módulo de e-learning
M. J. R. Malmierca
UDC, November 2010

DISSEMINATION ARTICLES

Article - Carmen Cotelo Queijo
Convocatoria CESGA-ICTS. Tres millóns de horas de cálculo
díxitos, 11, 2010

Article - María José Rodríguez Malmierca
Aula Cesga. Avaliación positiva. **díxitos**, 13, July 2010

Article - María José Rodríguez Malmierca
A escola rural na nube. **díxitos,** 15, November 2010

OTHER DISSEMINATION

Press release - *Investigadores Del CESGA, UDC, USC Y HP Desarrollan Software Para Evaluar El Rendimiento De Los Supercomputadores*

Press release - *La escuela rural se sube a la nube*

Press release - *El CESGA participa en un proyecto de investigación sobre la aplicación de Cloud computing para mejorar la escuela rural*

Web pages with information about **Rural Schools:**

www.elearningeuropa.info/out/?doc_id=23270&rsr_id=23493

http://www.elearningeuropa.info/directory/index.php?page=doc&doc_id=16845&doclng=6

http://www.supercomputingonline.com/latest/hp-labs-funds-cesga-e-learning-for-rural-schools

PARTICIPATION IN INTERNATIONAL CONFERENCES

JESÚS GONZÁLEZ, MARTA LOUREIRO, MIGUEL PAN, AURELIO RODRÍGUEZ, *Performance evaluation of HP SFS striping parameters,* **IBERGRID 2010,** 2010, pp.258 - 267

M. LOUREIRO, M. PAN, M. RODRÍGUEZ-PASCUAL, R. MAYO, D. POSADA, *MPI and Grid selection models of nucleotide substitution,* **IBERGRID 2010,** Poster. 2010

M. LOUREIRO, M. PAN, M. RODRÍGUEZ-PASCUAL, R. MAYO, D. POSADA, *Grid selection models of nucleotide substitution,* **HealthGrid 2010**, 2010, pp. 478 – 481

DAVID GARCÍA PÉREZ, JOSÉ CARLOS MOURIÑO GALLEGO, ANDRÉS GÓMEZ, *Accounting and Billing of Software Licenses,* **IBERGRID 2010,** 2010, pp. 333 – 343

TABOADA, J. M.; LANDESA, L.; OBELLEIRO, F.; RODRIGUEZ, J. L.; ARAUJO, M.; G. BERTOLO, J. M.; MOURINO, J. C. & GOMEZ, A. *Supercomputing challenges in electromagnetics. Antennas and Propagation,* **(EuCAP 2010),** 2010, pp. 1 - 4

DAMIÁN A. MALLÓN, J. CARLOS MOURIÑO, ANDRÉS GÓMEZ, GUILLERMO L. TABOADA, CARLOS TEIJEIRO, JUAN TOURIÑO, BASILIO B. FRAGUELA, RAMÓN DOALLO, BRIAN WIBECAN, *UPC Operations Microbenchmarking Suite*
The 25th International Supercomputing Conference (ISC' 10), Poster, 2010

