CENTRO DE SUPERCOMPUTACIÓN DE GALICIA

CESGA

Advanced computing services for the research community

(September 2009)

Ignacio López Cabido

(Technical Deputy Subdirector, Galicia Supercomputing Centre)

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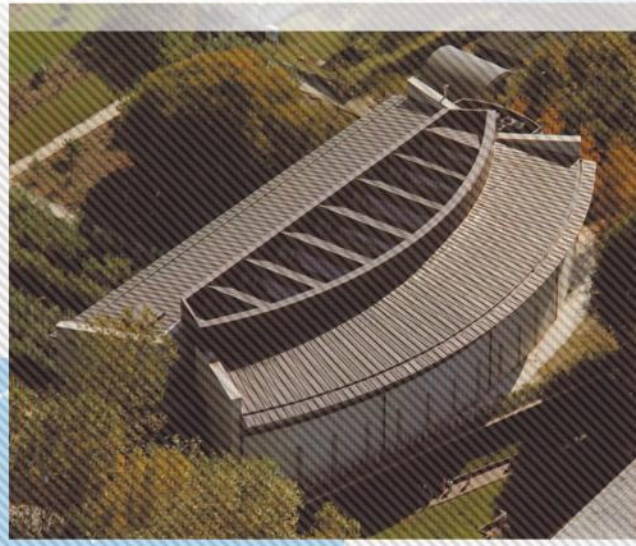
Outline

- Who we are
- Services
- Some plans
- Applications
- Challenges

ESTABLISHED IN 1993 IN SANTIAGO DE COMPOSTELA (SPAIN)

CESGA



CESGA

MISSION STATEMENT

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.

To promote high quality research in Computational Science in close collaboration with the research community from Galicia as well as from other regions or countries all over the world; contributing in this way to the advancement of science, to transfer technology to industry and administrations , and as consequence, to the welfare of society as a whole.

LEGAL ENTITIES

- Public Company
- Public Foundation

PARTNERS

- Regional Government of Galicia
- National Research Council of Spain

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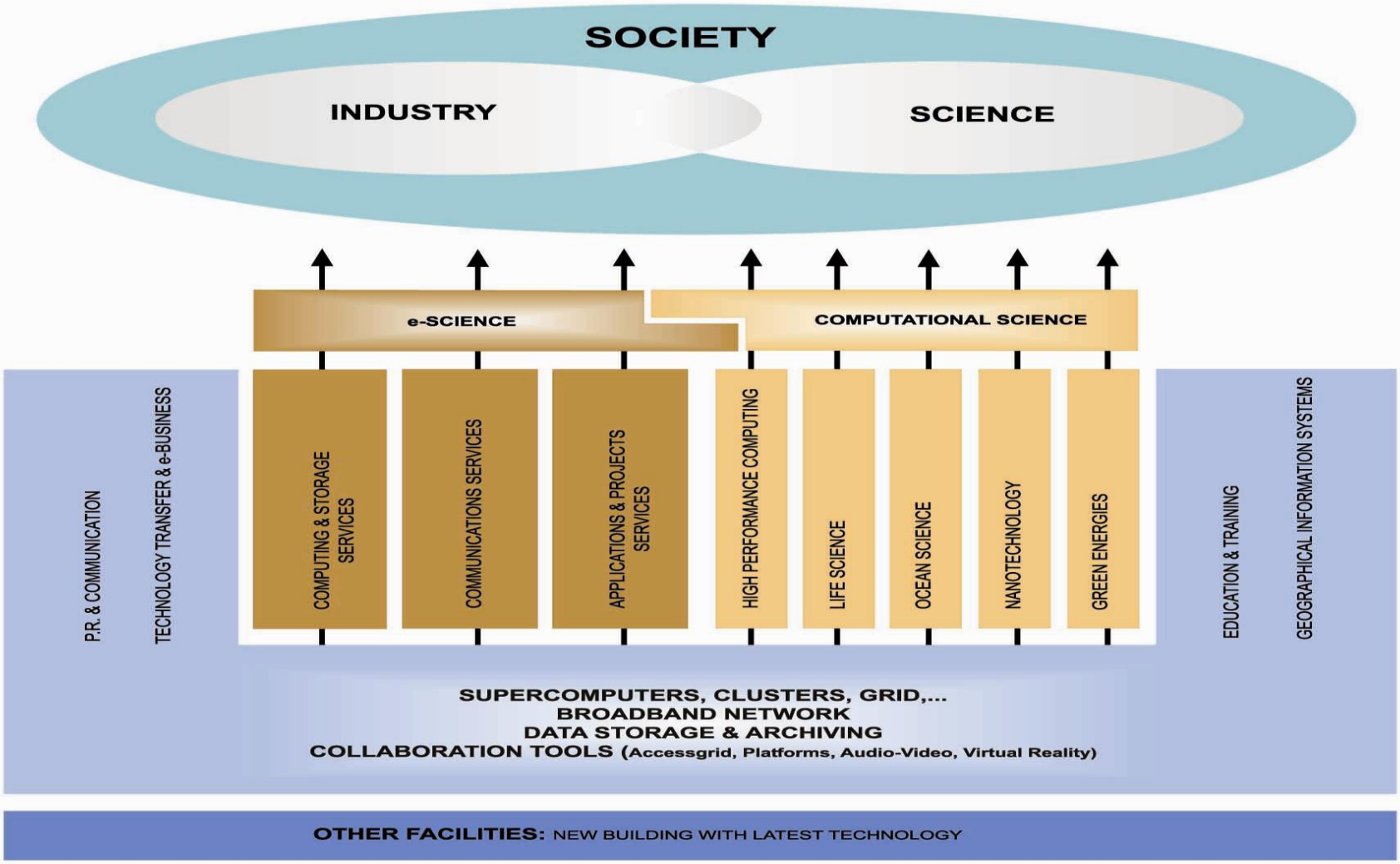
CSIC

FUNCTIONAL SCHEME



AREAS OF ACTIVITY

RESEARCH

CESGA - C²SRC

(CESGA – Computational Science Research Centre)

- Starting date: 2009
- Staff: 115 Researchers & Technicians(recruiting)

ADVANCED SERVICES & INNOVATION

- Starting date: 1.993
- Staff: 60, currently

CESGA - C²SRC

CESGA COMPUTATIONAL SCIENCE RESEARCH CENTRE

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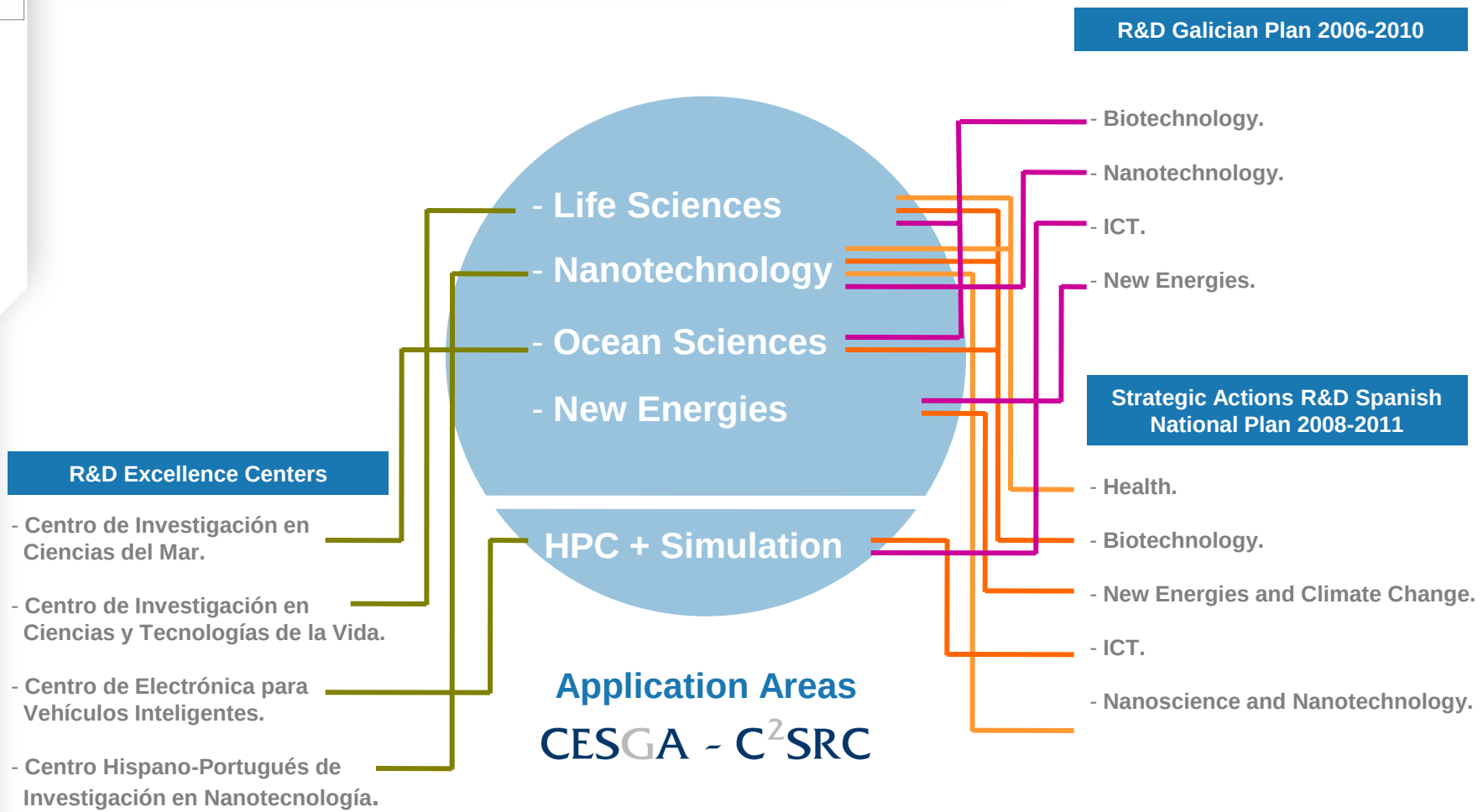
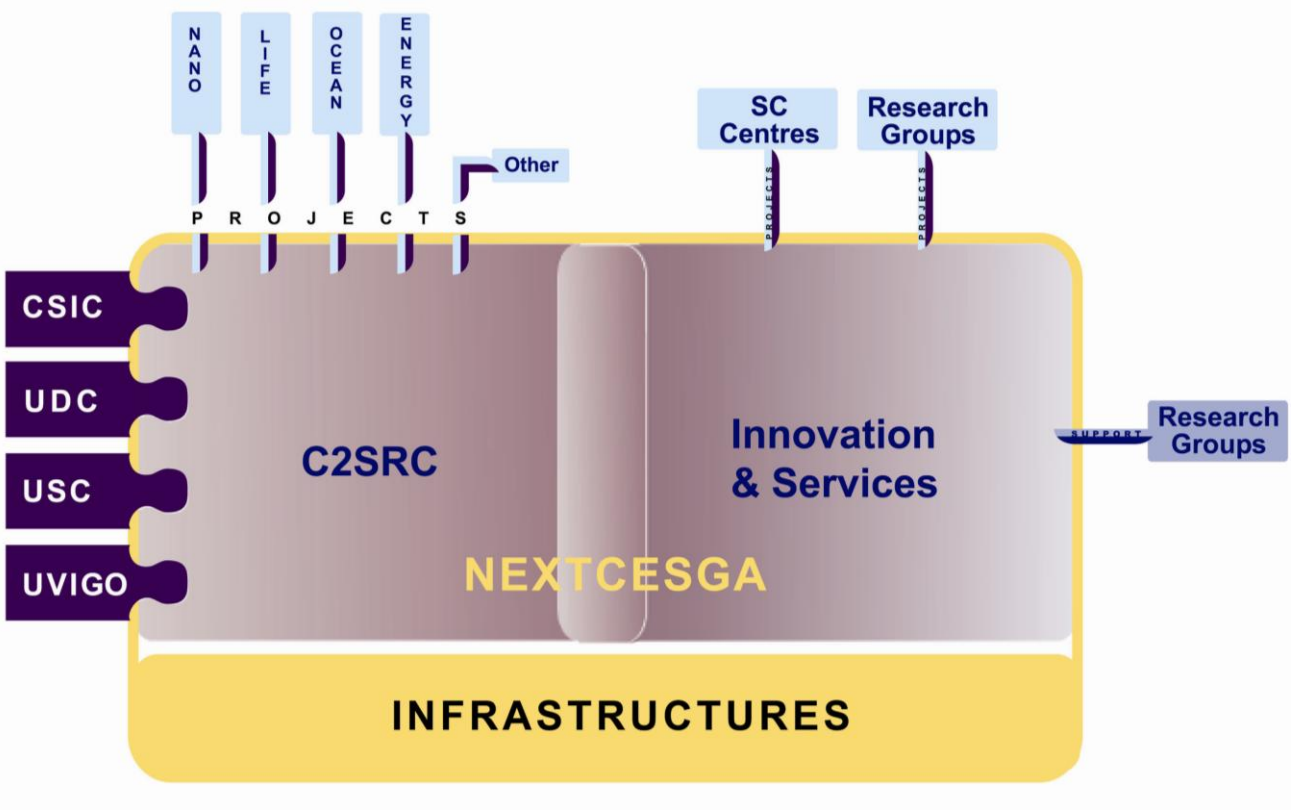
- **Application Areas:**
  - Strategic for Galicia.
  - High demand of HPC resources.
  - Research experience in Galicia and CSIC.
  - Singular in Galicia and CSIC.

