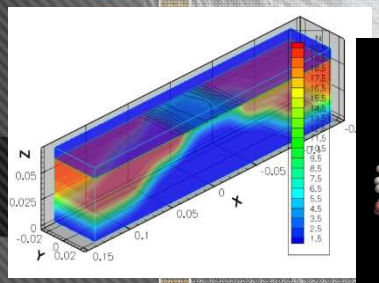
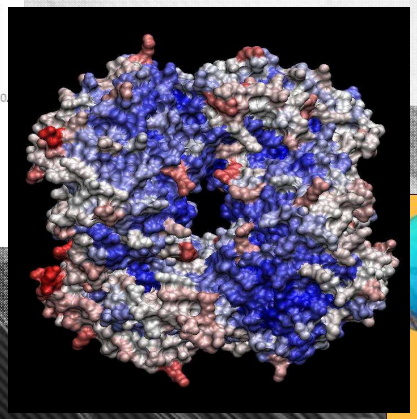
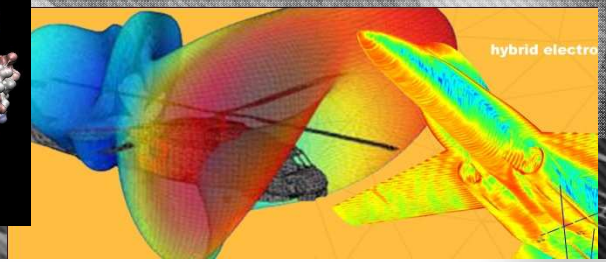
Computational challenges at CESGA-FinisTerrae Supercomputer in Molecular Simulations

FINISTERRAE







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XUNTA DE GALICIA
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CSIC CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

MINISTERIO DE CIENCIA E INNOVACIÓN

FEDER
FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL

ESTABLISHED IN 1993 IN SANTIAGO DE COMPOSTELA

CESGA

CESGA

MISSION STATEMENT

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

To promote the use of new information and communication technologies applied to research within the scientific community of Galicia.

To become a consolidated RTD Centre of Excellence serving as international scientific and technological reference in the field of computational science and numerical simulation.

LEGAL ENTITY

- **Public Foundation**

PARTNERS

- **Regional Government of Galicia** **70%**
- **National Research Council of Spain** **30%**

Xunta de Galicia

CSIC

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CURRENT CESGA'S COMMUNITY OF USERS

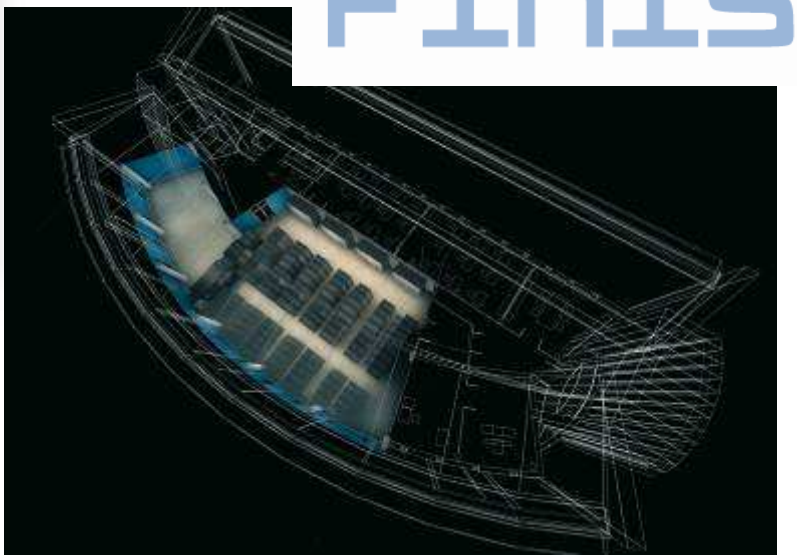
- **Galician Universities**
- **Spanish National Research Council (CSIC) Centres**
- **Galician Regional Government Research Centres**
- **Any researcher from Europe or CYTED Countries (through ICTS call, 20% Finis Terrae)**
- **Other public or private enterprises and institutions**
  - Hospital Laboratories
  - Private Industries R&D Departments
  - Technological & Research Centres
  - Other Universities worldwide
  - Non-profit R&D organizations

SERVICES

- **HPC, HTC & GRID Computing**
- **User Data Storage**
- **Support to scientific application development**
- Advanced Communications Network
- Video streaming broadcast & on-demand
- Remote Learning & Collaboration Room Network
- e-Learning & Collaboration Tools
- GIS (Geographical Information Systems)
- Transfer and Innovation Consulting
- R&D&I Project management

FINIS TERRAE (2007)

FINISTERRAE



HPC (December 2007)

More than **16 TFLOPS** and **19TB RAM** Memory

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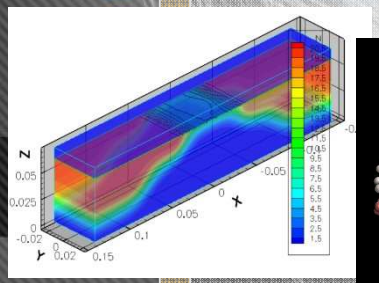
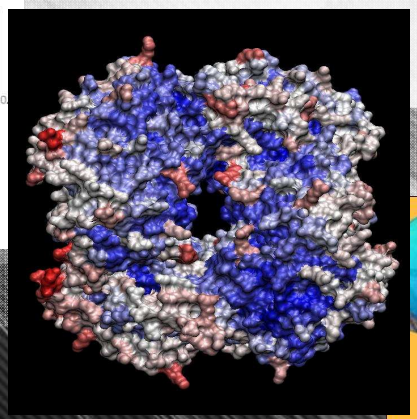
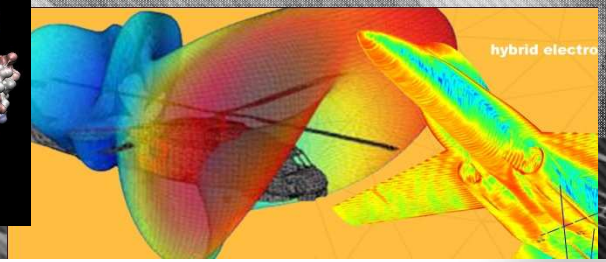
Usage Evolution







