

Servicios del CESGA a la Comunidad Científica del CSIC

II Encuentro en Computación de Alto Rendimiento en Simulaciones Moleculares

FINISTERRAE

**Aurelio Rodríguez,
Técnico Superior de
aplicaciones**

aurelio@cesga.es

CSIC Madrid, SPAIN, June 2008

ÍNDICE

❑ CESGA

- ✓ Plataformas de cálculo científico

❑ DEP. APLICACIONES Y PROYECTOS

- ✓ Aplicaciones y herramientas en FT
- ✓ Pruebas de rendimientos
- ✓ Soporte y nuevas aplicaciones

CSIC Madrid, SPAIN, June 2008

ESTABLISHED IN 1993 IN SANTIAGO DE COMPOSTELA



CESGA



SANTIAGO DE COMPOSTELA



CSIC Madrid, SPAIN, June 2008



COMUNIDAD DE USUARIOS DEL CESGA

- **Universidades gallegas**
- **Centros de Investigación de la Xunta de Galicia**
- **Centros del CSIC**
- **Otras instituciones públicas y privadas de I+D**

CSIC Madrid, SPAIN, June 2008

EVOLUCIÓN TECNOLÓGICA DEL CESGA

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

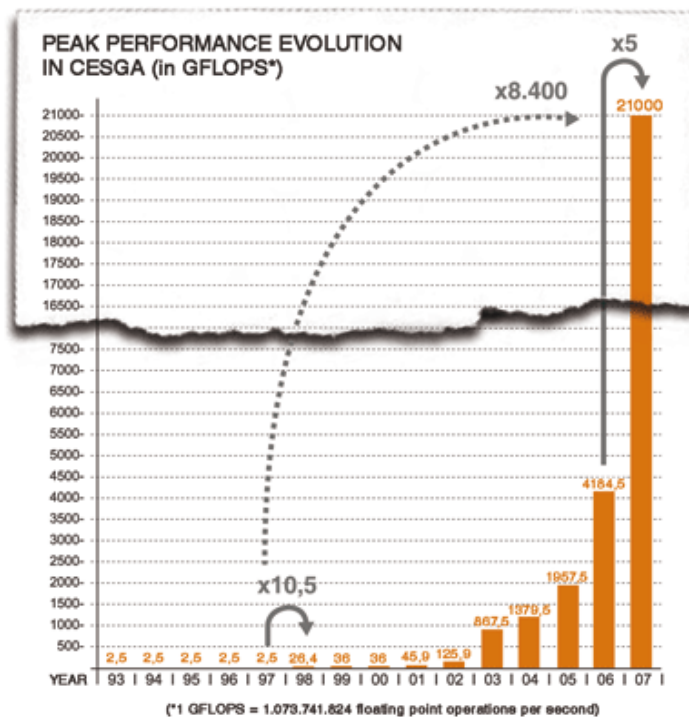


16,000 GFLOPS

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

Madrid, SPAIN, June 2008

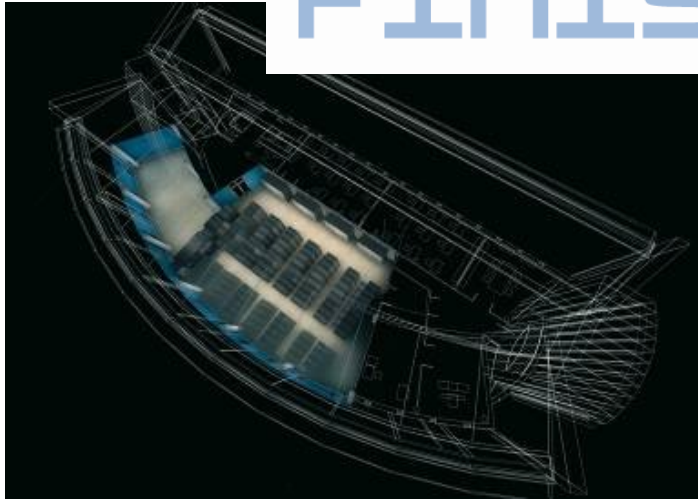
Evolución en rendimiento



CSIC Madrid, SPAIN, June 2008

FINIS TERRAE

FINISTERRAE



New Server HPC (December 2007)

on production (April 2008)