CENTER STRUCTURE



CENTER STRUCTURE FOR THE FUTURE



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CESGA-ADVANCED SERVICES And INNOVATION

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CURRENT CESGA's COMMUNITY OF USERS

- **Galician Universities**
- **Galician Regional Government Research Centres**
- **Spanish National Research Council (CSIC) Centres**
- **Other public or private organizations worldwide**
  - Hospital R&D Departments
  - Industries R&D Departments
  - Technological & Research Centres
  - Other Universities worldwide
  - Non-profit R&D organizations

USERS´ SERVICES

- HPC, HTC & GRID Computing
- User Data Storage
- Advanced Communications Network
- e-Learning & Collaboration Infrastructures
- GIS (Geographical Information Systems)
- Technology Transfer to Industry and e-Business
- Public Relations Department

TECHNOLOGY
CESGA'S TECHNOLOGICAL EVOLUTION: INSTALLED SERVERS

1993
VP 2400

2.5 GFLOPS

1998
VPP 300 **AP 3000**

14.1 GFLOPS 12 GFLOPS

1999
HPC 4500

9.6 GFLOPS

2001
SVG

9.9 GFLOPS

2002
HPC 320 **BEOWULF**

64 GFLOPS 16 GFLOPS

2003
SUPERDOME

768 GFLOPS

2004, 2005, 2006
SVG

3,142 GFLOPS

2007
FINISTERRAE

16,000 GFLOPS

Installation Year	1993	1998	1999	2001	2002	2003	2004	2005	2006	2007
Capacity				SVG			SVG	SVG	SVG	
Capability	VP2400	VPP300E AP3000	HPC4500		HPC320	SUPERDOME				FINIS TERRAE

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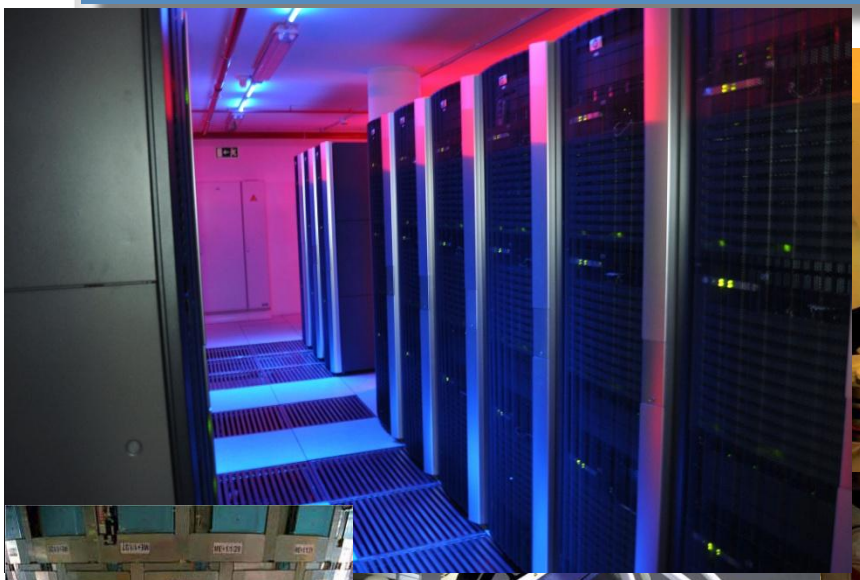
FINIS TERRAE

Spanish National Singular Scientific & Technological Infrastructure

More than: **16,000 GFLOPS** **2,580 CPUs** **19,640 GB Memory**

LINUX, UNIX, WINDOWS

ICTS: Unique S &T Infrastructure
Required to conduct research that strives for excellence



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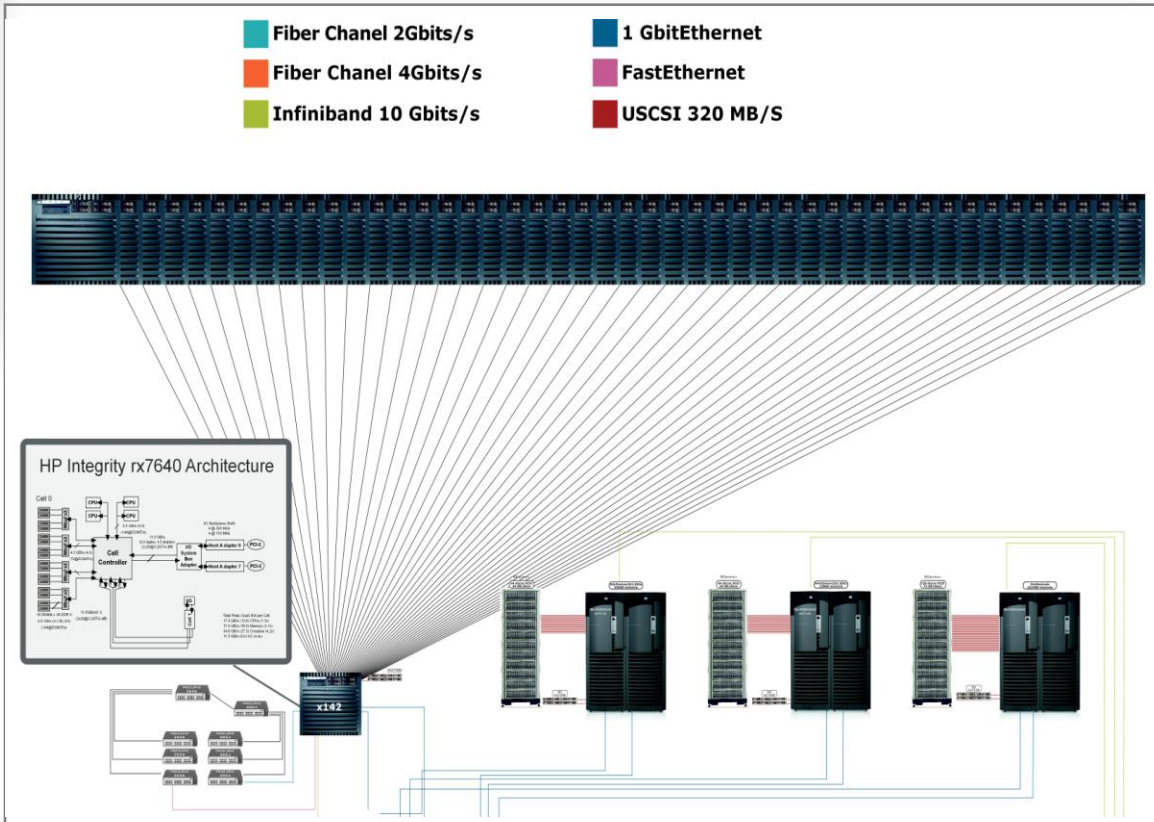
FINIS TERRAE – COMPUTING NODES



SUPERCOMPUTING NODES:

147 cc-NUMA Nodes with Itanium CPUs connected through a high efficiency INFINIBAND network

- **1 node: 128 cores, 1,024 GB memory**
- **2 nodes: 64 CPUs, 128+256 GB memory**
- **142 nodes: 16 cores, 128 GB memory**
- **2 nodes: 4 cores, 4 GB memory for testing**