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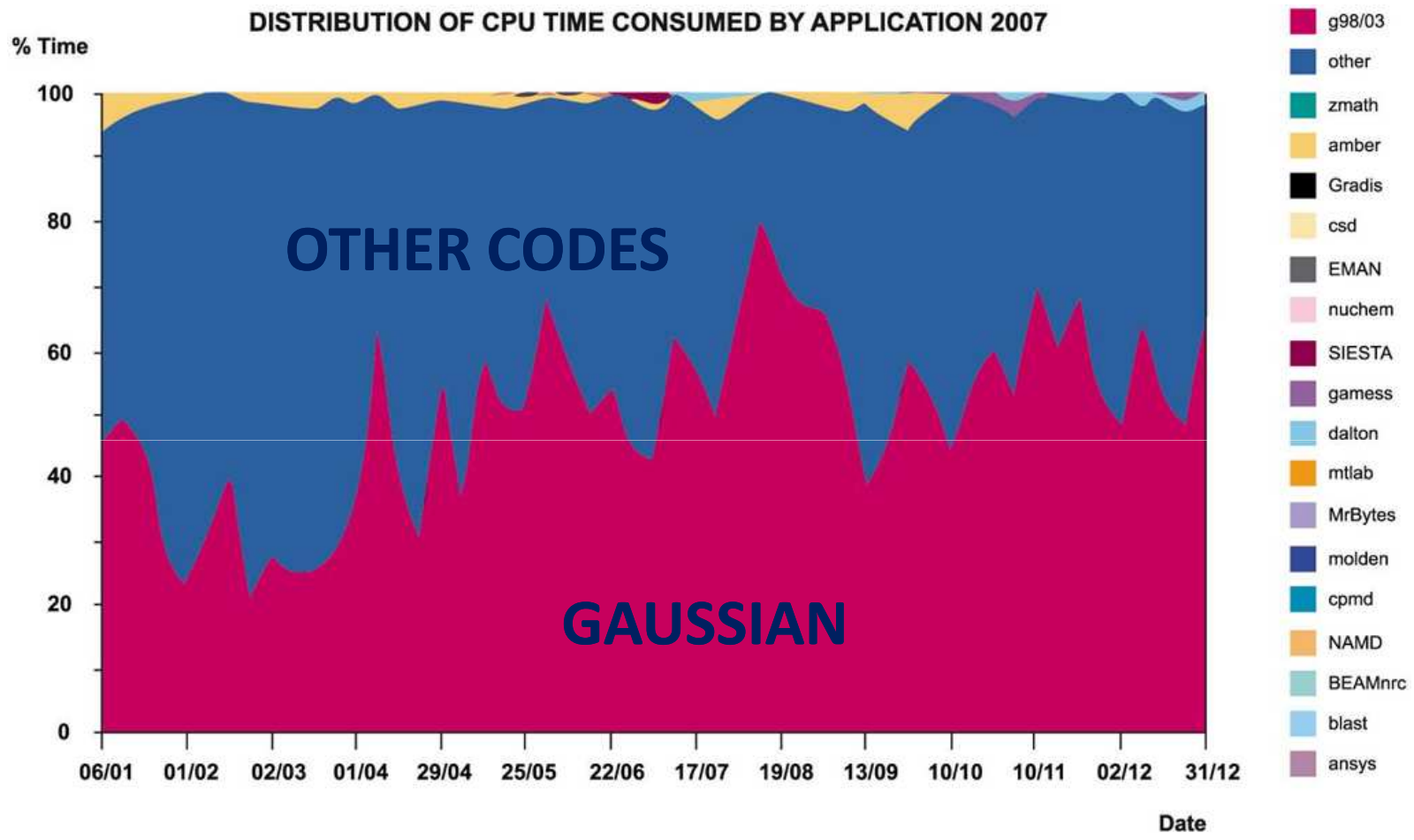
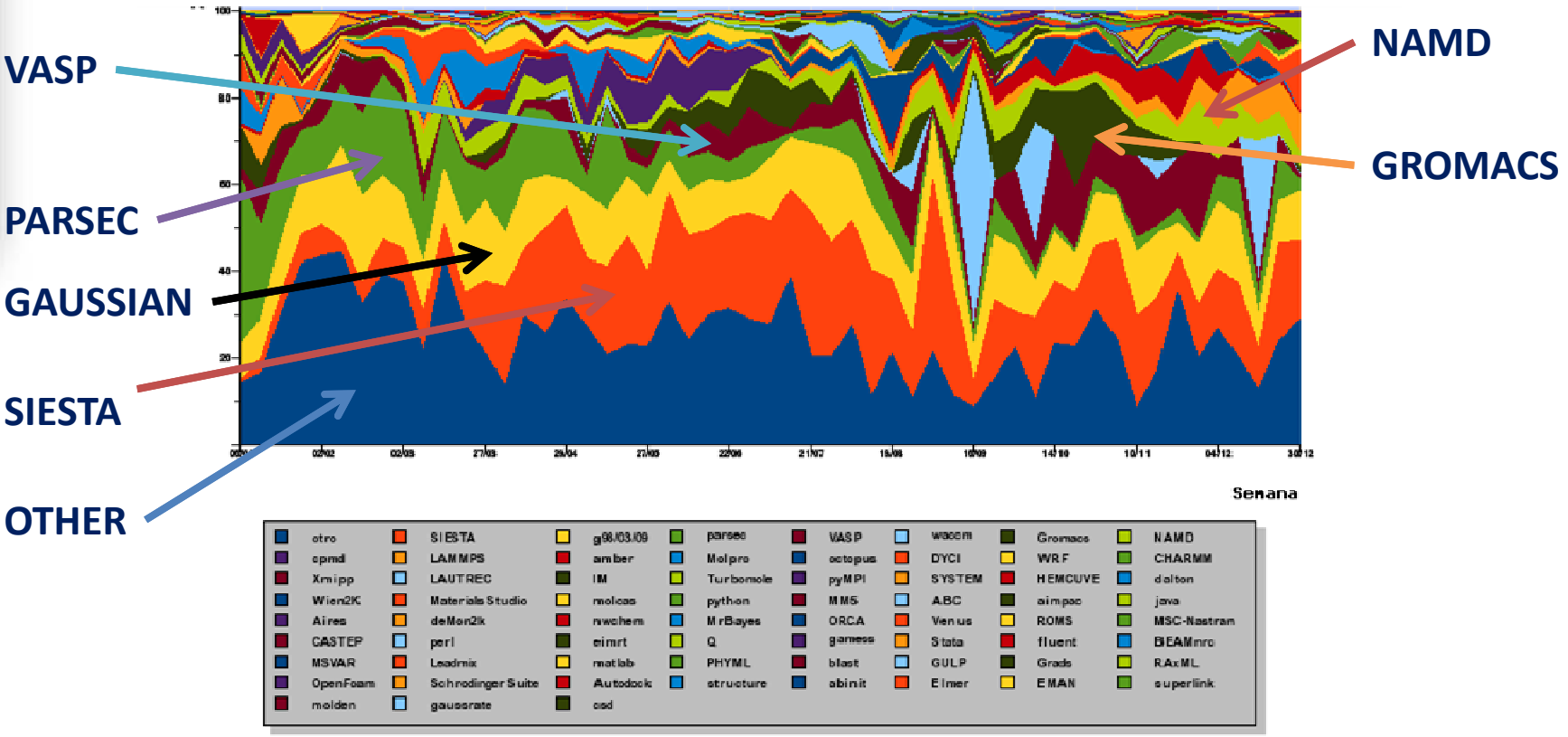
Application distribution 2007