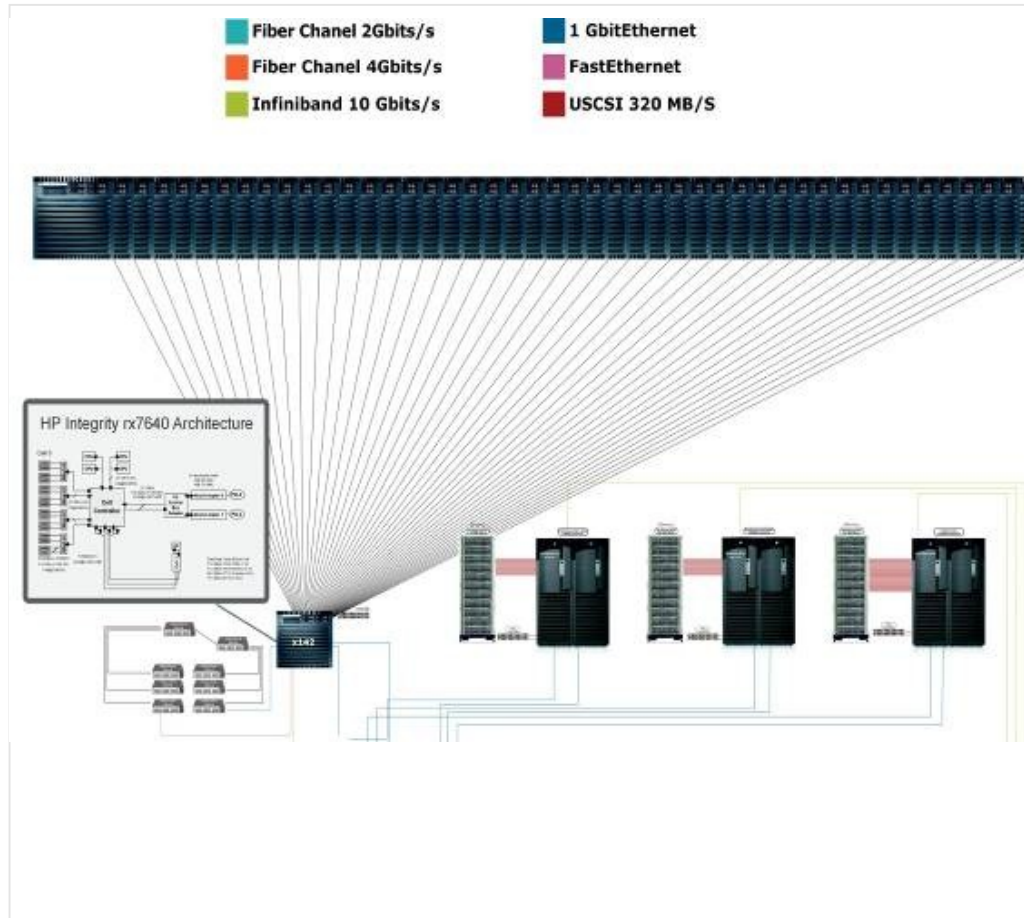
More than **16 TFLOPS** and **19TB RAM** Memory
Plus Agreement among



CSIC Madrid, SPAIN, June 2008



FINIS TERRAE – COMPUTING NODES



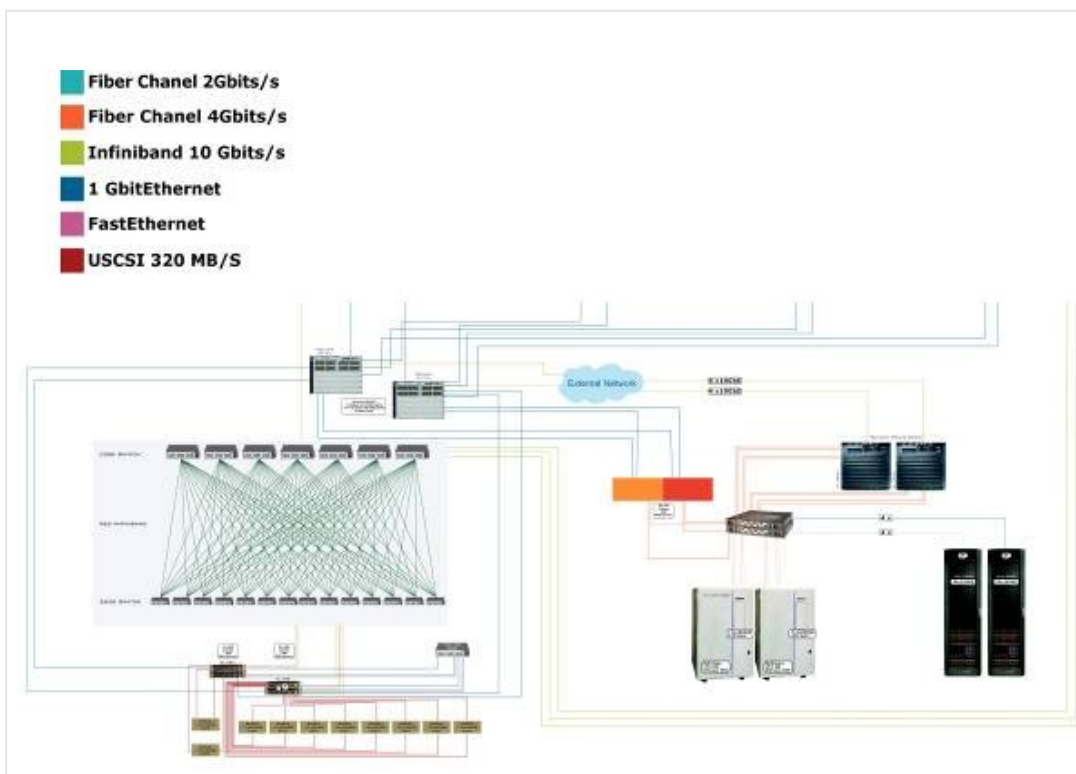
SUPERCOMPUTING NODES:

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

- 1 node: 128 cores, 1.024 GB memory
- 2 nodes: 64+64 CPUs, 256+128 GB memory
- 142 nodes: 16 cores, 128 GB memory

CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – Recursos de almacenamiento



DATA STORAGE:

- 22 nodes with 44 cores for storage management.
- 390 TB disk.
- 1 PB Robot Tape Library.

```
aurelio@fs001:~> df -H /sfs
S.ficheros          Tamaño Usado  Disp Uso% Montado en
84.21.168.199:/sfs  156T  5.8T  142T  4%  /sfs
```

CSIC Madrid, SPAIN, June 2008

OTRAS INFRAESTRUCTURAS

SVG	
Architecture	PC Farm (Self Made), Beowulf Cluster
Number of Processors	Over 96 processors
Type of Processor	Intel Pentium III 1GHz up to P4 3,2 GHz
Peak Performance	528 GFLOPS (nodo CESGA)
Interconnect	Myrinet and Gigabit Ethernet
Memory	1GB - 2GB per node
Disc	9 up to 160 GB per node (over 12TB global)
OS	Linux
Year Installed	2000 (first stage)

