

Cesga's User
Scientific Production

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

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

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

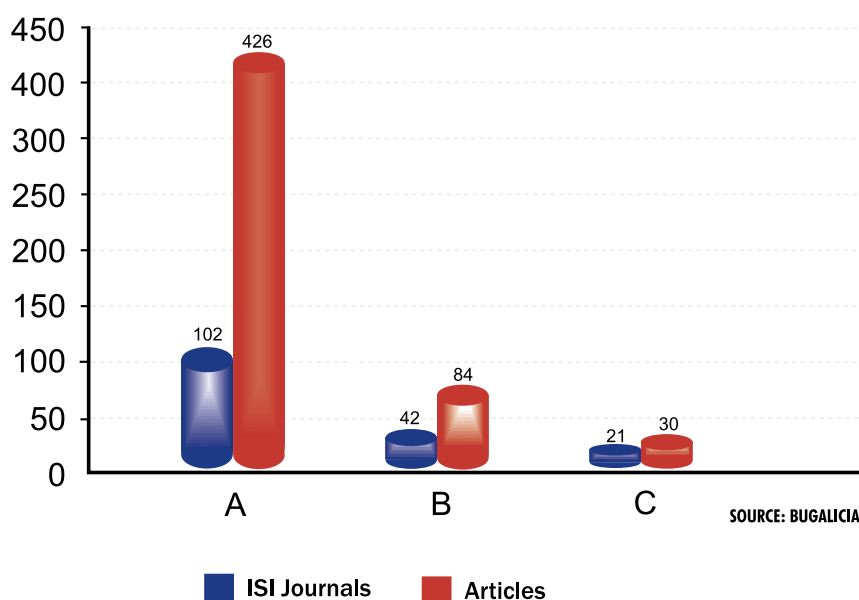
The first of these studies was conducted by BUGALICIA, the Consortium of University Libraries in Galicia, classifying and analysing all of the scientific publications reported by the users between 2002 and 2007. During this period, the scientific production in ISI publications multiplied by 3.18 (from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

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

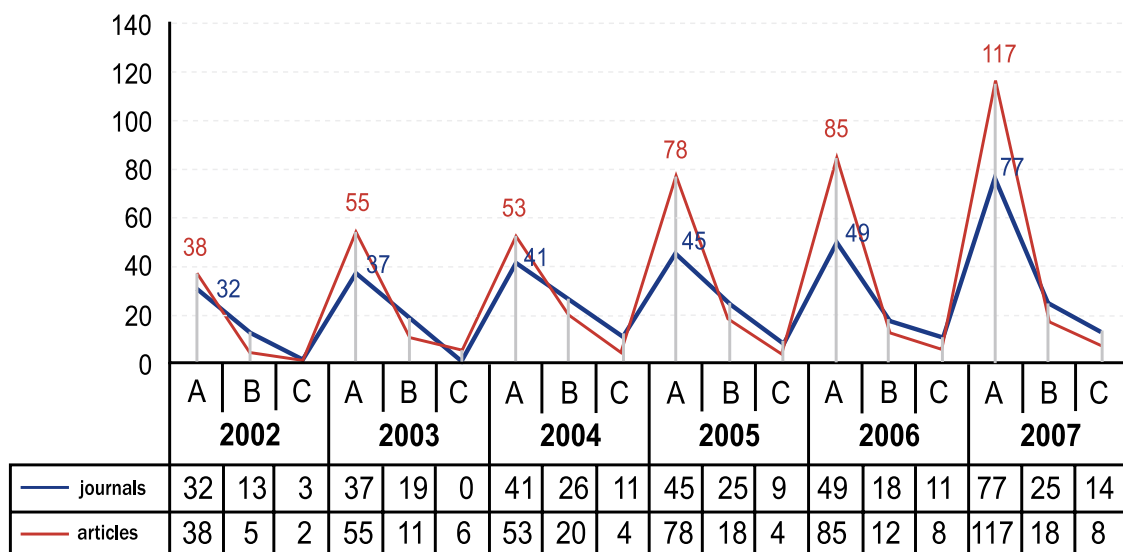
cles were produced was Physics, Atomic, Molecular, and Chemistry.