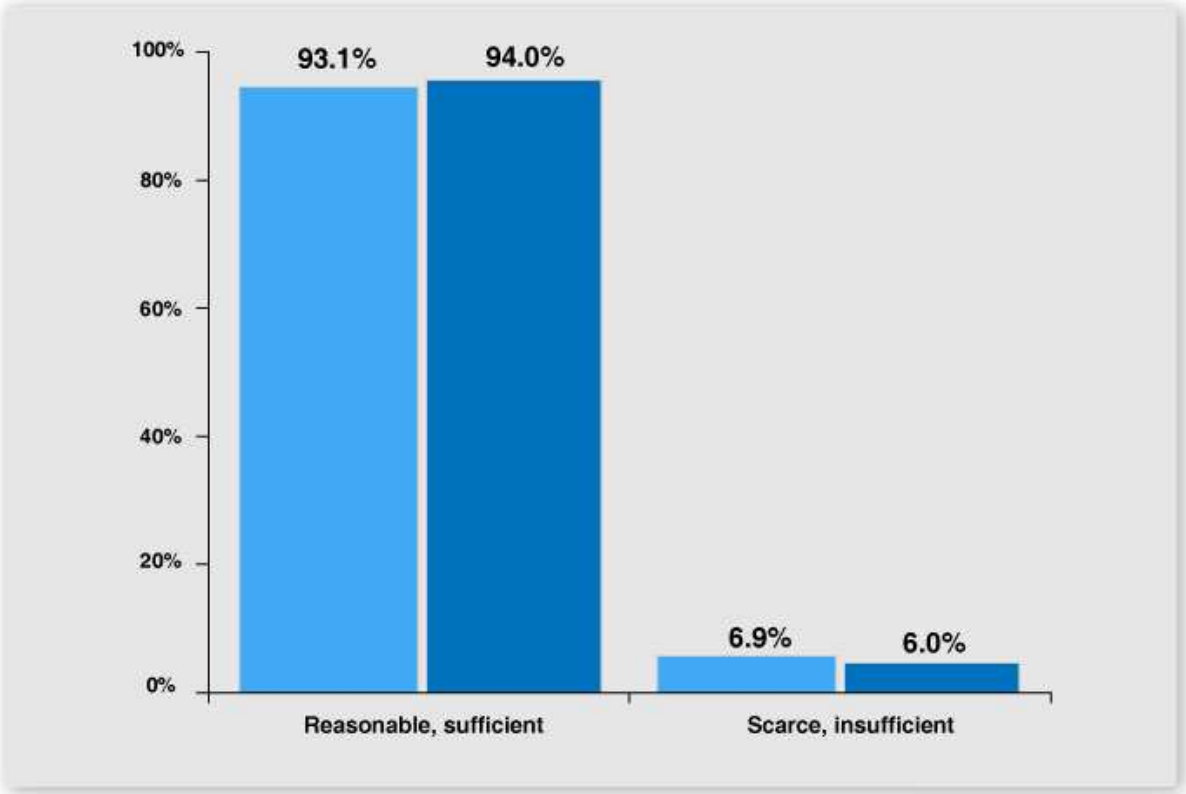


Application distribution 2009



Users' surveys

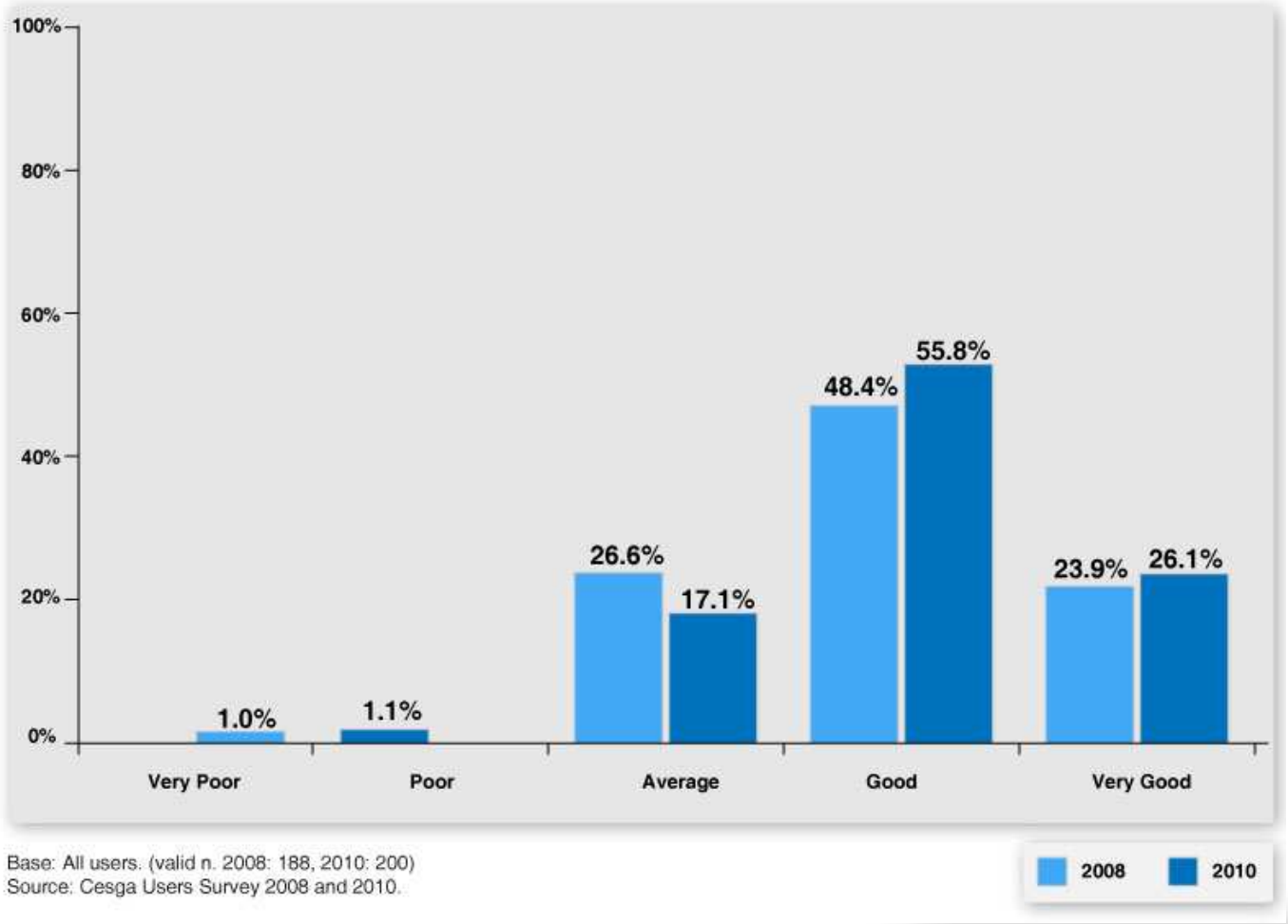
Graph 6: User assesment of the scientific application repertoire avaliable at CESGA. Years 2008 and 2010. Data in Percentages.