GRID	
Architecture	Blades Dell PowerEdge 1955
Number of Processors	40
Type of Processor	Intel quad-core: 36 Intel Xeon 5130 1.6GHz 4 Intel Xeon 5355 2.66GHz
Peak Performance	2183 GFLOPS
Interconnect	Gigabit Ethernet
Memory	4GB (nodos Xeon 5130) 8GB (nodos Xeon 5355)
Disc	SAS 73.4GB (nodos 5130) 2x SAS 73.4GB (nodos 5355)
OS	Linux
Year Installed	2007

CSIC Madrid, SPAIN, June 2008



EGEE Infraestructura:

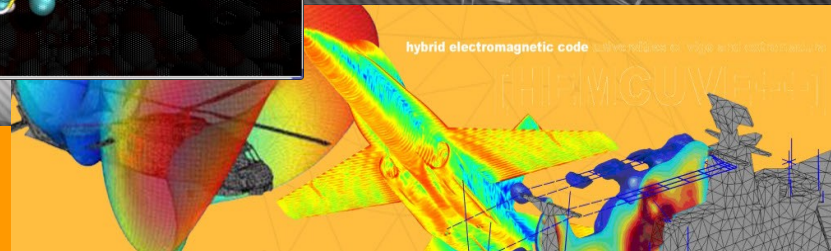
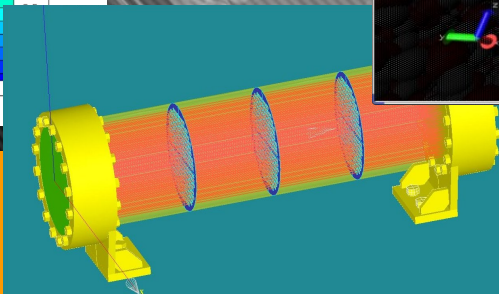
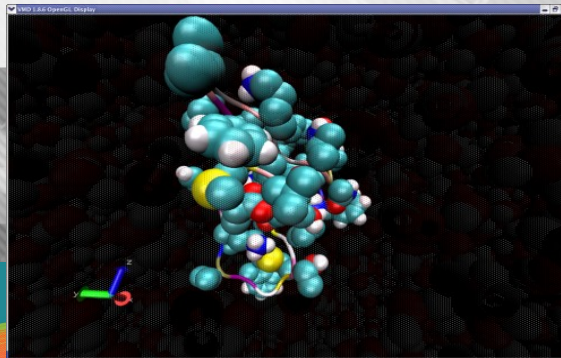
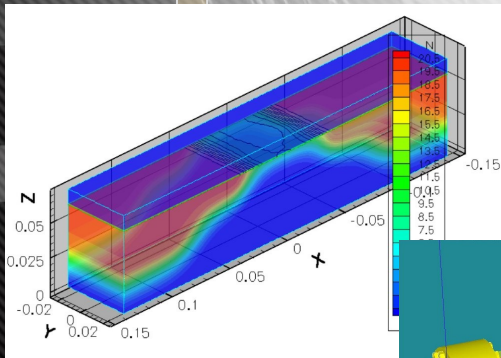
- > 240 sitios en más de 50 países
- > 40.000 CPUs
- > 15 PB almacenamiento de media
- > 20.000 trabajos concurrentes por día
- > 120.000 trabajos por día
- > 6.000 usuarios en más de 100 VOs

CSIC Madrid, SPAIN, June 2008

DPTO. APLICACIONES Y PROYECTOS



FLUJIS TERRAE



DPTO. APLICACIONES Y PROYECTOS

□ 3 + 1 TÉCNICOS DE SOPORTE APLICACIONES

- ✓ Dr. en Física
- ✓ Dr. en Química Computacional
- ✓ Dr. en Ingeniería Informática
- ✓ Licenciada en Matemáticas (Aplicadas, i-MATH)

□ TÉCNICO DE INNOVACIÓN

□ CONTRATADOS DE PROYECTOS

CSIC Madrid, SPAIN, June 2008

DPTO. APLICACIONES Y PROYECTOS (i)

- ❑ INSTALACIÓN Y COMPILACIÓN DE APLICACIONES DE CÁLCULO
- ❑ SOPORTE TÉCNICO APLICACIONES Y PROGRAMACIÓN CIENTÍFICA
 - ✓ Paralelización
 - ✓ Librerías
 - ✓ Herramientas y lenguajes
 - ✓ Rendimiento
- ❑ DESARROLLO DE PEQUEÑAS APLICACIONES DE CÁLCULO