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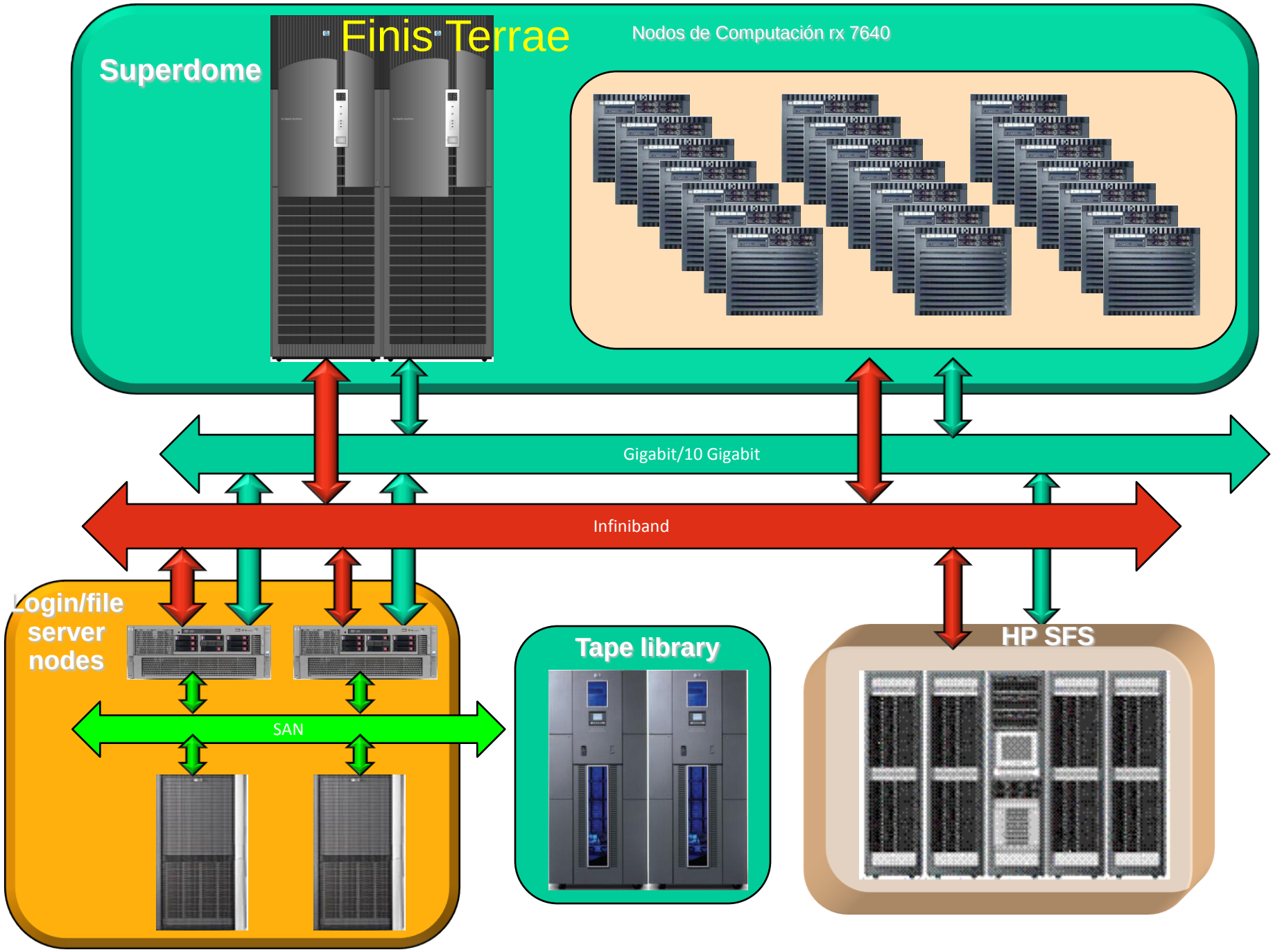
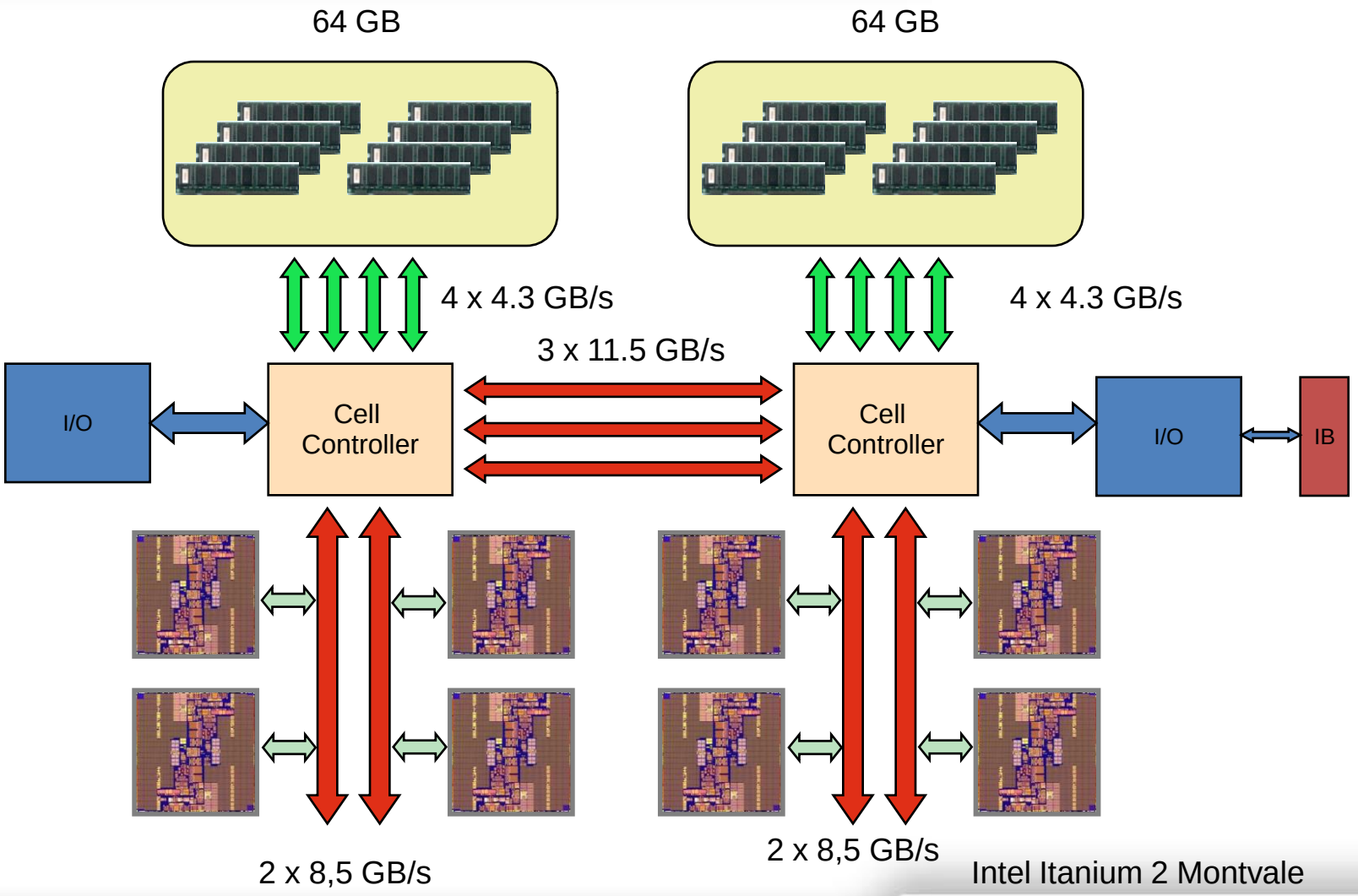
ERDF European Regional Development Fund
FEDER FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL

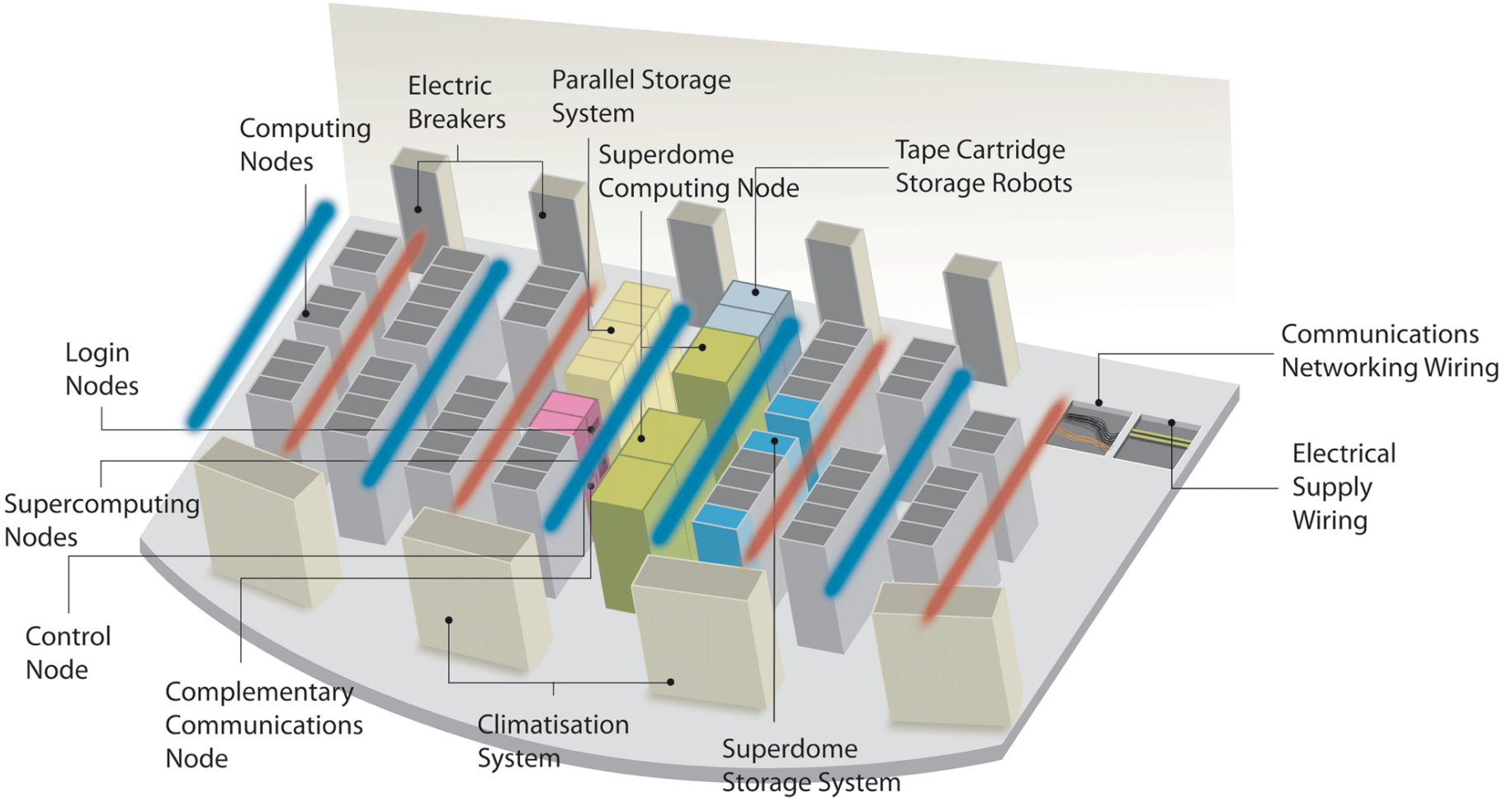

Finis Terrae
Superdome
Nodos de Computación rx 7640
Gigabit/10 Gigabit
Infiniband
Login/file server nodes
SAN
Tape library
HP SFS

RX 7640 Architecture



Intel Itanium 2 Montvale

The Finis Terrae Cluster



Technical Specs.