Base: All users. (valid n. 2008: 189, 2010: 200)
Source: Cesga Users Survey 2008 and 2010.

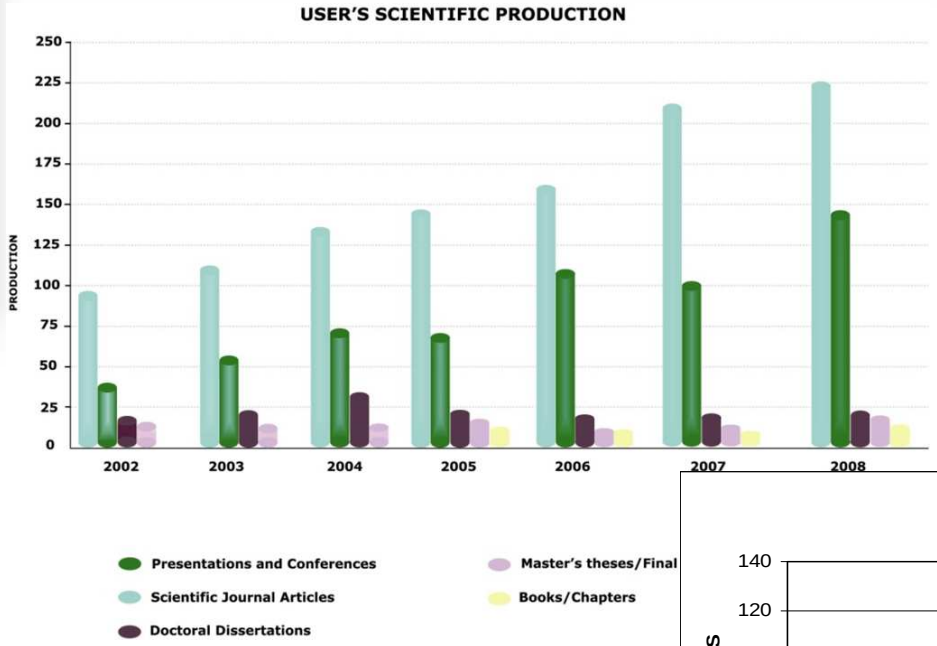
Users' surveys

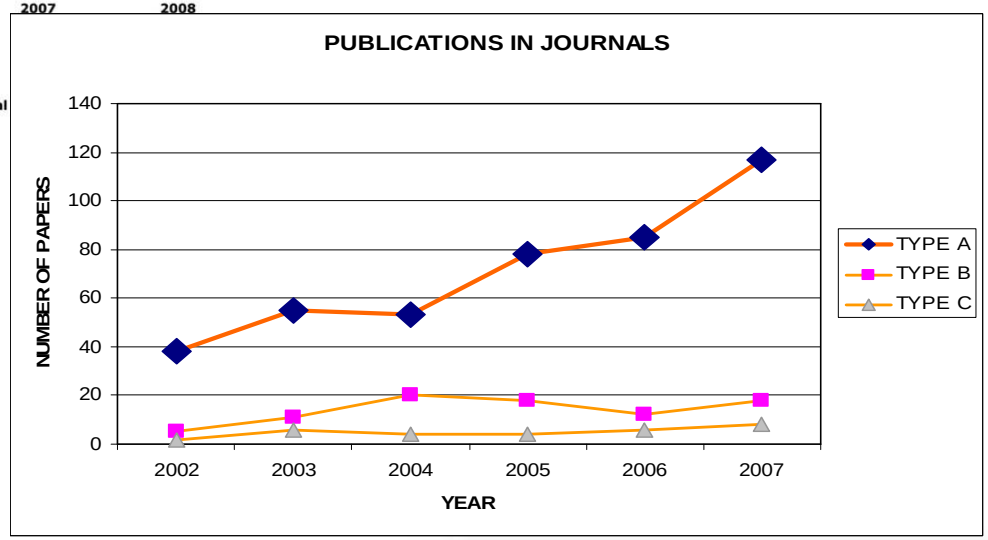
Graph 7: User assesment of the applications support service. Years 2008 and 2010. Data in percentage.



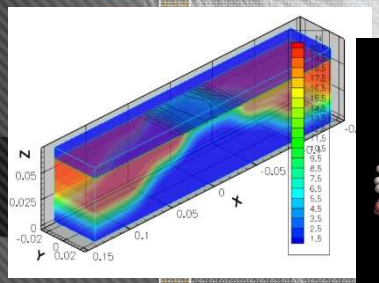
Base: All users. (valid n. 2008: 188, 2010: 200)
Source: Cesga Users Survey 2008 and 2010.