CSIC Madrid, SPAIN, June 2008

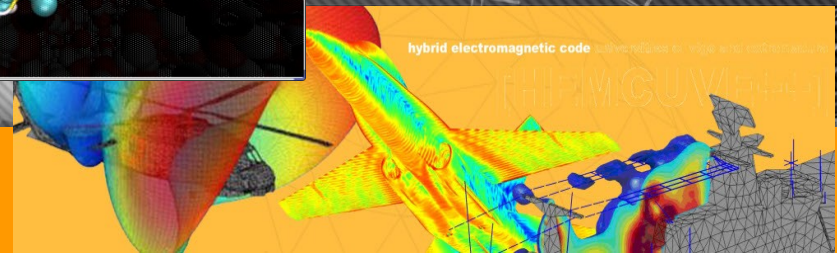
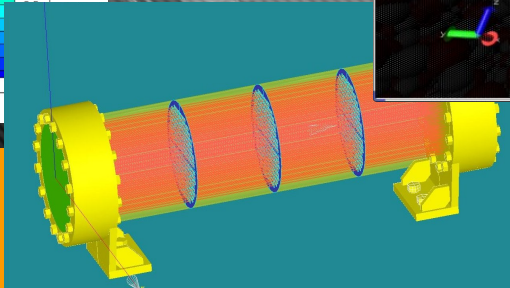
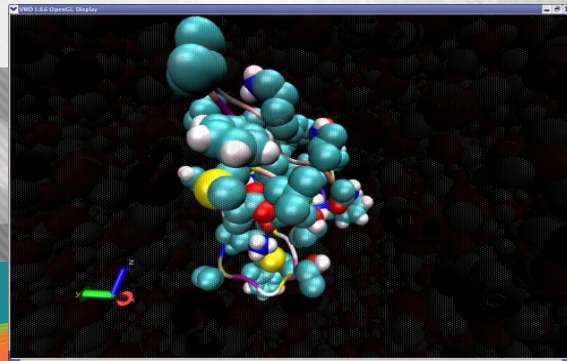
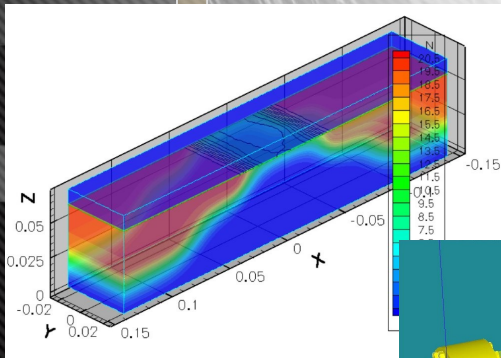
□ REALIZACIÓN DE PROYECTOS DE I+D+i

- ✓ Europeos (SMARTLM, EGEE, BEINGRID, ETC)
- ✓ Nacionales (i-MATH, RETELAB, IFEC)
- ✓ Regionales (g-Fluxo, ISEC, e-IMRT, etc).
- ✓ Siempre en colaboración
- ✓ Orientación de investigación aplicada

APLICACIONES EN FINIS TERRAE



FINIS TERRAE



APLICACIONES INSTALADAS ABRIL 2008

Cálculo Estructural,
Flúidos y Magnetismo

Elmer



Cálculo Molecular

Amber

X

Amber

Gaussian 03

X

SIESTA

X

Gaussian 03



Gromacs

X

LAMMPS

X

LAMMPS Molecular Dynamics Simulator

NAMD

X

NAMD
Scalable Molecular Dynamics

[VER LISTA ACTUALIZADA EN](#)
[WWW.CESGA.ES O EN MODULES](#)

CSIC Madrid, SPAIN, June 2008

APLICACIONES INSTALADAS ABRIL 2008

```
aurelio@fs001:~ - Terminal - Konsole
Sesión  Editar  Vista  Marcadores  Preferencias  Ayuda

aurelio@fs001:~> module av

----- /usr/share/modules -----
3.1.6                modulefiles/module-info modulefiles/use.own
modulefiles/dot      modulefiles/modules
modulefiles/module-cvs modulefiles/null

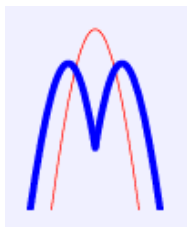
----- /usr/share/modules/modulefiles -----
dot                module-cvs  module-info  modules      null          use.own

----- /opt/cesga/modules -----
amber/9(default)    hp-mpi      mkl/10.0.2.018
attach              icc/10.1.012 mkl/9.1(default)
cmkl/10.0.011       icc/9.1.052(default) mlib/9.6(default)
cmkl/9.1            idb/10.1.012 molpro/2006.1-par(default)
elmer               idb/9.1.052(default) molpro/2006.1-par-ext
fftw/2.1.5          ifort/10.1.012 molpro/2006.1-serie
fftw/3.0.1          ifort/9.1.052(default) namd/2.6(default)
fftw/3.1.2(default) impi/3.0    namd/2.6b1
g03/c1              impi/3.1    netcdf/3.6.1
g03/d2              impi/3.1.038(default) netcdf/3.6.2(default)
g03/e1(default)    intel/10    numpy
gamess/mar2007(default) intel/9(default) pyMPI
grads               itac/7.1/impi3 siesta
gromacs/3.3.1       lammps/22Jan2008(default) stata/10.0(default)
gromacs/3.3.2(default) lammps/22Jan2008-impi uunits
gromacs/3.3.3       mkl/10.0.011
aurelio@fs001:~> |
```

CSIC Madrid, SPAIN, June 2008

APLICACIONES CSIC EN EL FINIS TERRAE

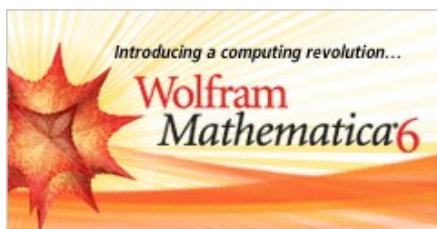
INSTALADAS:



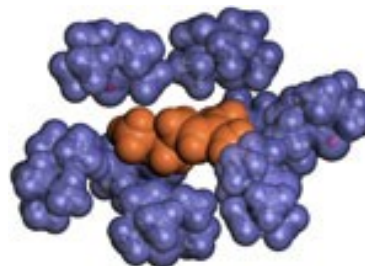
Molpro quantum chemistry package



PRÓXIMAMENTE:



Materials Studio



PODEMOS INSTALAR APLICACIONES CON LICENCIA CSIC

CSIC Madrid, SPAIN, June 2008

HERRAMIENTAS DE DESARROLLO

HERRAMIENTAS

Intel C++
Compiler

X

Intel Fortran
Compiler

X

Modules

X



LIBRERÍAS



MKL

X



HP's Mathematical Software Library (MLIB)

Developer & Solution Partner Program (DSPP)

MPI	HP MPI	X
	Intel MPI Library	X



HP Message Passing Interface library (HP-MPI)