Surface Area: 140 m²

Weight:
35.000 Kg

Storage:
2.200.000 GB on tape
390.000 GB on disk

Memory:
19.670 GB

2.528 Processing Cores
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

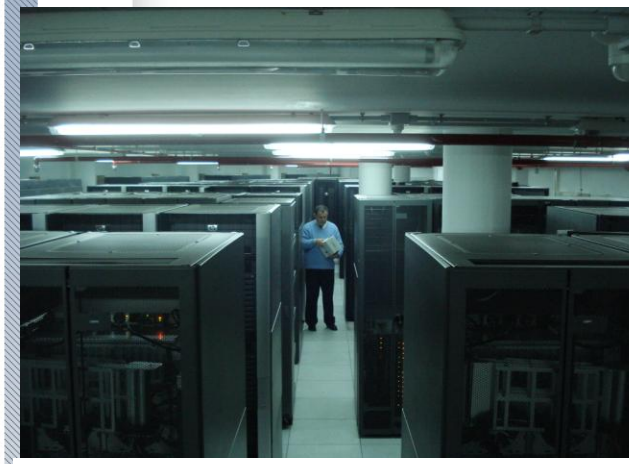
Node Interconnect INFINIBAND 4x DDR at 20 Gbps
85 Km of interconnect cable
Open Software: Linux, Lustre, Globus...

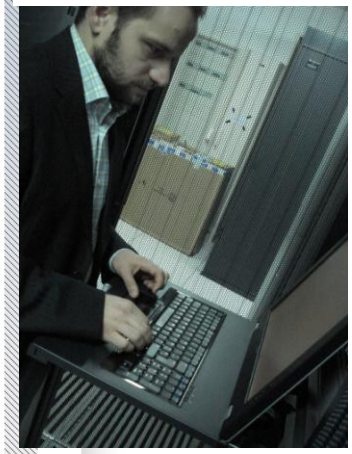
ISO 9001

DNV

CERTIFICATED FIRM

FINISTERRAE





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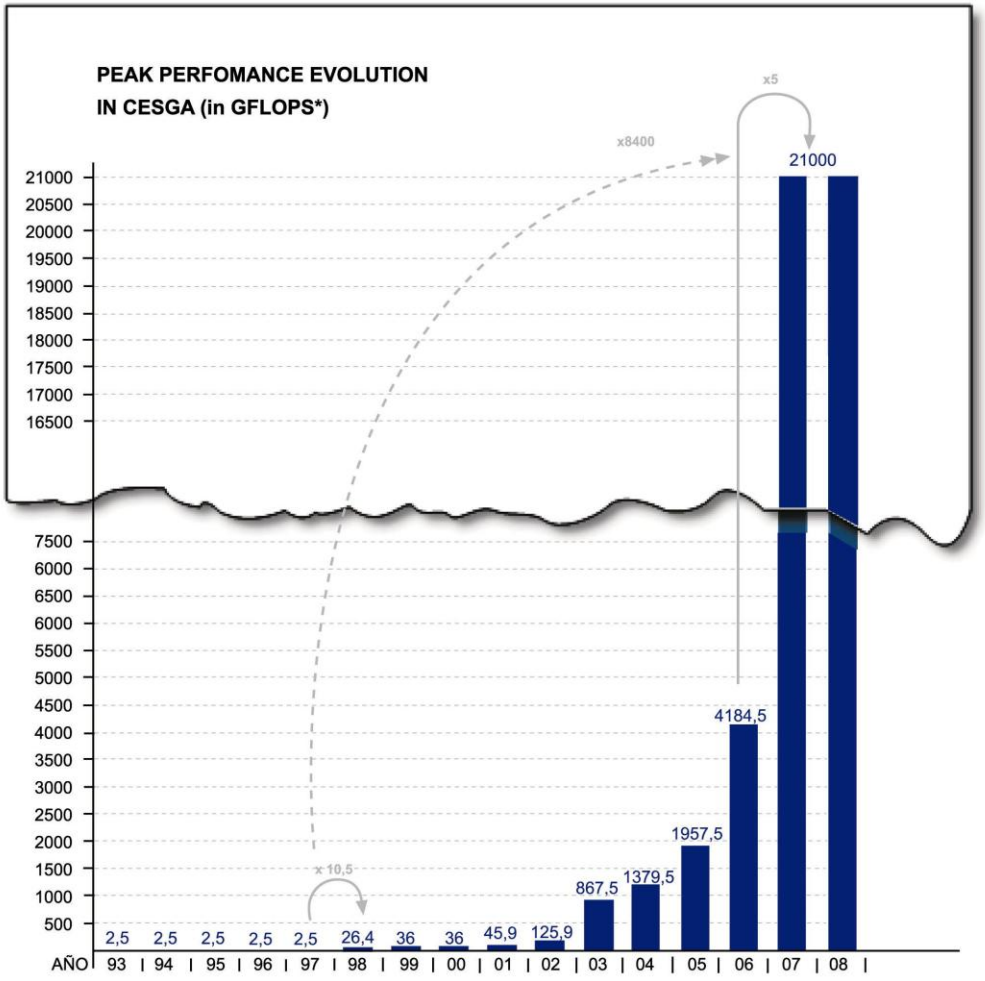
CESGA'S PEAK PERFORMANCE EVOLUTION



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

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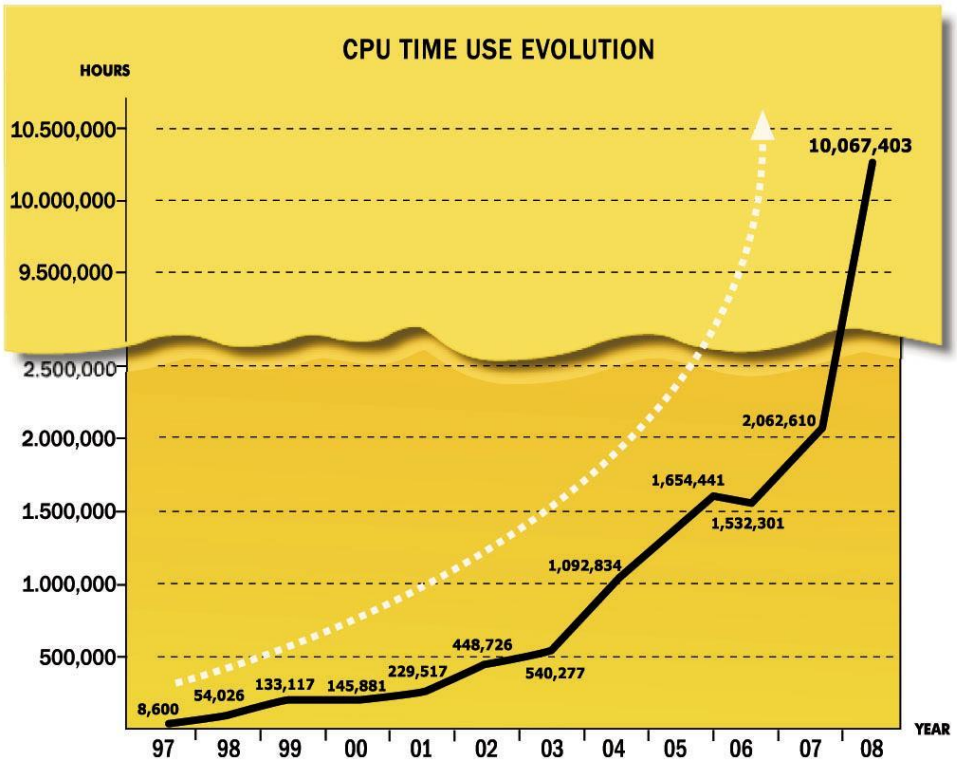
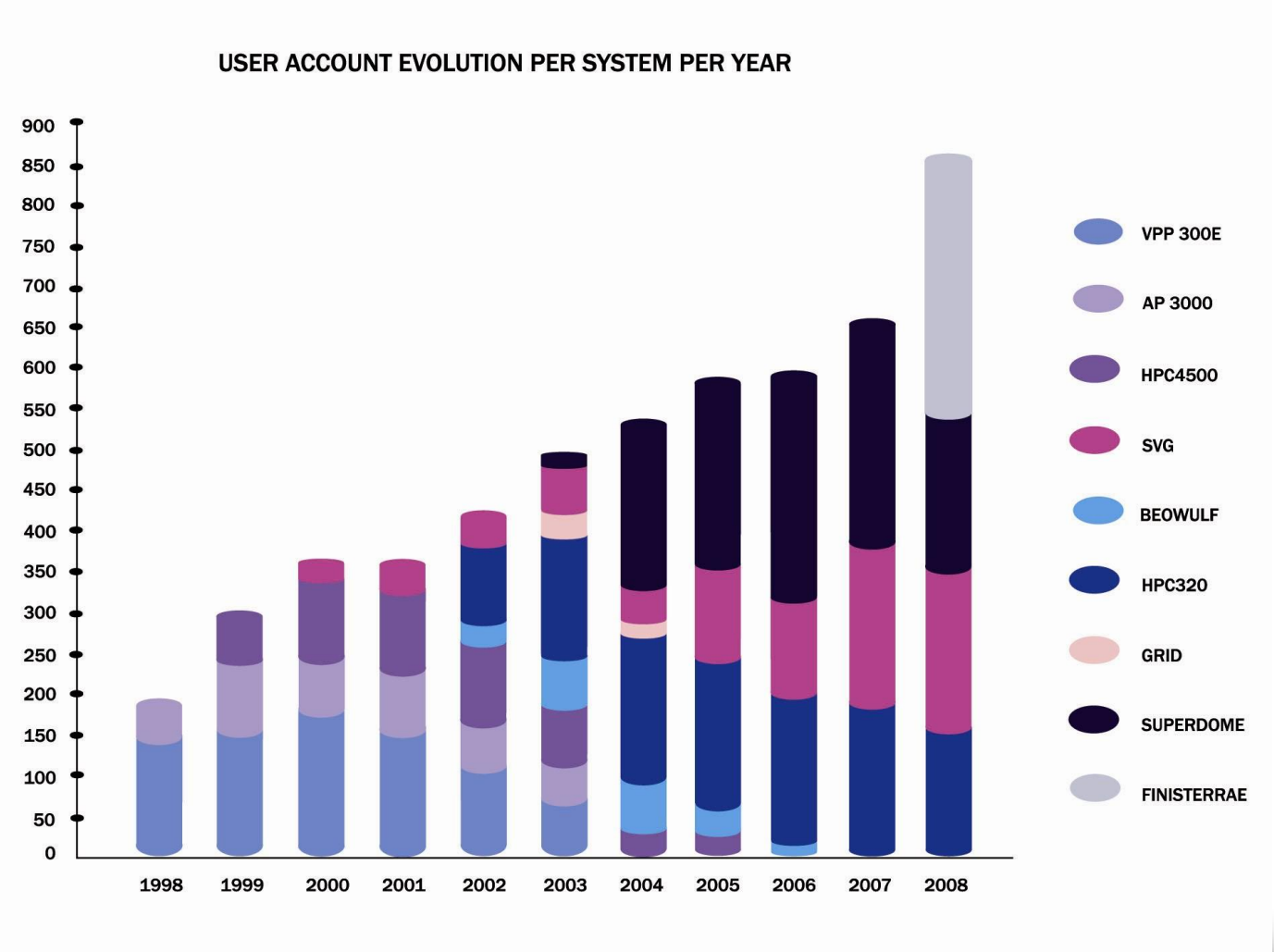
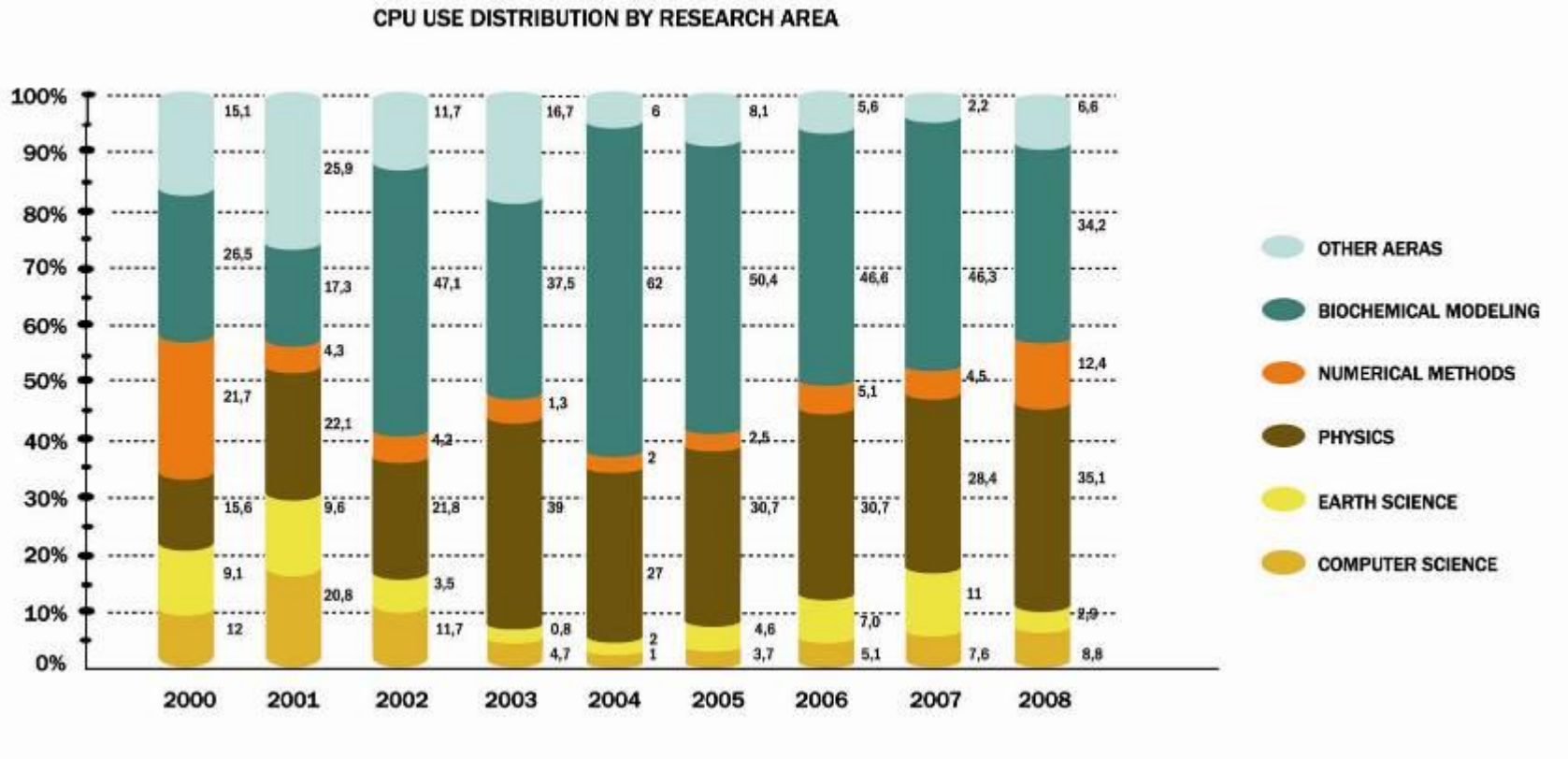
CPU TIME USE EVOLUTION AT CESGA