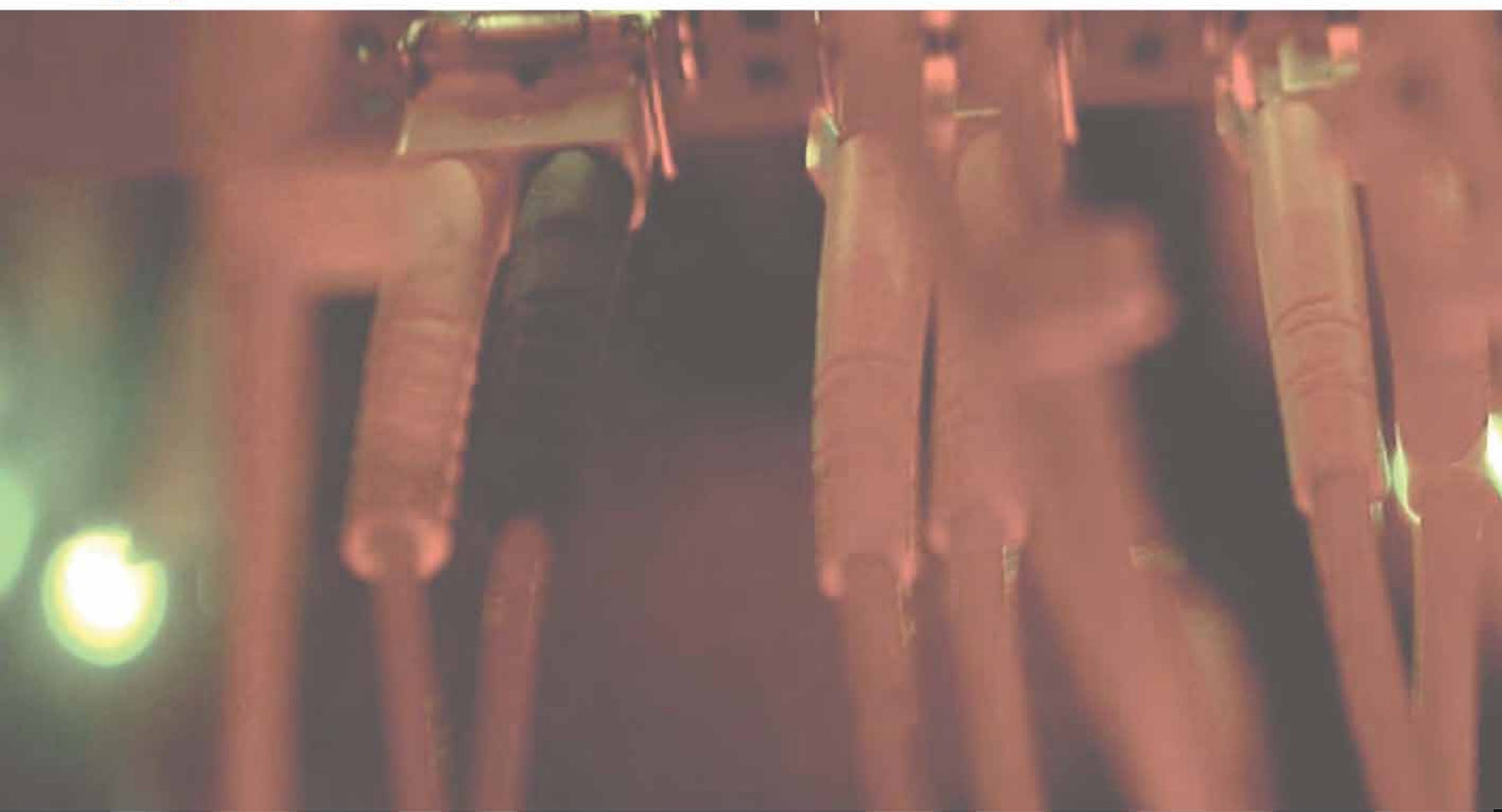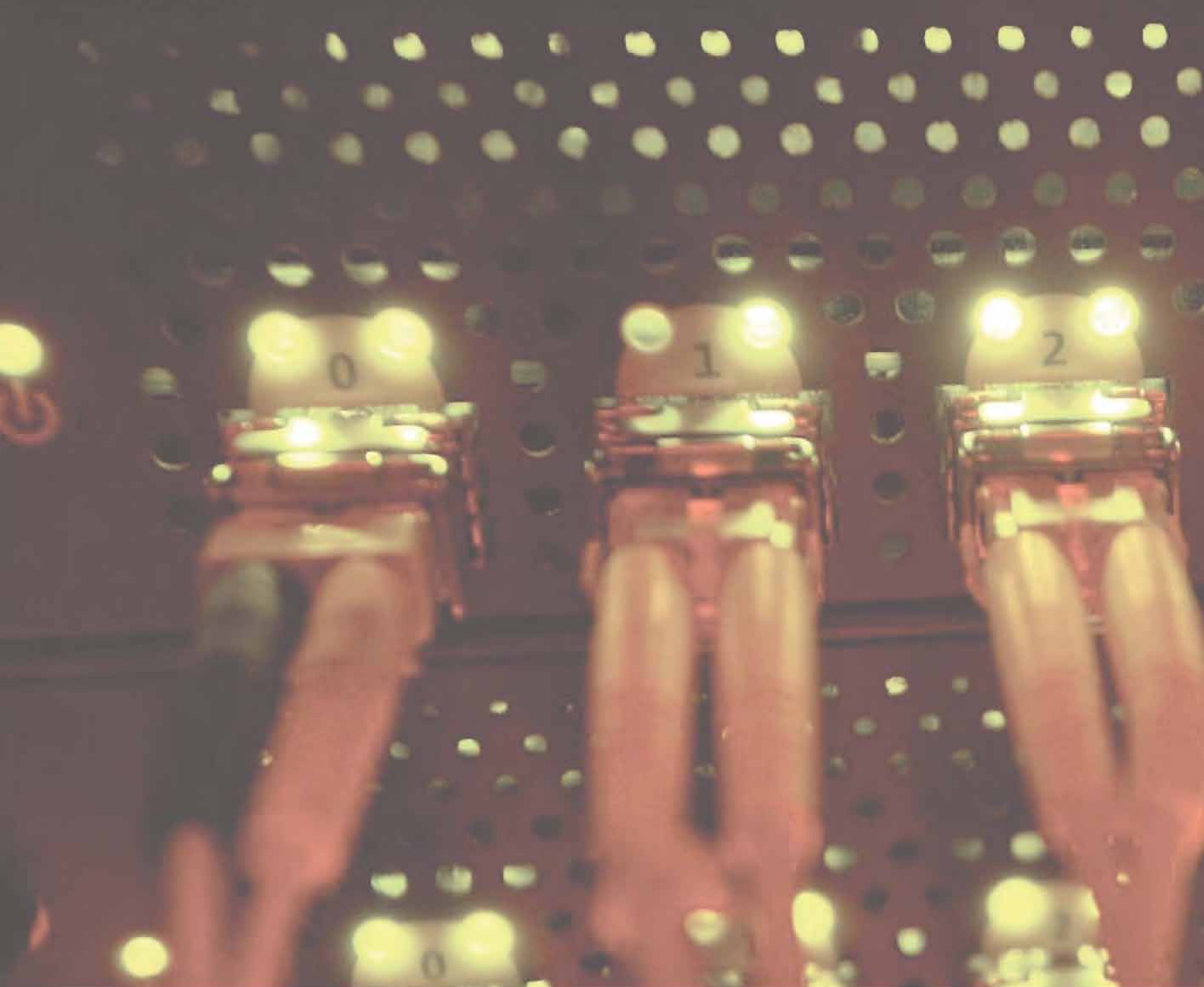FREIRE, E.; SIMÓN, A.; FERNÁNDEZ, C.; LÓPEZ, J.; DÍEZ, R.; DÍAZ, S.; REY, P., BORGES, G.