Developer & Solution Partner Program (DSPP)

PRÓXIMAMENTE:

HP Caliper

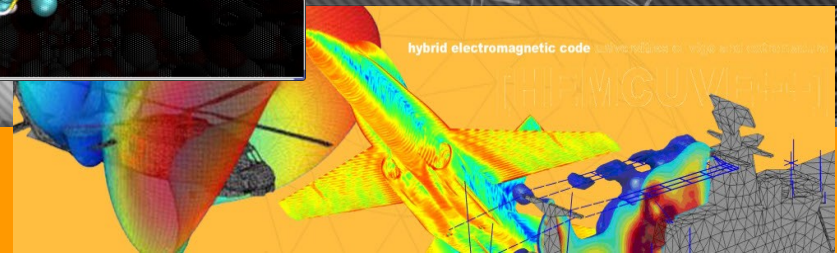
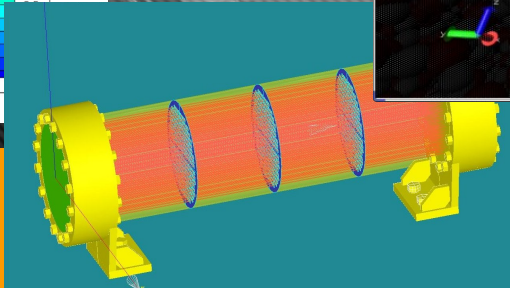
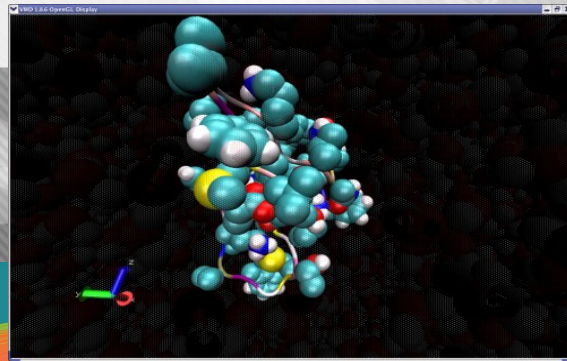
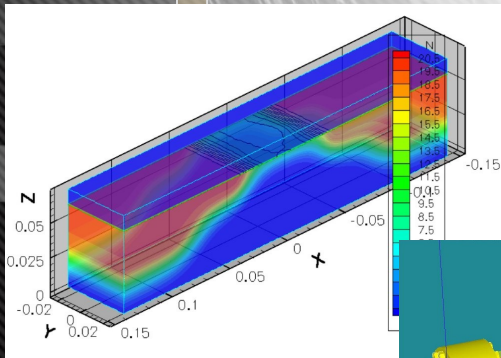