DEMAND OF COMPUTING RESOURCES AT CESGA



CPU USE DISTRIBUTION BY RESEARCH AREAS



ISO 9001
DNV
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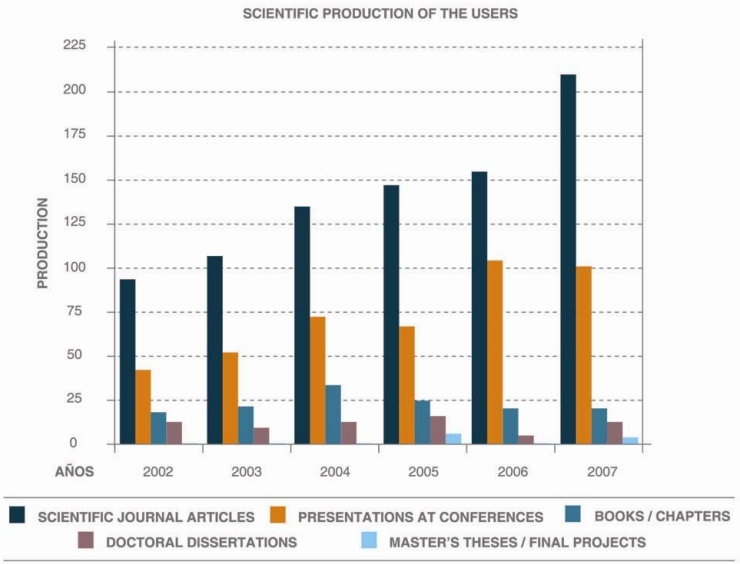
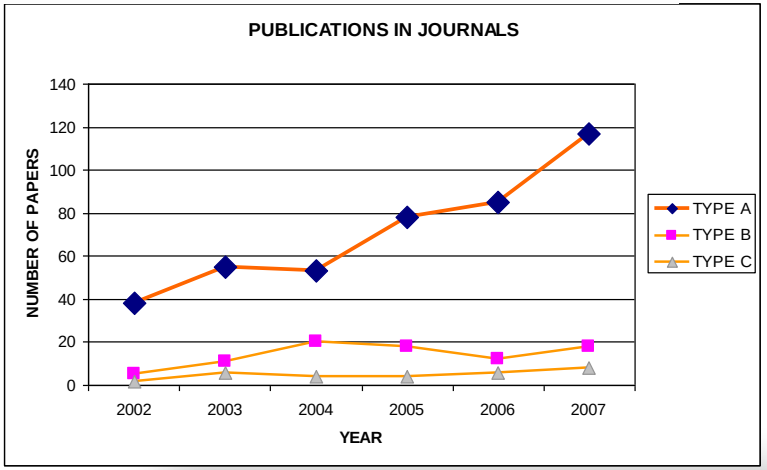
CESGA USERS'S SCIENTIFIC PRODUCTION 2002-2007



DISTRIBUTION OF SCIENTIFIC PRODUCTION PER YEAR

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

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



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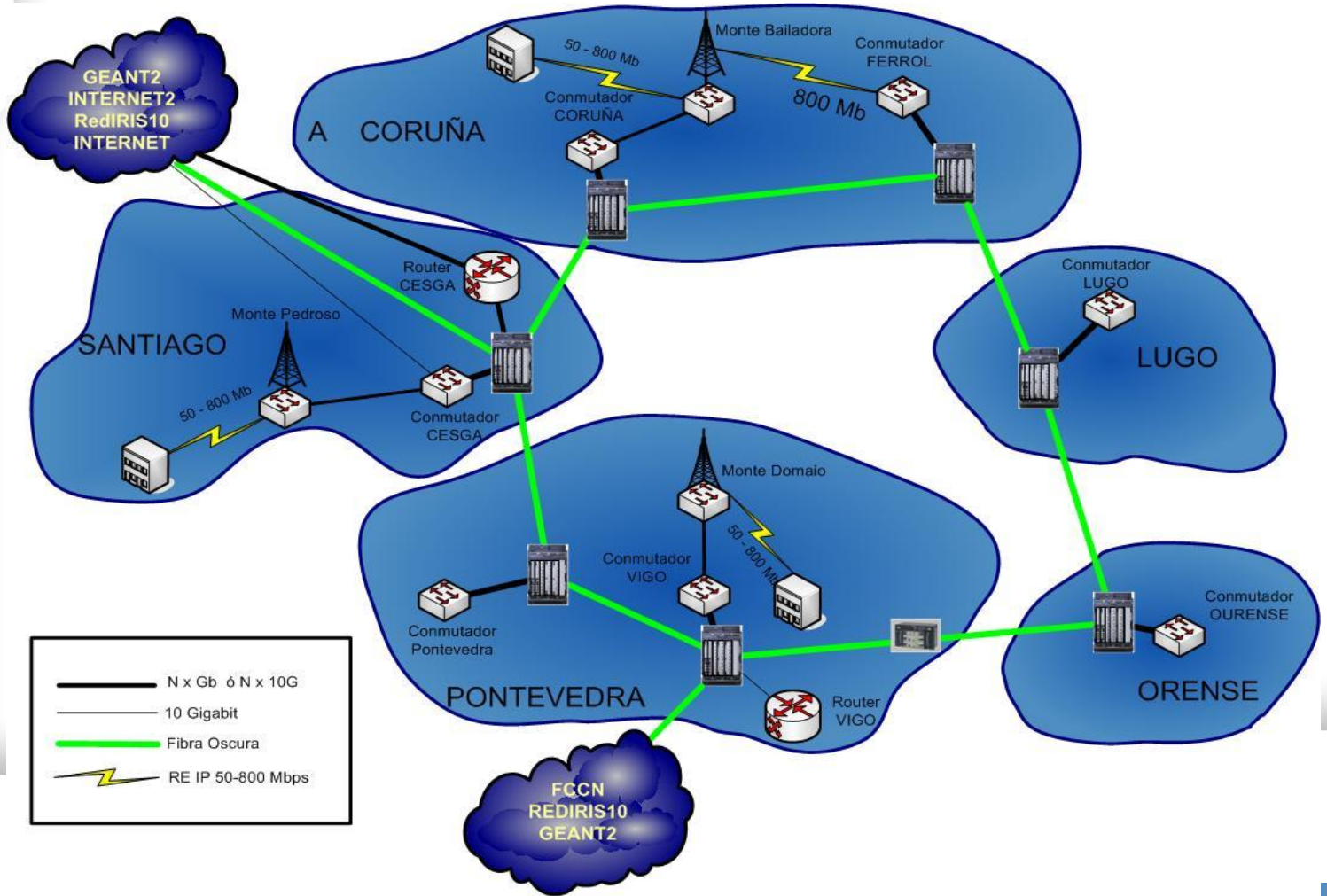
RECETGA NOVA

58 points of presence in Galicia

RECETGA-Rediris Link: Dark fiber (Increase ~ 80 times)



CESGA - C²SRC

CESGA
STRATEGIC PLAN 2010-13

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VISION

Achieving and maintaining international recognition as a high level and high quality supercomputing facility and as a Research Centre of Excellence in the area of Computational Science

KEY ACTIONS

- **Upgrade the computing and associated facilities**
  - Design, building and installing Finis Terrae II;
  - Upgrade of SVG (the CESGA HTC computer);
  - Design and deployment of a new on-line storage;
  - Actualization of RedIris Nova lines;
  - New visualization and collaboration facilities;
  - Security infrastructure to guarantee a good usage of the systems.