The road to Production: SGE Integration Process with CREAM-CE, **IBERGRID 2010,** 2010, pp. 71-8
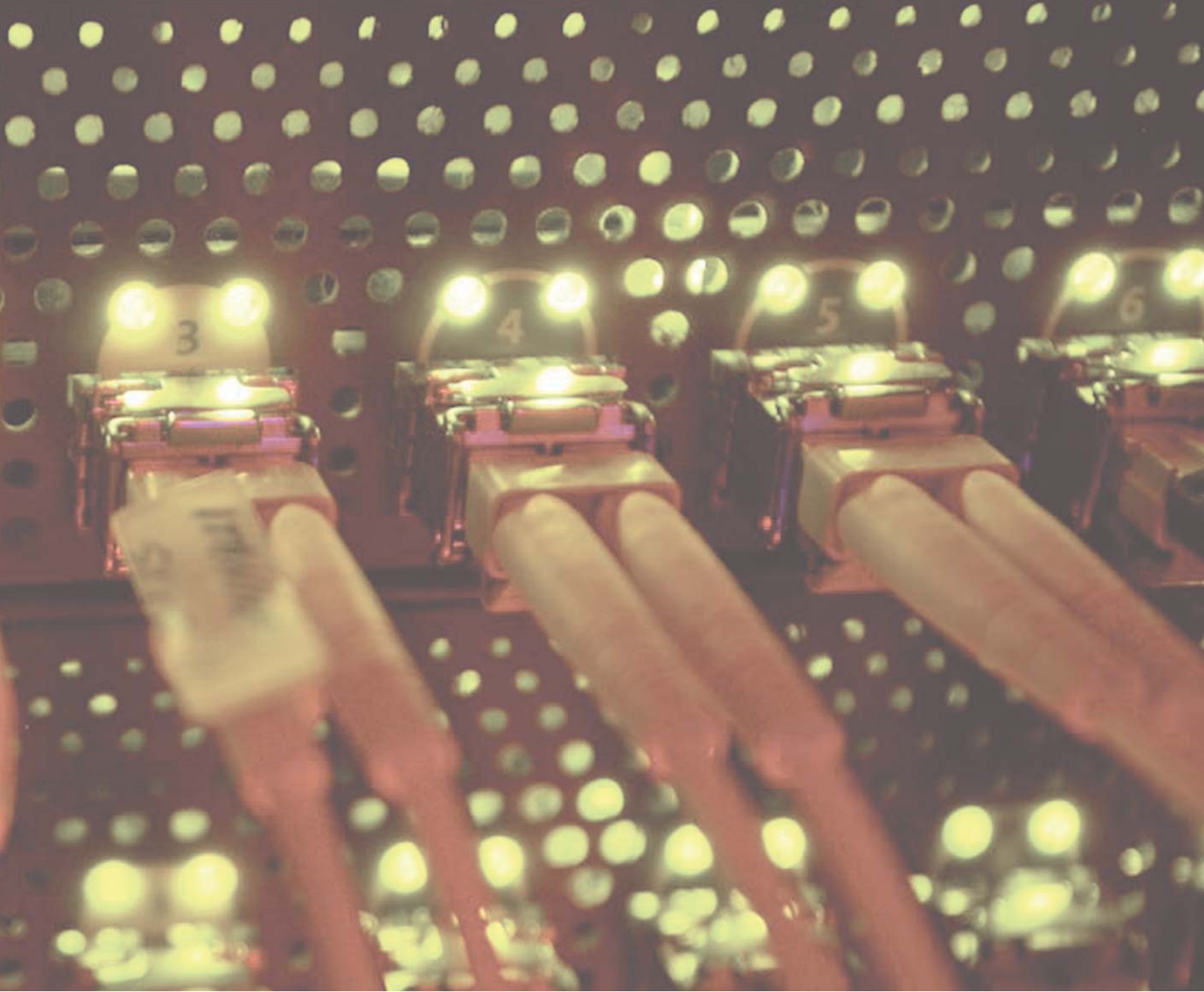
CACHEIRO, J. L.; BORGES, G.; GOMES, J.; DAVID, M.; GOMES, H.; FERNÁNDEZ, C.; SIMÓN, A.; CAMPOS, I.; LÓPEZ, A., ORVIZ, P., *Provisioning of Grid Middleware for EGI in the framework of EGI-InSPIRE.* **IBERGRID 2010,** 2010, pp. 36-48