CSIC Madrid, SPAIN, June 2008

PRUEBAS Y RENDIMIENTO

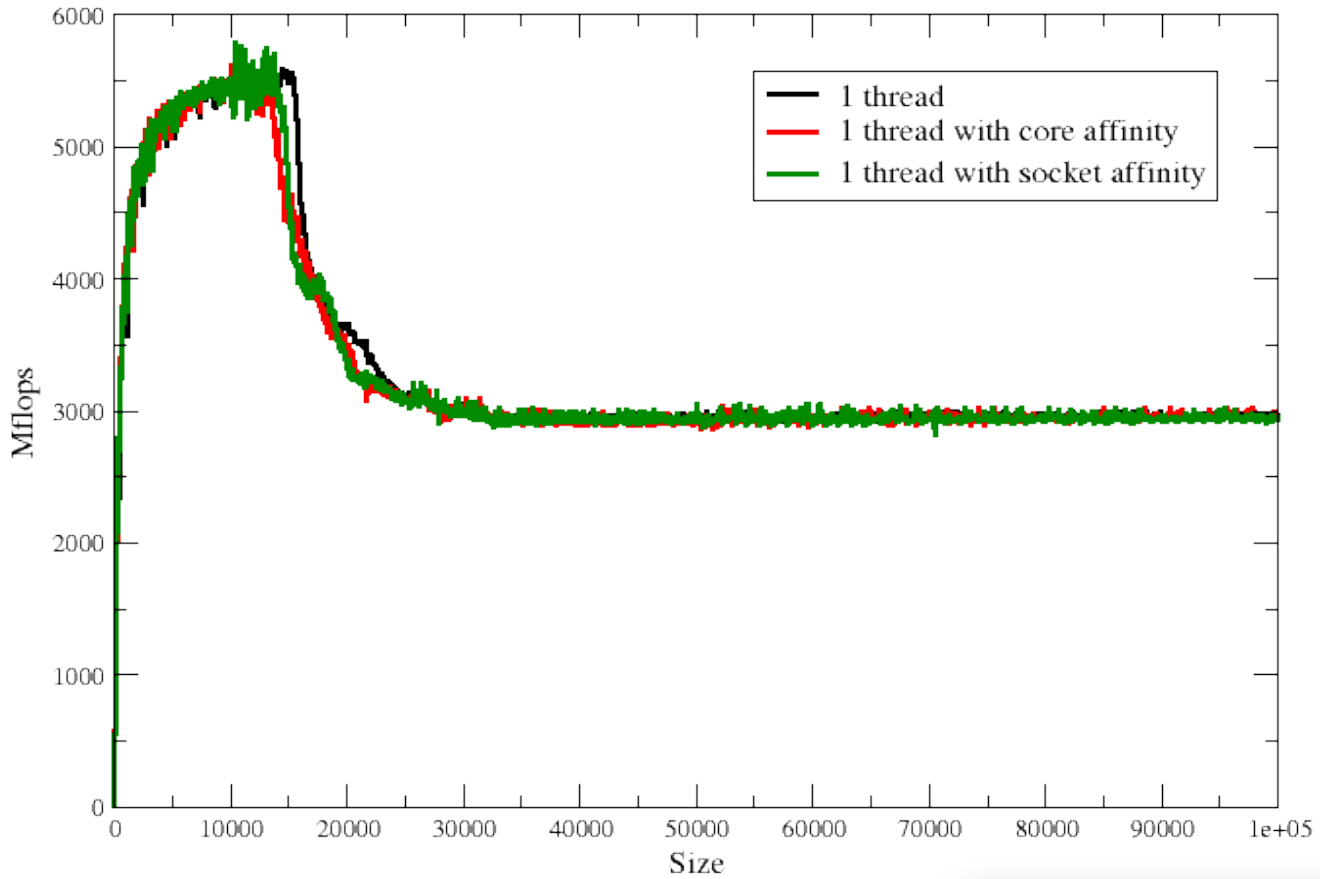


FELICISTERRAE



FINIS TERRAE – MKL Performance

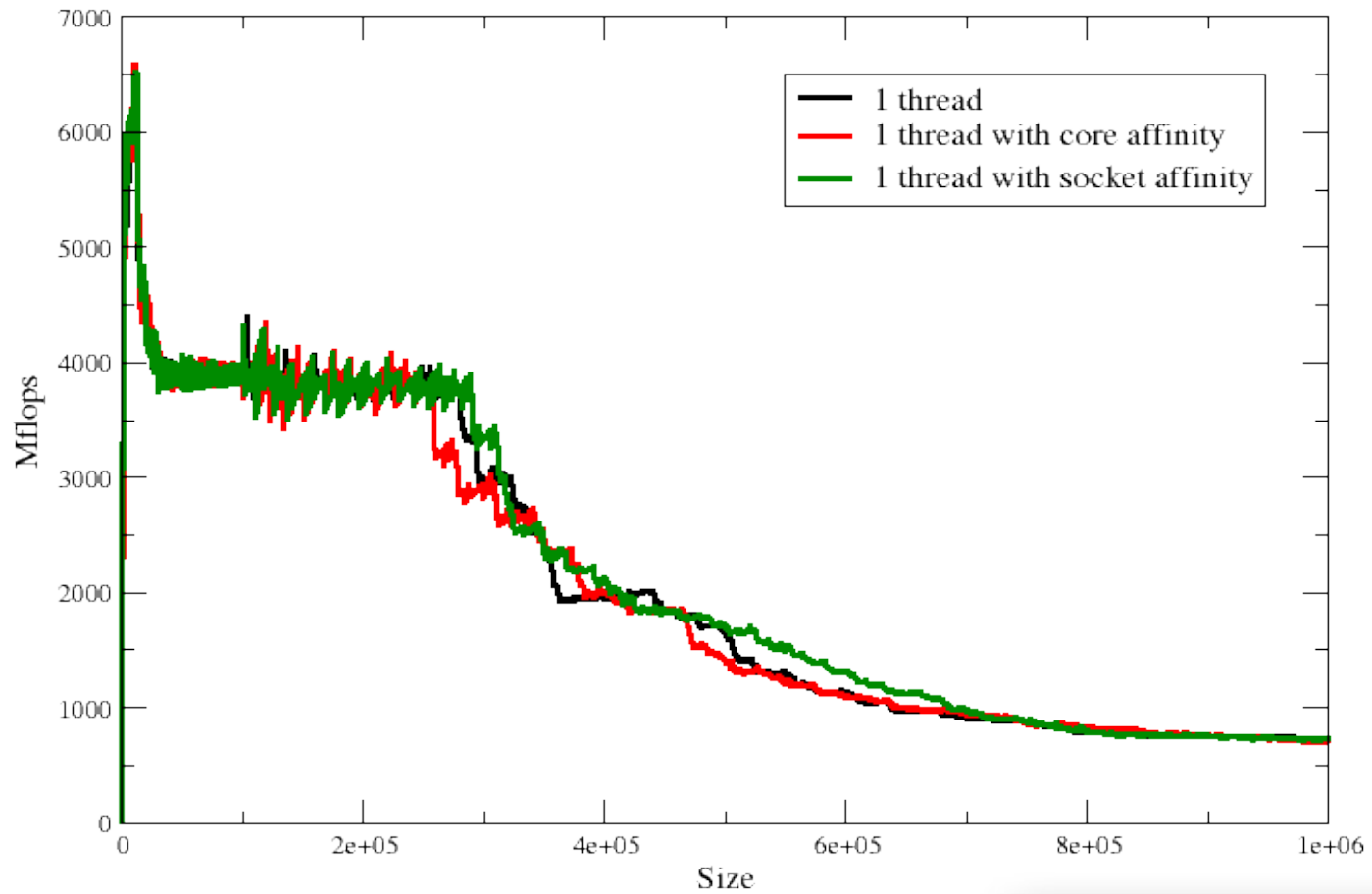
DAXPY from MKL in FINIS TERRAE



CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – MKL Performance

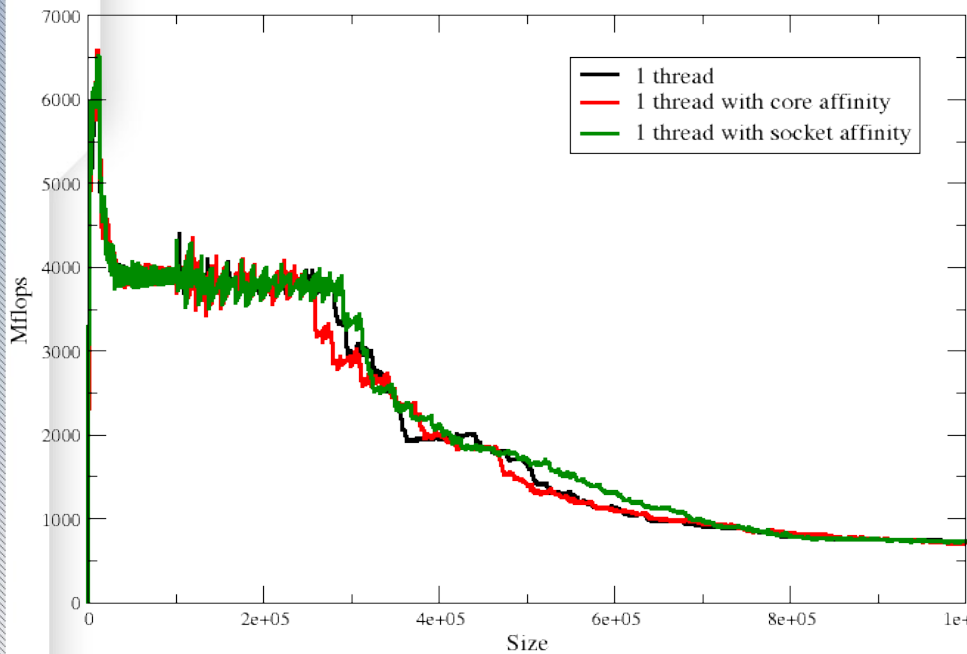
DDOT from MKL in FINIS TERRAE



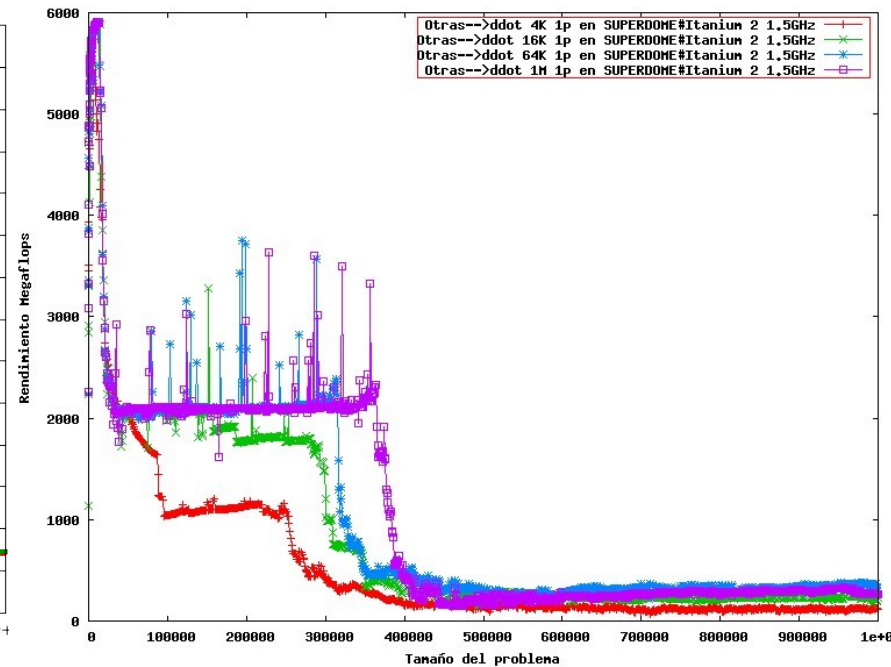
CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – SUPERDOME