- **Start and foster new high added-value services for scientists:**
  - Specialized storage and archiving services,
  - Improve scientific development application support,
  - Specialized visualization services

- **Improve IT departments' research and support activities:**
  - E-learning and other collaboration tools,
  - Innovation and technological support.

CHANGES IN ORGANIZATION

- **Improvement of and new services**
  - Scientific application support
  - Storage and archiving support .

- **Focusing current services toward computational science:**
  - E-Learning
  - E-Business and technological transfer
  - GIS

TECHNOLOGICAL PLAN: INVESTMENTS

SUPERCOMPUTING. FINIS TERRAE II:

❑ Year 2H2010-11

- Constitution of a scientific and technical committees to determine the best architecture of Finis Terrae II:
  - Gather information about users current and future users requirements.
  - Gather information about technology: industry and other Centres.
  - Proposal of the new supercomputer: scientific, technical, logistic, and economical conditions.

❑ Year 2012:

- Call for tenders.
- Deployment of Finis Terrae II

❑ Year 2013:

- Finis Terrae II: open production.

TECHNOLOGICAL PLAN: INVESTMENTS (II)

HTC/GRID:

- **Year 2010:**
  - Upgrade of HTC/GRID servers: 1.000 cores

CARE AND DATA STORAGE:

- **Year 2010:**
  - Update of storage subsystem: Very High throughput, permanent storage of large datasets, multiprotocol

TECHNOLOGICAL PLAN: INVESTMENTS (and III)

COLLABORATION AND VISUALIZATION TOOLS:

❑Year 2012:

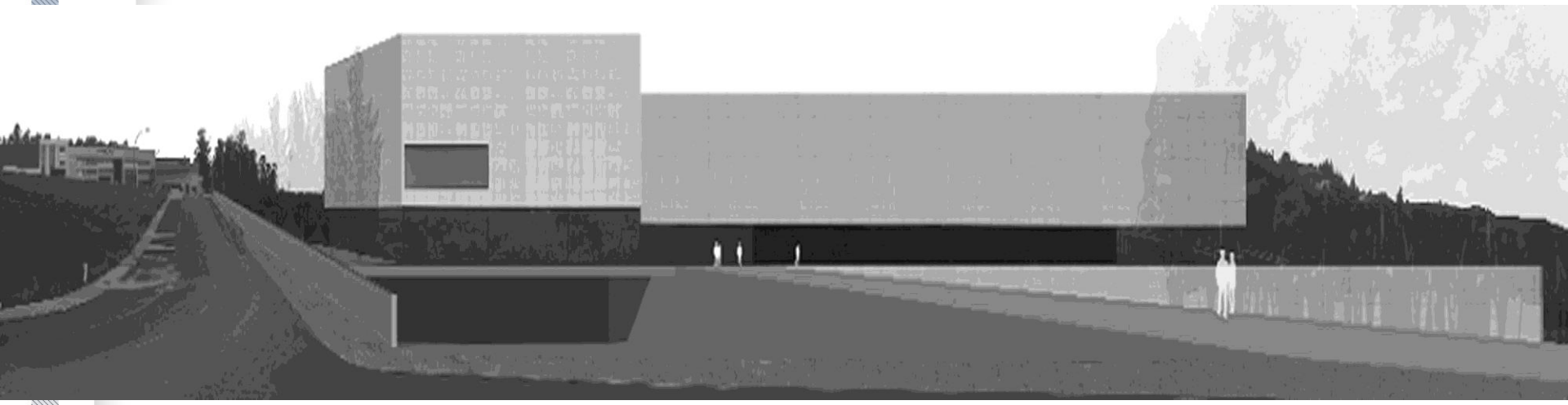
- Deployment of two AccessGrid Rooms
- Deployment of one Auditorium in the new building
- Virtual reality: one AccessGrid room with VR.

LOCAL AREA NETWORK:

❑Year 2012:

- Deployment of new internal local area network. Improving: bandwidth, availability, serviceability, reliability, security, integrity and quality

NEW FACILITIES



Molecular Simulation Applications

- abinit
- Amber
- CPMD
- Dalton
- Gamess
- Gaussian 03
- Gaussian 98
- Gromacs
- LAMMPS
- Molden
- NAMD
- NWChem
- Octopus
- Schrodinger Suite
- SIESTA

LAMMPS Molecular Dynamics Simulator

- Molecular Dynamics Calculations:
  - Small memory per proccess requirement
  - Highly scalable

Amber

Gromacs

NAMD Scalable Molecular Dynamics

Gaussian 03

- Electronic Structure Calculations:
  - Large memory per proccess requirement
  - Not so scalable usually poorly scalable

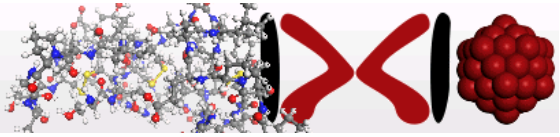
NWChem high performance computational chemistry software

GAMESS

See up-to-date list in WWW.CESGA.ES

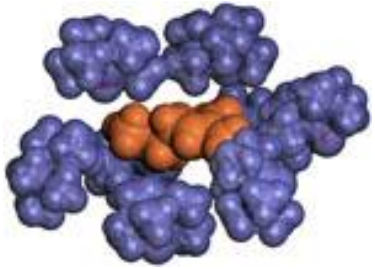
Users Licensed Applications installed at CESGA

TURBOMOLE GmbH



Molpro quantum chemistry package

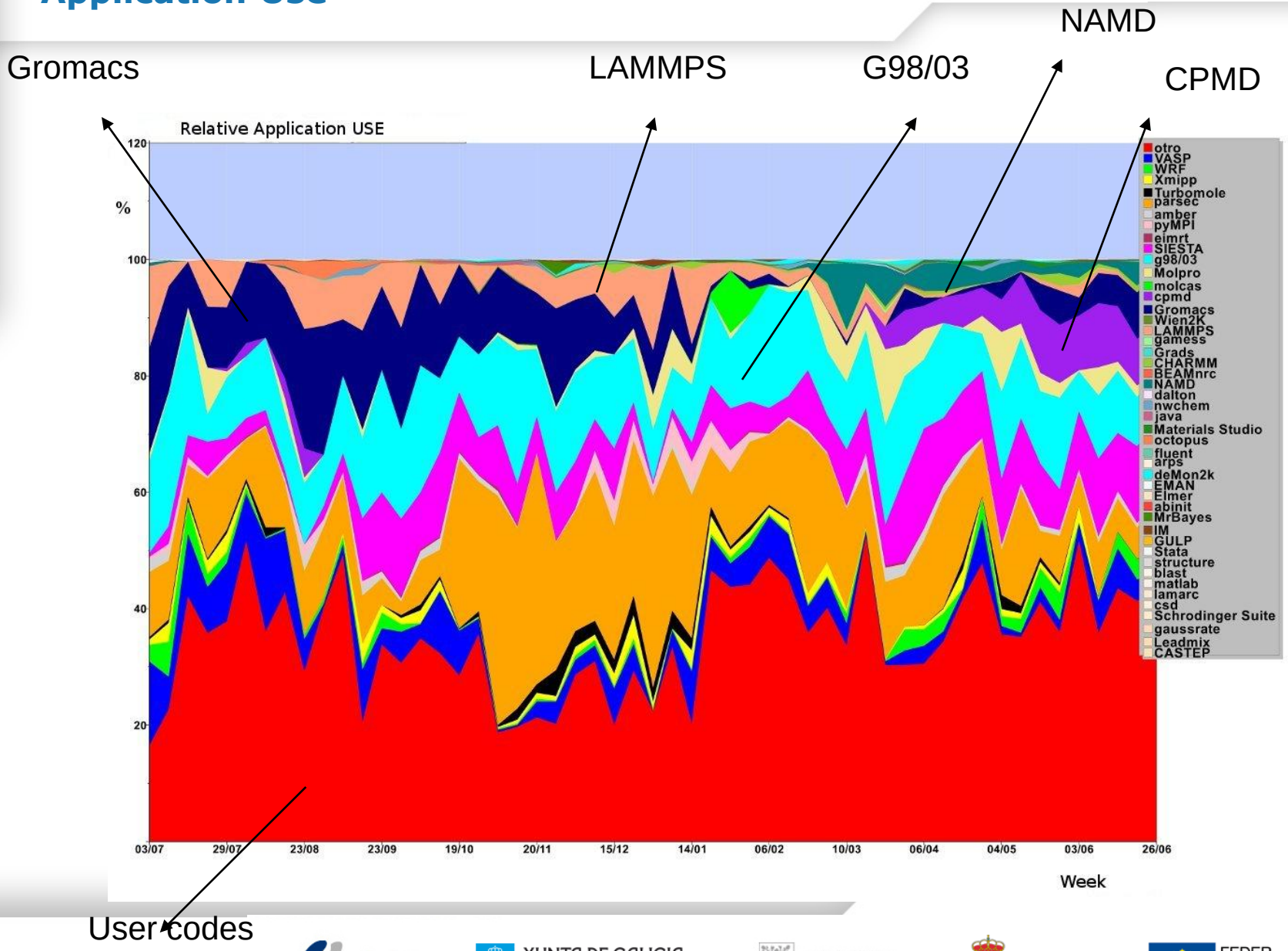
Materials Studio



MOLCAS

It is possible in many cases run private applications on CESGA servers (the license must admit it)