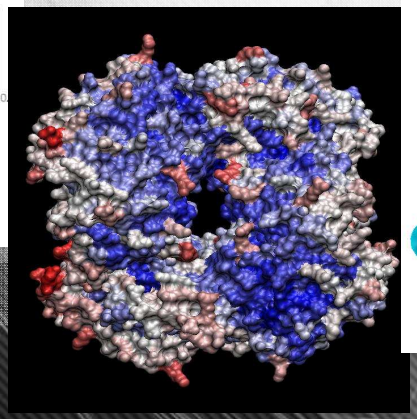
Users' Scientific Production CESGA 2002-2008

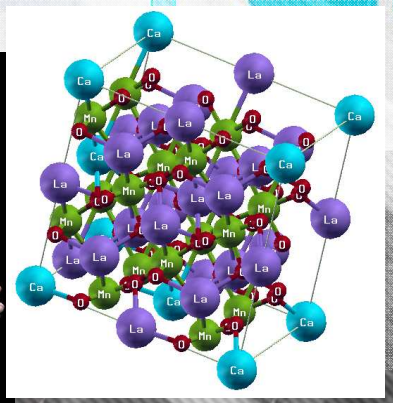




SOME RESULTS







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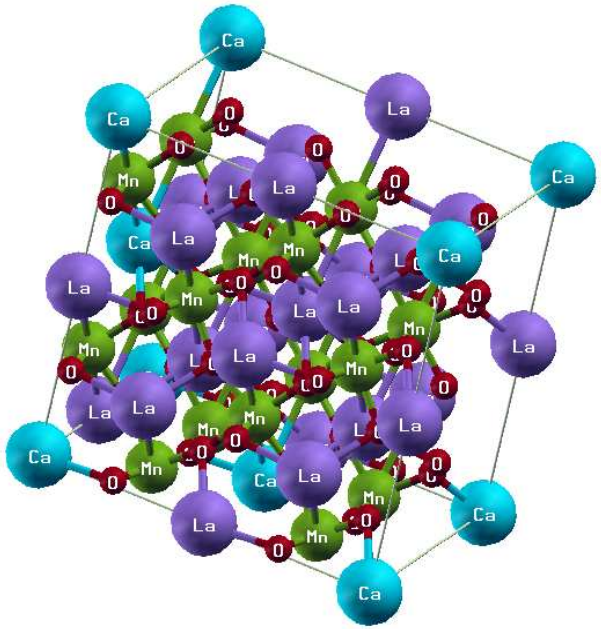
Special Projects: Phase Separation (I)



Phase separation

La1-xCaxMnO3

4º physics problem for American Physical Society (APS)

TNT 2009

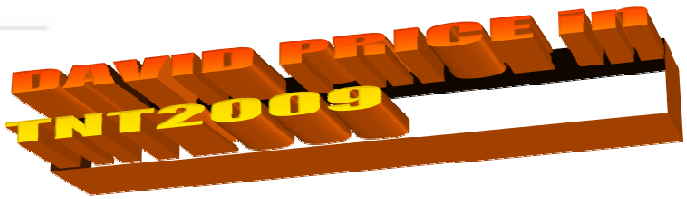
Influence of the Ca^{2+} inhomogeneity distribution in the physical properties of $La_{0.625}Ca_{0.375}MnO_3$

A. Piñeiro[1,2*], V. Pardo[1,2], D. Baldomir[1,2], F. Rivadulla[3], A. Rodriguez[4], A. Gómez[4], J. E. Arias[2], J. Rivas[1,3]

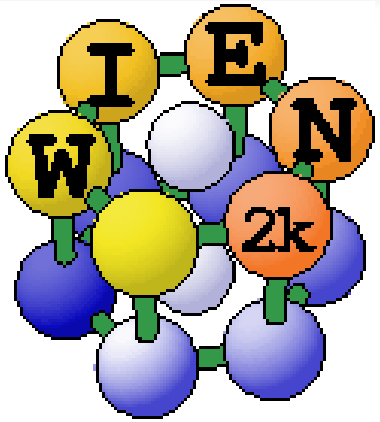
Article first published online: 16 AUG 2010

DOI: 10.1002/pssc.200983822

Issue



Special Projects: Phase Separation (II)



Research Group Resources: cluster with 20 nodes.

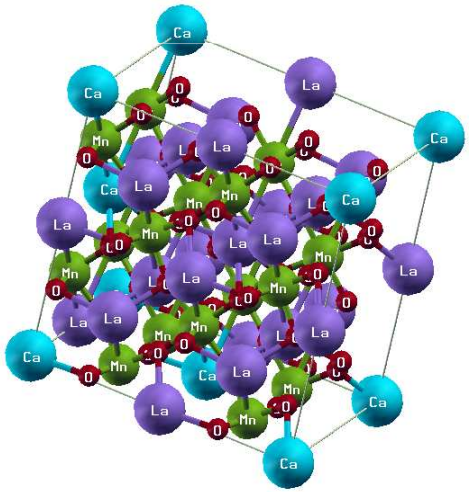
Estimated time: 1 year

Problem: Not enough memory per core

Unfeasible!!!

Resources used at Finis Terrae:

- 24 nodes: 384 cores
- 2-4 GB of memory per core
- Around 70000 CPU hours



Job Done in one month

Special Projects: Phase Separation (III)

Ab-initio calculations.

- Density functional theory-based calculations.
- Augmented Plane Wave + local orbitals methods (APW+lo).
- Program package: WIEN2k v8.1.

Computational details.

- Full potential, all electron scheme, electronic structure calculations.
- Muffin-tin radius (RMTs) values. La: 2.43 a.u. Ca: 2.29 a.u. Mn: 1.96 a.u. O: 1.73 a.u.
- Exchange-correlation effects:
  - Generalized Gradient Approximation (GGA) [3] for structural relaxations calculations.
  - Local Density Approximation + U (LDA+U) [4].
  - Structural relaxation: reduction of 3% of the RMTs.