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

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

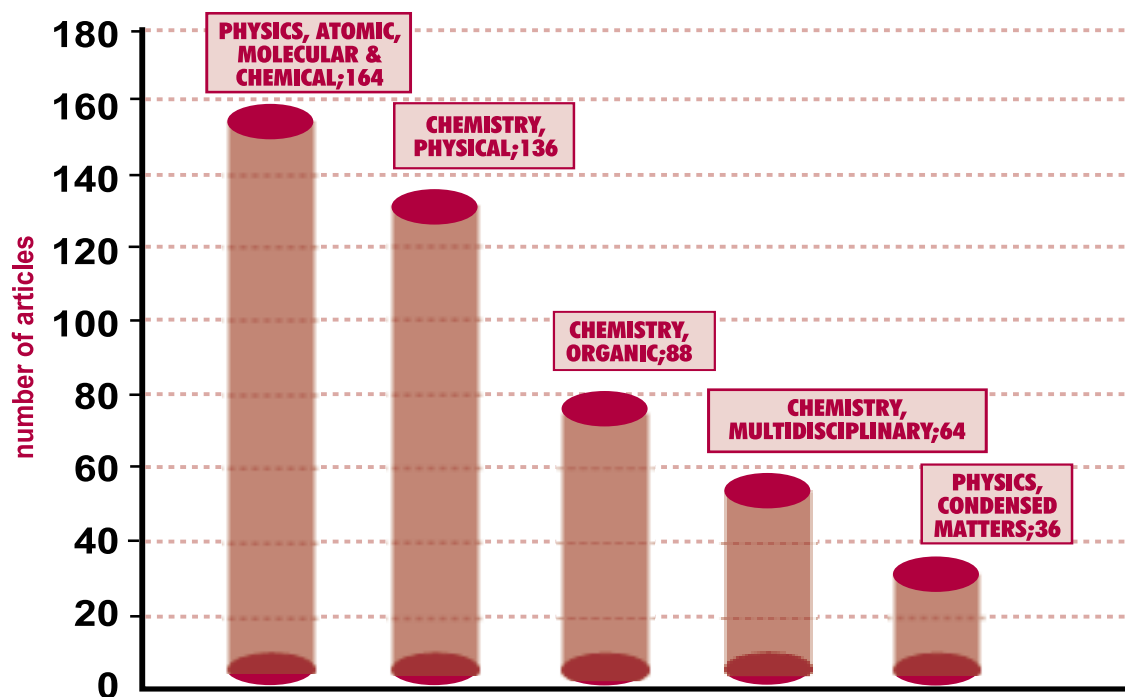


**CESGA'S USERS SCIENTIFIC PRODUCTION 2002-2007
ARTICLE & JOURNAL DISTRIBUTION PER TYPE (A,B,C) AND YEAR**



SOURCE: BUGALICIA

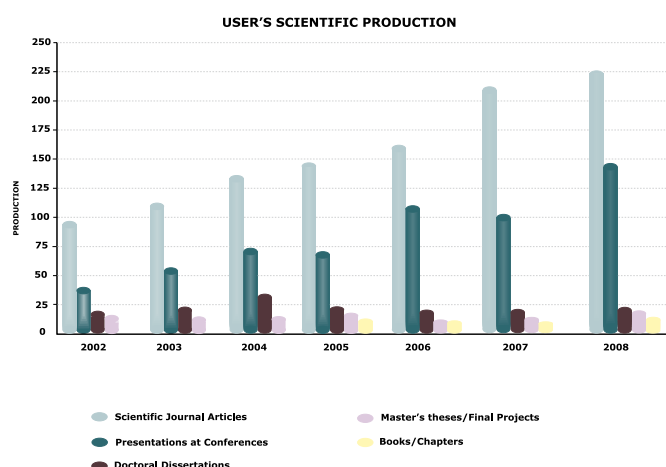
**CESGA'S USERS SCIENTIFIC PRODUCTION 2002-2007
ISI CATEGORIES SHOWING THE HIGHEST PRODUCTION**



SOURCE: BUGALICIA

scientific production reported by CESGA'S users in 2008

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



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

DISTRIBUTION OF SCIENTIFIC PRODUCTION PER YEAR

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

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

DISTRIBUTION OF SCIENTIFIC PRODUCTION DECLARED

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

CESGA AND SERGAS NOT INCLUDED

scientific production reported by CESGA'S users

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

SPANISH NATIONAL RESEARCH COUNCIL (CSIC)

Scientific Articles Published



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

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

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

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

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

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

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

Presentations at Congresses/Conferences

2008 ECOLOGICAL SOCIETY OF AMERICA, ANNUAL MEETING.

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

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

37th INORGANIC REACTION MECHANISMS GROUP MEETING.

Barcelona (Spain), January 2008.

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

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

4th INTERNATIONAL MEETING ON MOLECULAR ELECTRONICS.

Grenoble, (France). 2008.

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

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

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

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

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

San Antonio, Texas (USA). November 2008.

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

CONGRESO MEXICANO DE ECOLOGIA.

Mérida, Yucatán (México) November 2008.

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

ESPA-2008.

Mallorca (Spain) 2008.

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

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

EUROICE2008 AN EXPLORATORY WORKSHOP DE LA EUROPEAN SCIENCE FOUNDATION.

Granada, 1-4th October 2008.

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

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

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

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

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

IBER-2008.

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

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

Crete (Greece). 2008.

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

II ENCUESTRO HPC - CSIC.

Madrid (Spain) 3rd June, 2008.

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

MaCoMuFi 2nd YEARLY MEETING.

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

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

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ANGEL RIVERA CALZADA.

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