Application Use



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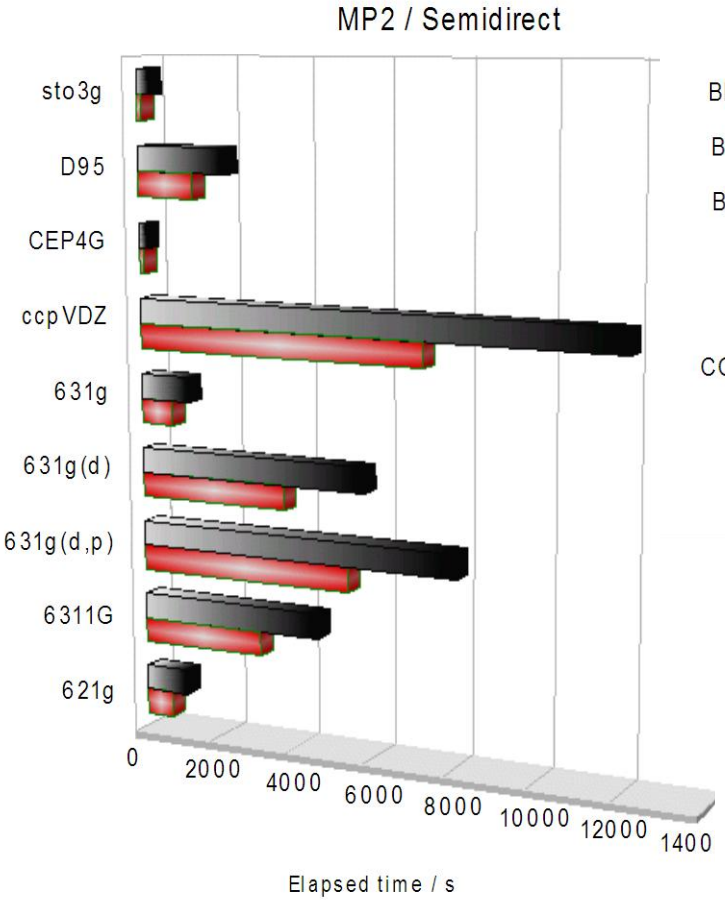
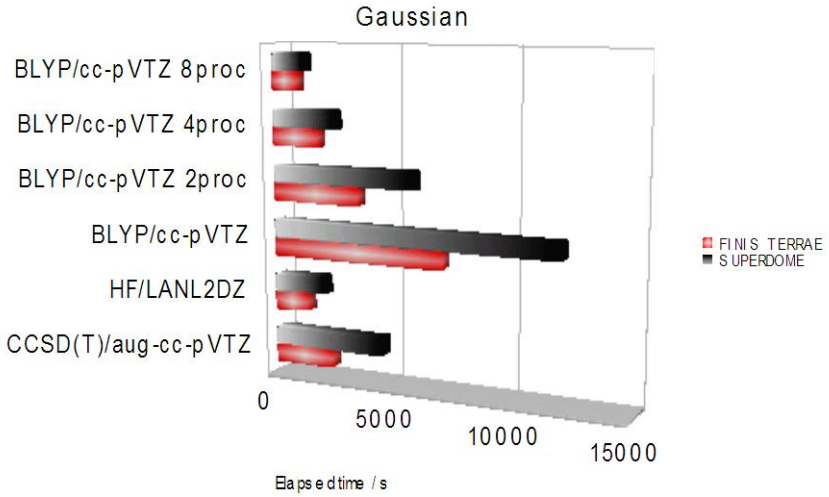
Electronic Structure – Gaussian Performance

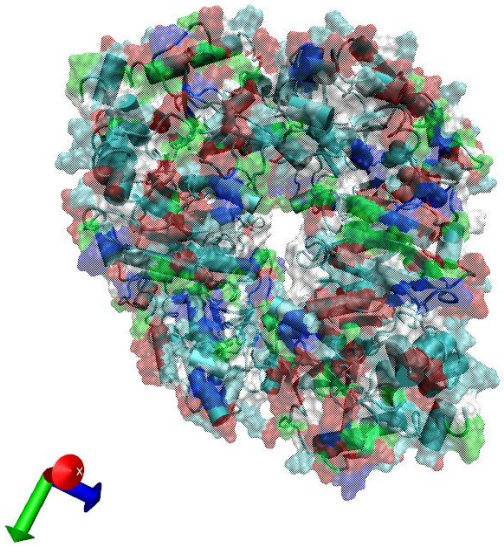


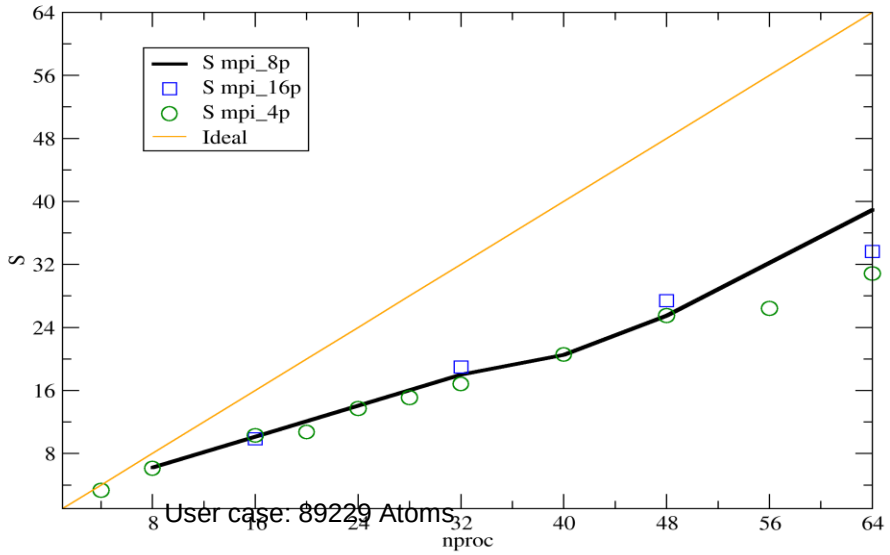


- Improved performance over 1core ia64
- Good scaling inside a node (OpenMP) using direct calculations

MOLECULAR DYNAMICS APPLICATIONS – Gromacs

- Gromacs: Highly Efficient Molecular Dynamics
  - Usually poor scaling. Improved in version 4.0
    - Optimum number of PME nodes (all to all communications)
    - Thick nodes problem (how many processes per node?)

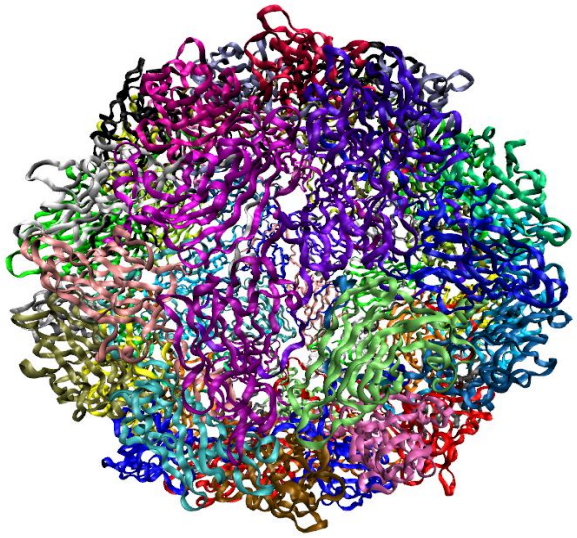


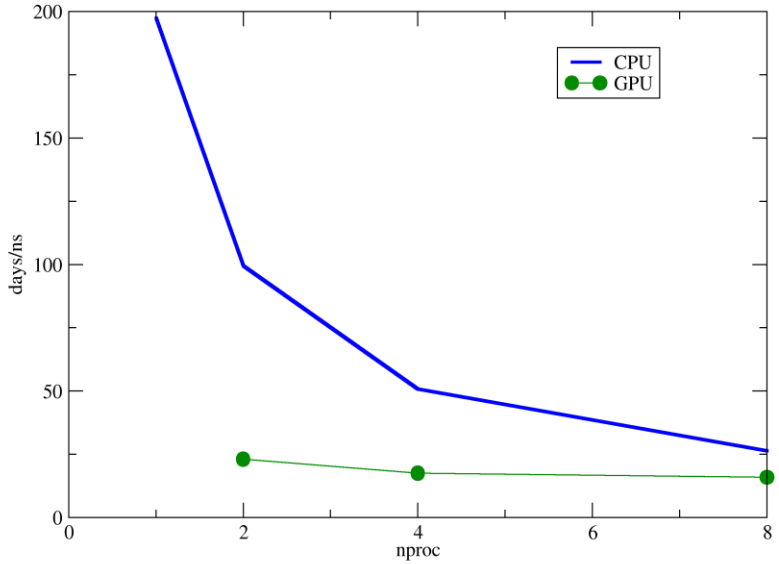


User case: 89229 Atoms

New Architectures (GPUs): NAMD Performance

- NAnoscale Molecular Dynamics (NAMD) is a highly scalable molecular dynamics (MD) code.
- NAMD is especially geared towards the simulation of large biomolecular systems.
- Benchmark: Satellite Tobacco Mosaic Virus (STMV) (1,066,628 atoms)
- Platform: A 8 cores Nehalem E5520 with a NVIDIA Tesla C1060





Single GPU acceleration: 1GPU = 4-6 cores

Finis Terrae : Grand challenges

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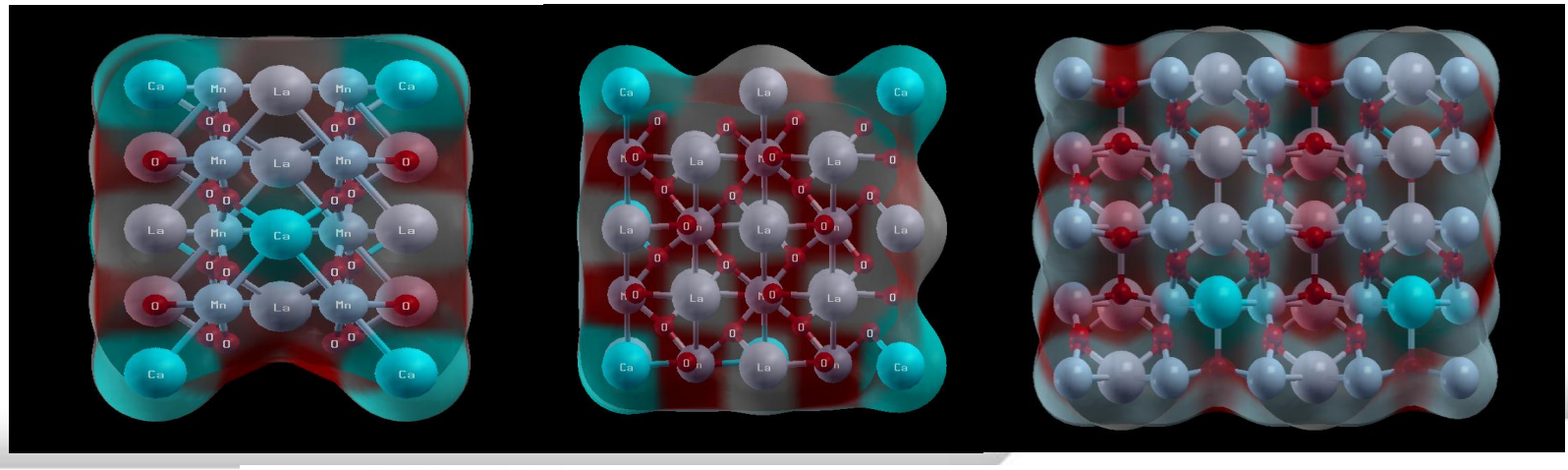
FEDER
FONDO EUROPEO DE DESENVOLVEMENTO REXIONAL