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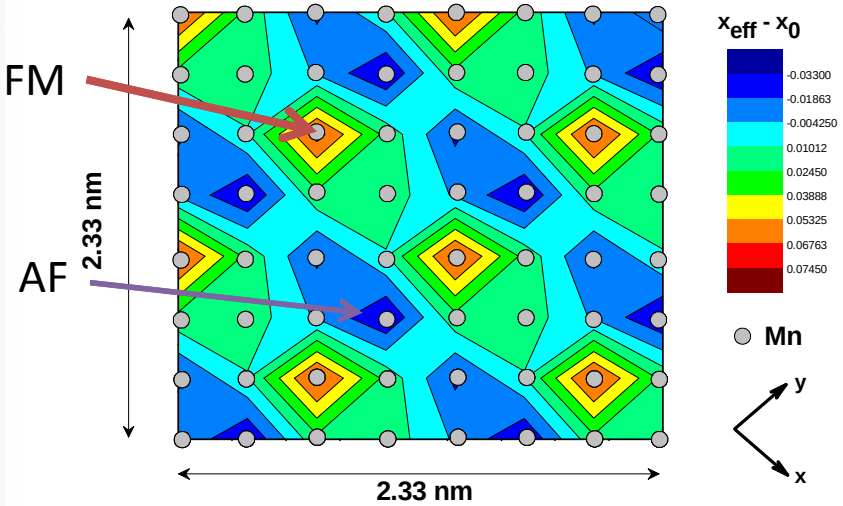
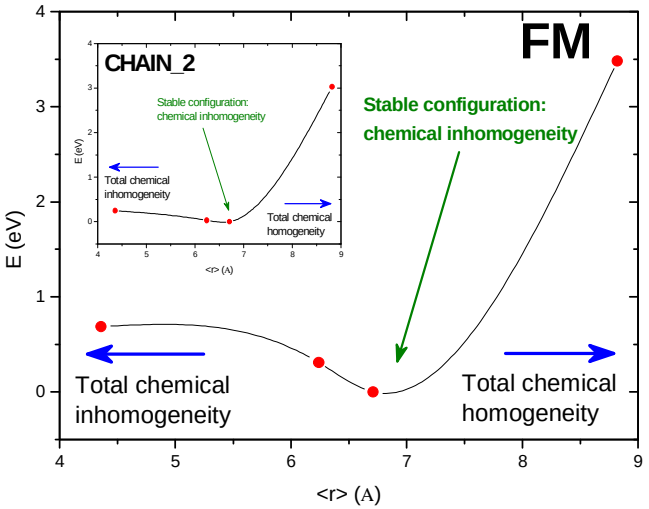
Special Projects: Phase Separation (IV)

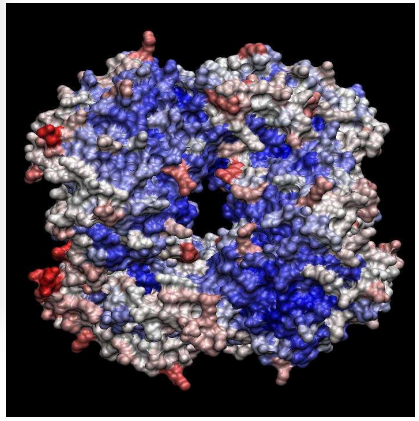
Results.

- magnetism alone cannot drive phase separation.
- nanoscale doping inhomogeneities are the driving force of the phase separation phenomenon in manganites.





Dynamic Enzyme Response against Temperature

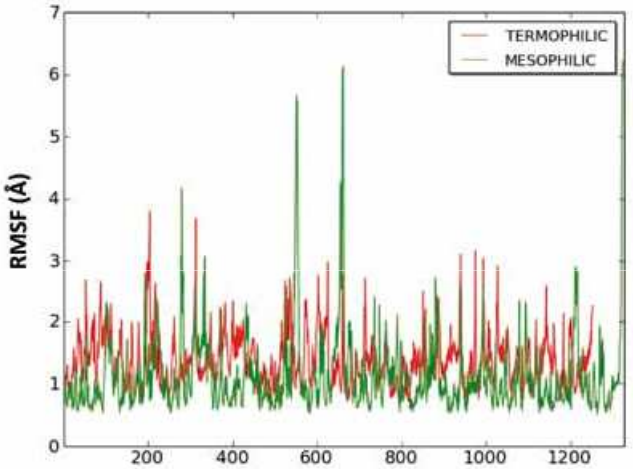


OBJECTIVE: Better understand the relationship between the structure/dynamic/enzyme activity

Institut de Química Avançada de Catalunya

TOOLS:

- *Gromacs 4.0*
- *Scaling up to 72 cores (8 cores/node)*
- *more than 10 ns/day*



RESULTS:

Mesophilic enzymes are unstable at high temperatures, whereas thermophilic enzymes have highest activity at these elevated temperatures.

Although the thermophilic enzyme is more flexible, its flexibility is more homogeneous.

Mesophilic organism has some regions of extremely high mobility which can potentially lead to denaturation of the enzyme and, consequently, loss of function

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Development Support: MAD-WAVE3

Special example of support in parallelization (using MPI) and optimization of a Quantum Molecular Dynamics user code:

✔ Better Performance

✔ Improved Scaling

As result: A collaborative publication ...

14488 *J. Phys. Chem. A* **2009,** *113,* 14488–14501

Differential Cross Sections and Product Rotational Polarization in A + BC Reactions Using Wave Packet Methods: $H^+ + D_2$ and Li + HF Examples†

A. Zanchet,‡ O. Roncero,*,‡ T. González-Lezana,‡ A. Rodríguez-López,§ A. Aguado,⊥ C. Sanz-Sanz,‡,# and S. Gómez-Carrasco‡,¶

Instituto de Física Fundamental, CSIC, Unidad Asociada UAM-CSIC, Serrano 123, 28006 Madrid, Spain, Centro de Supercomputación de Galicia, Av. de Vigo s/n (Campus Sur), 15706 Santiago de Compostela, Spain, and Departamento de Química Física, Facultad de Ciencias C-XIV, Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, 28049, Madrid, Spain, School of Chemistry, University of Birmingham, Edbaston, Birmingham B15 2TT, United Kingdom, and Theoretical Chemistry Department, Institute of Physical Chemistry, University of Heidelberg, Im Neuenheimer Feld 229, D-69120 Heidelberg, Germany

Received: April 28, 2009; Revised Manuscript Received: June 24, 2009

A service for Development Support

Development Support

A service helping to the development of user software.

✔ Programing help and collaboration in several languages

✔ Optimization of the already existing code

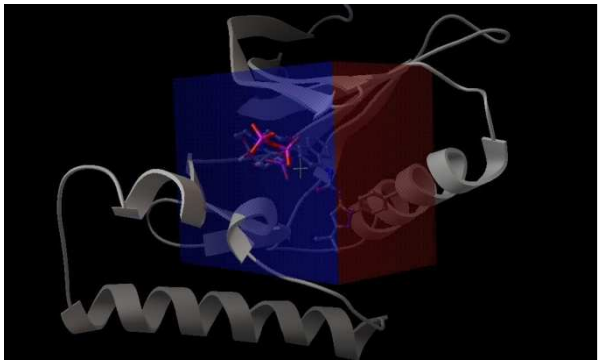
✔ Help for the implementation of solutions combining different computing technologies.