CACHEIRO, J. L.; BORGES, G.; GOMES, J.; DAVID, M.; GOMES, H.; FERNÁNDEZ, C.; SIMÓN, A.; FREIRE, E.; DÍEZ, R.; CAMPOS, I.; LÓPEZ, A., ORVIZ, P.
Ibergrid Transition to EGI, **IBERGRID 2010,** 2010 , pp. 24-36
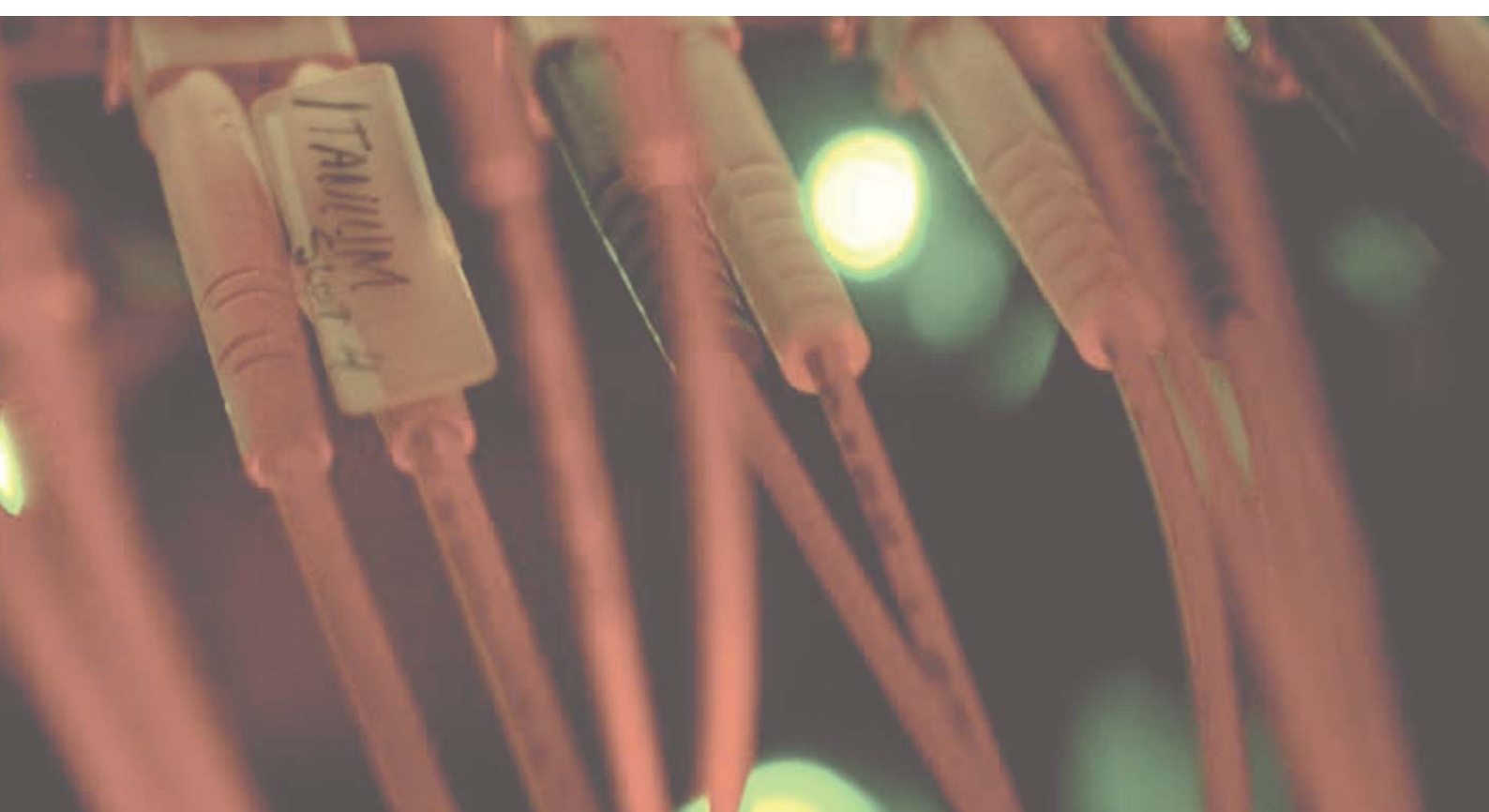
SIMÓN, A.; FERNÁNDEZ, C.; FREIRE, E.; LÓPEZ, J.; DÍEZ, R.; DÍAZ, S., REY, P., *The Metrics Portal: A tool to get statistics about EGEE operations*, **IBERGRID 2010**, 2010, pp. 48-60

VALÍN, R.; SEOANE, N.; GARCÍA-LOUREIRO, A.; ALDEGUNDE, M. & LÓPEZ, J., SMNANOS
Submitting and Monitoring Nanoelectronic Simulation in the VO-MOSFET, I**BERGRID 2010,** 2010, pp. 121-132

2010 Annual Report

www.cesga.es

CESGA