- Different scientific fields / know-how
- Coming from different groups / Institutions / research projects
- Computationally highly demanding

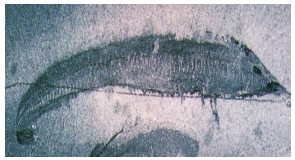
"PHASE SEPARATION"

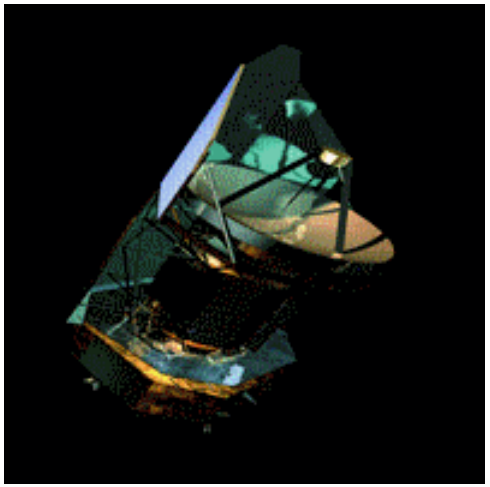
- Condensed Matter Physics: Materials Design
- 3rd/4th physics most important problem of decade (AIP)
- Wien2k: electronic structure calculations of solids using density functional theory (DFT).
- Two levels parallelism:
  - Coarse grain: k points
  - Fine grain: ScaLapack
- 24 nodes: 384 cores, 100G memory, 300G disk -> 68.000h



"GENETIC ALGORITHM FOR THE ASTROPHYSICS OF MASSIVE STARS"

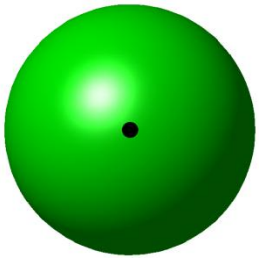
- Molecular and Infrared Astrophysics
- Genetic Algorithms: PIKAIA multimodal optimization problems / FASTWIND
- MPI master slave schema:
  - master task took care of the GA-related operations
  - slave tasks to perform the model calculations
- 20.000 – 40.000 models (15 min each)
- 80 cores

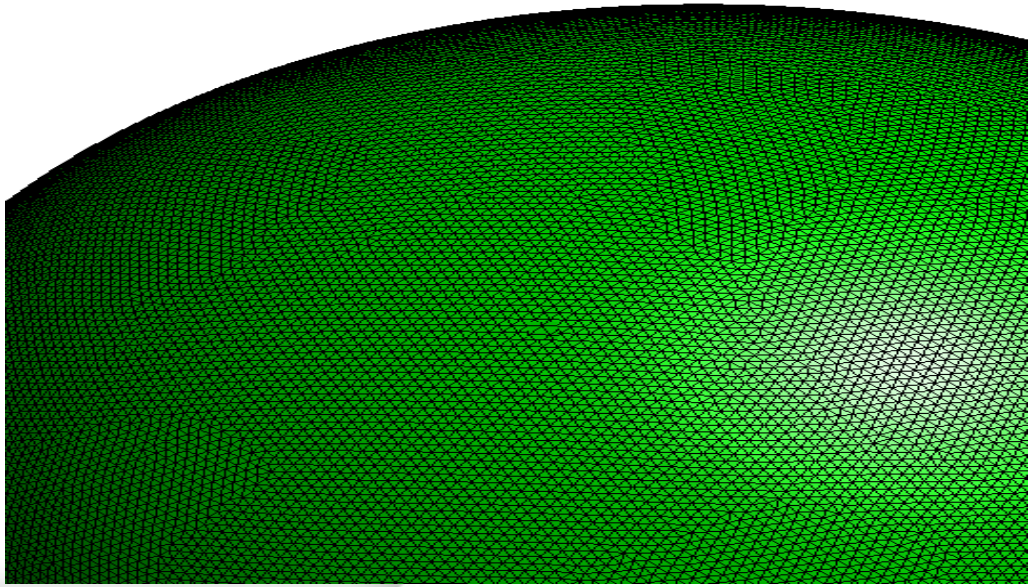




"FEKETE POINTS"

- I-MATH: Applied Maths (Potential theory/Numerical methods)
- Forces Method -> Estimation of Fekete points
- 7th Smale: Mathematical problems for 21st century
- Several parallelizations paradigms:
  - MPI
  - OpenMP
  - MPI/OpenMP
  - High Throughput
- 1024 cores
- 350.000 hours
- 50 million executions



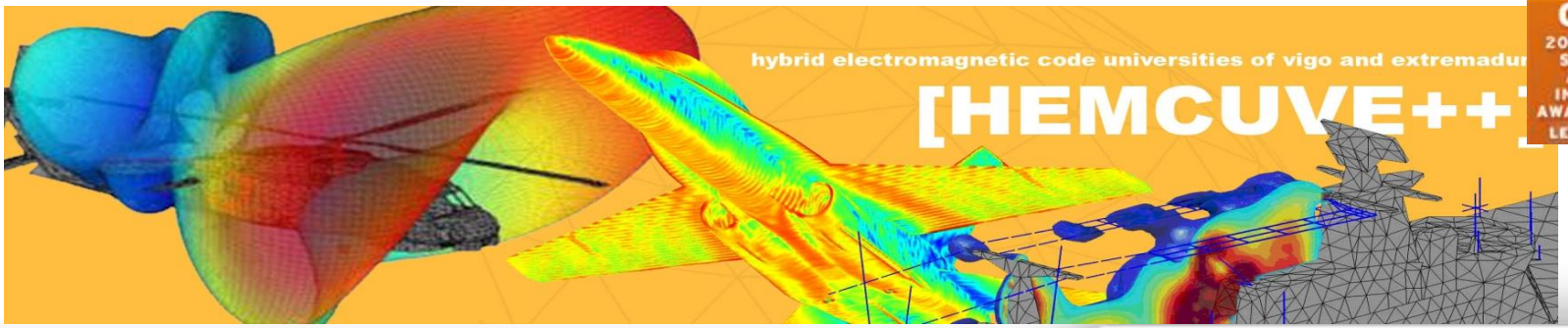


ELECTROMAGNETICS
WORLD RECORD
0.5 billion unknowns

HEMCUVE"

PRACE
Award 2009
presented at
ISC
INTERNATIONAL SUPERCOMPUTING CONFERENCE

- Electromagnetic problems in large structures
- HEmCUVE++: Electromagnetic calculations based on FAST MULTIPOLE methods
- MPI/OpenMP
- Highly demanding on memory per process: Balance between CPU time and memory
- 1024 cores, 6T of memory



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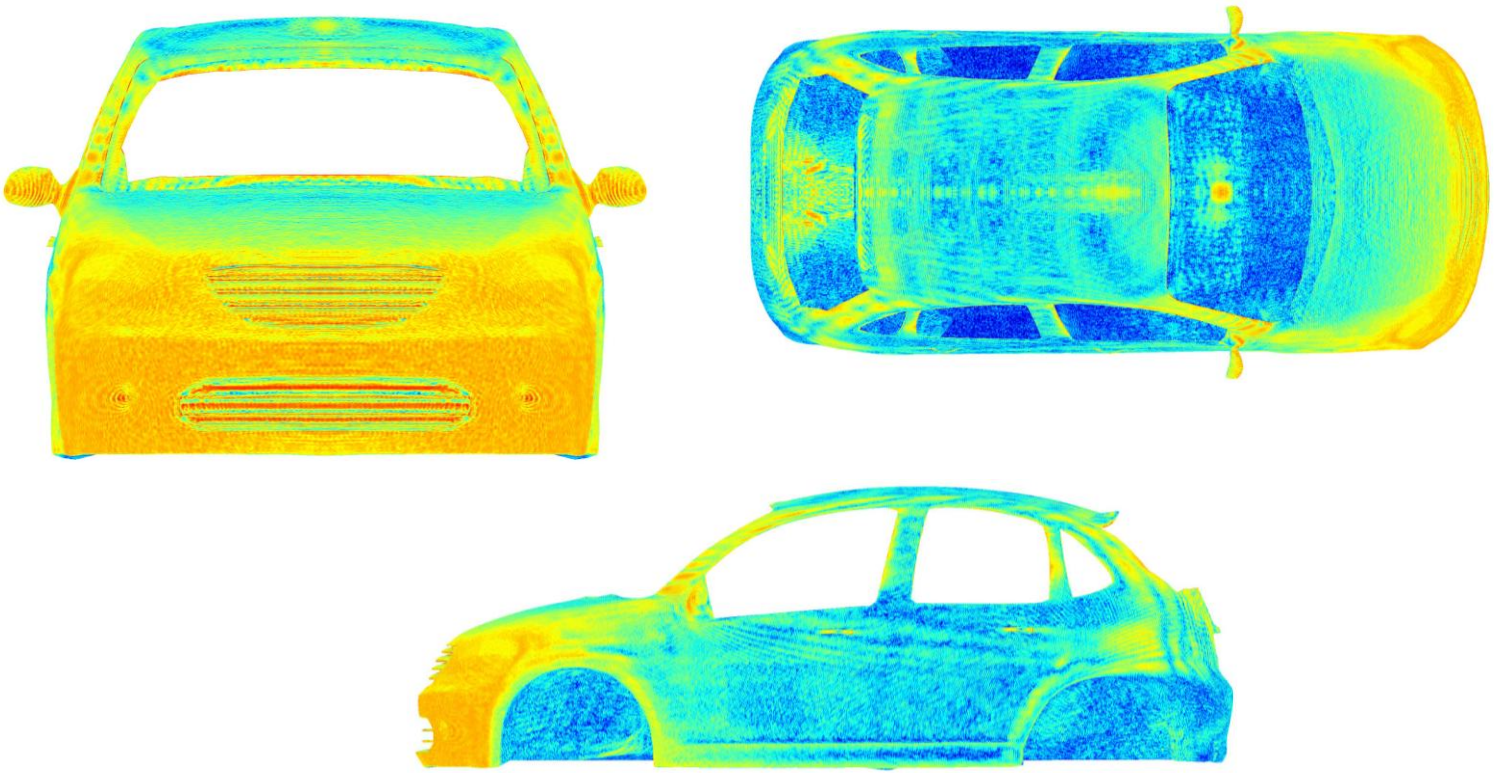
"HEMCUVE"

Citröen C3 at 24.125 GHz (radar frecuency) 40M unknowns



In progress 79 GHz: 300M – 400M unknowns