✔ Development of projects of a maximum of 4 months with tight collaboration between the user and the technician.

http://www.cesga.es/File/Computacion/DO_Solicitud_Servicio_desarrollo_v1_en.doc

Scientists Against Malaria (SAM) Synergy Pilot project

OBJECTIVE: Virtual Screening on Pf-MAPK using Vina (MGLab) and Glide (Schrödinger)



TOOLS: Cloud Computing for Virtual Screening

Collaborative experience between:

- Research Group Fundación Pública Galega de Medicina Xenómica
- Centro de Supercomputación de Castilla y León
- CESGA

FCSCL

Fundación Pública Galega de Medicina Xenómica

40 nodes (320 cores Intel Xeon E5520 @ 2.27GHz)

Vina:

- Over 1280000 molecules
- 13 days computation time

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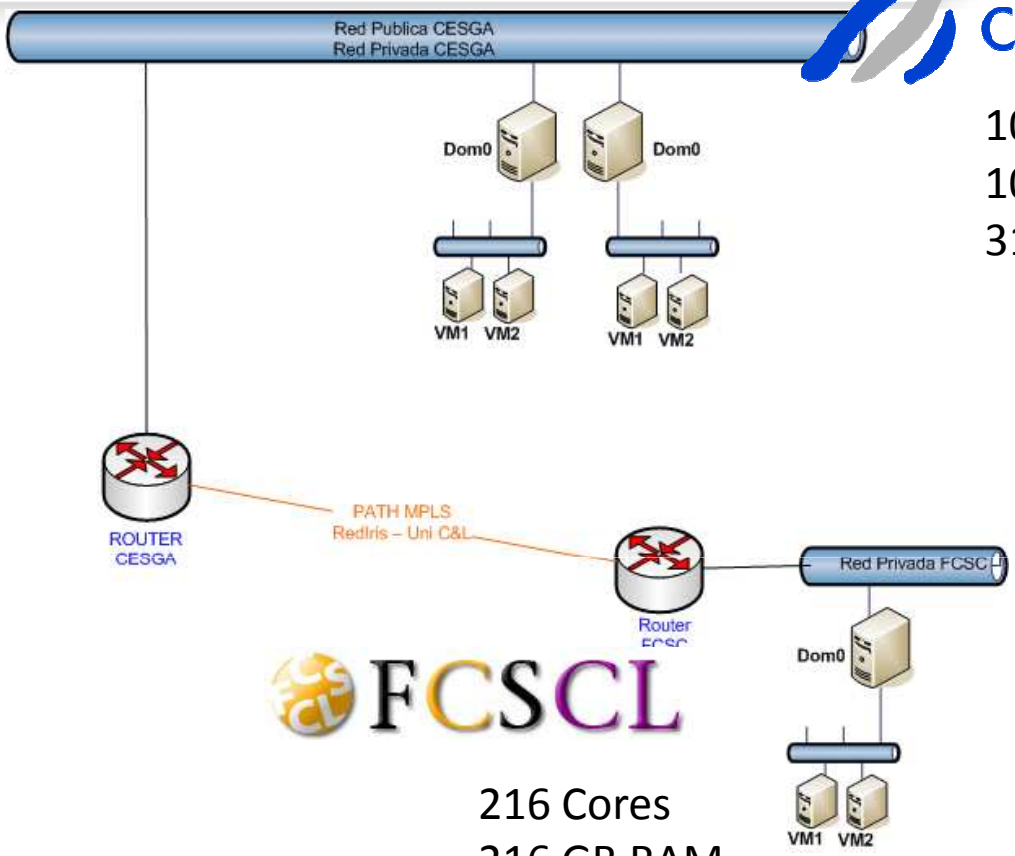
Scientists Against Malaria (SAM) Synergy Pilot project



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106 Cores
106 GB RAM
313 GB HD

FCSCL

216 Cores
216 GB RAM
1420 GB HD

OpenNebula.org
The Open Source Toolkit for Cloud Computing

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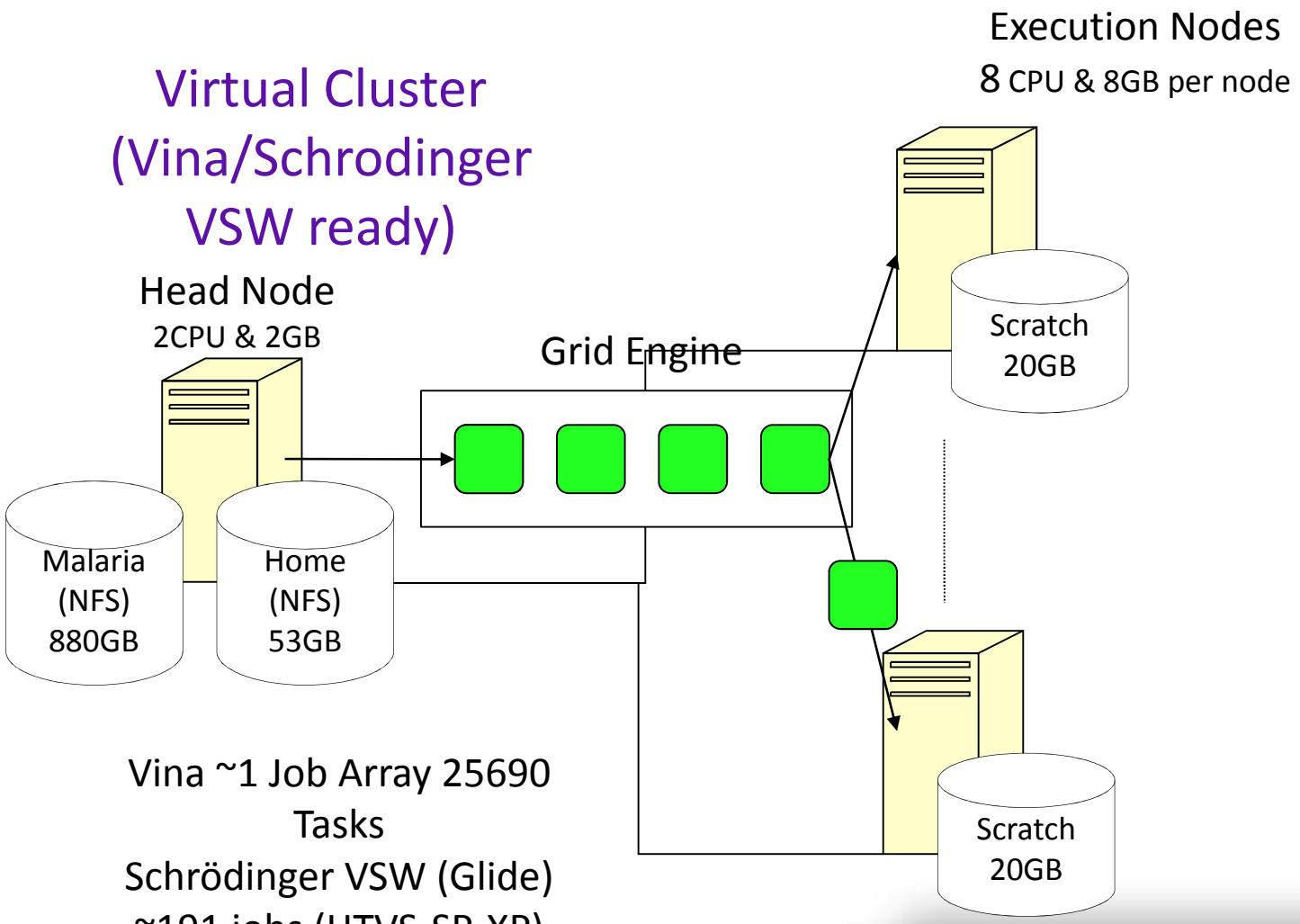
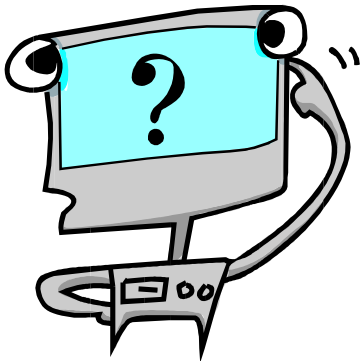


END

THANK YOU!

QUESTIONS



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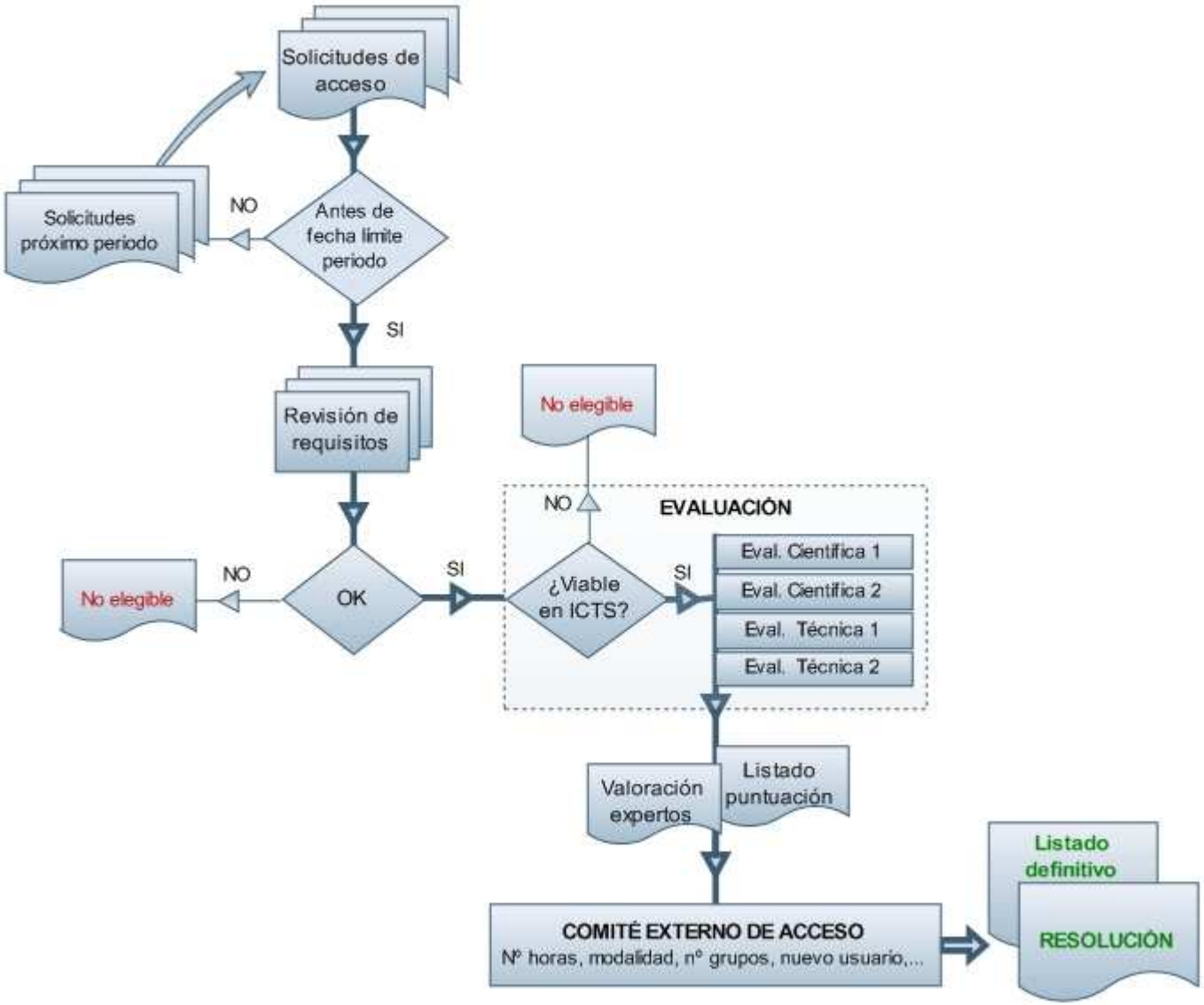
http://www.cesga.es

ICTS- Selection



ICTS-Projects

Period 1

	Nº access	Priority Hours	Non-Priority Hours	Total Hours
Modality 1:	4	261.000	0	261.000
Modality 2:	12	1.711.202	627.838	2.339.040
TOTAL	16	1.972.202	627.838	2.600.040
Period 2				
Modality 1:	3	222.000	228.000	450.000
Modality2:	7	376.000	609.000	985.000
TOTAL	10	598.000	837.000	1.435.000
AÑO 2010				
TOTAL	**26**	**2.570.202**	**1.464.838**	**4.035.040**