DDOT from MKL in FINIS TERRAE



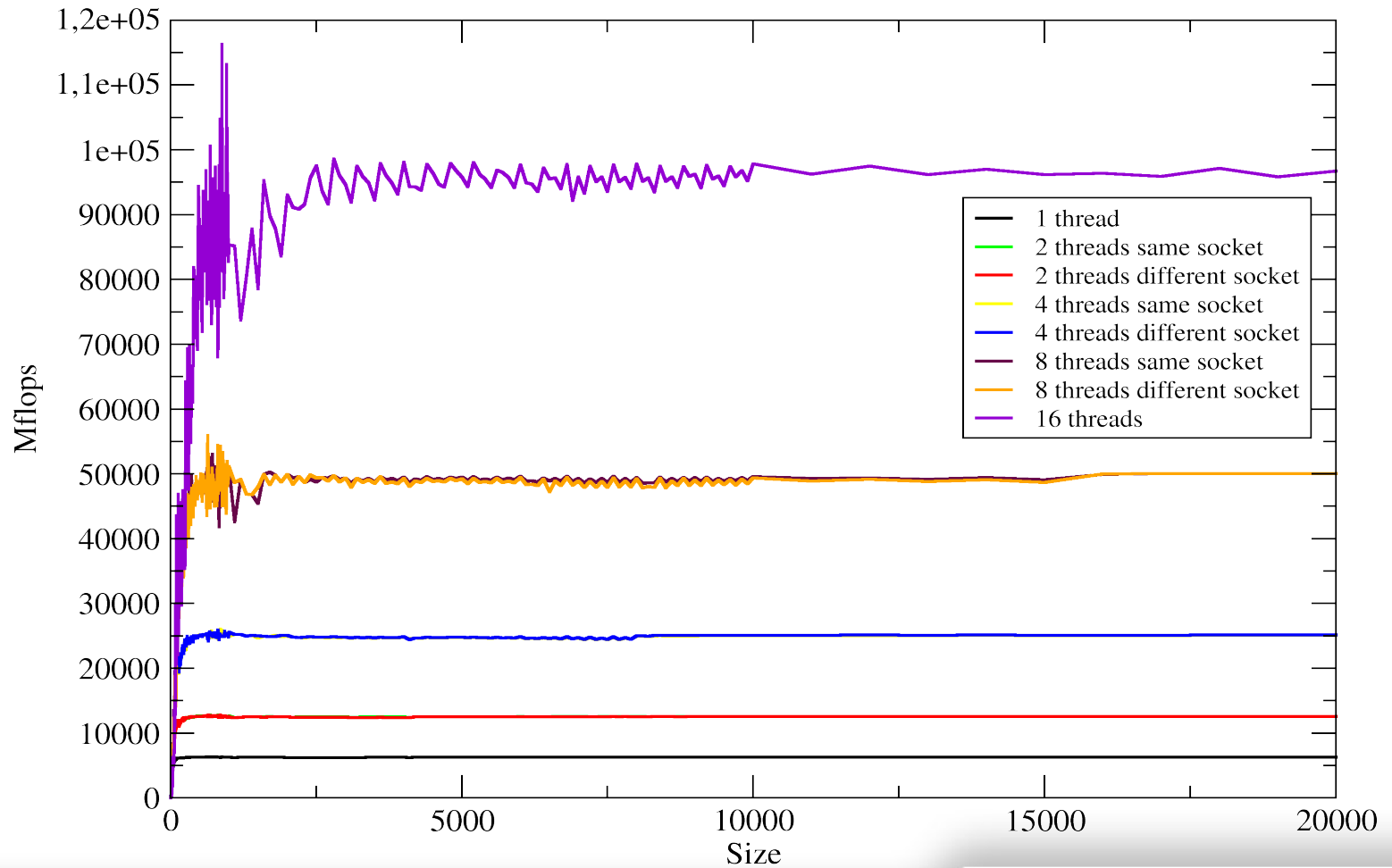
SUPERDOME HP-UX -MLIB



CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – MKL Performance

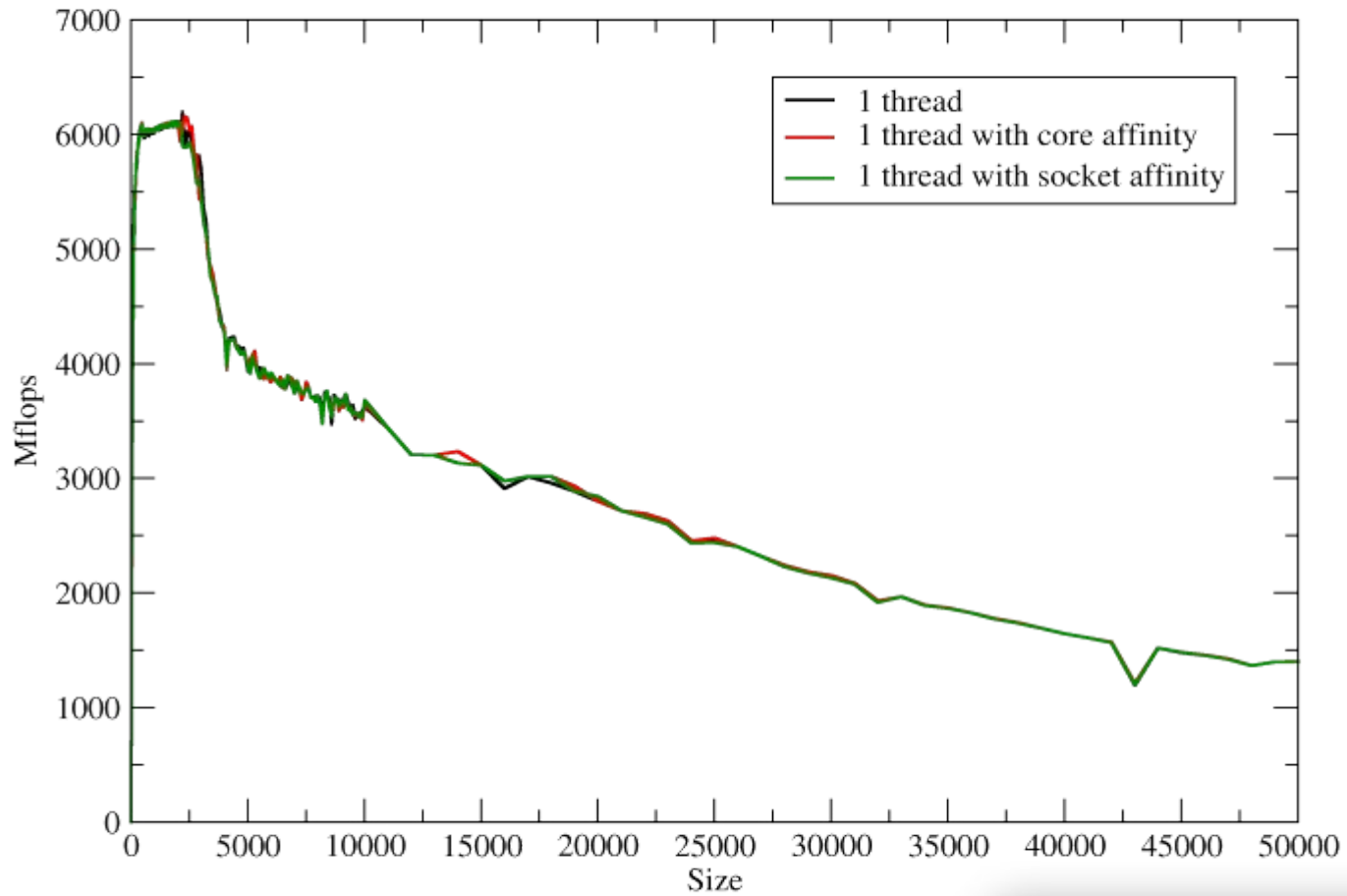
DGEMM from MKL in FT



CSIC Madrid, SPAIN, June 2008

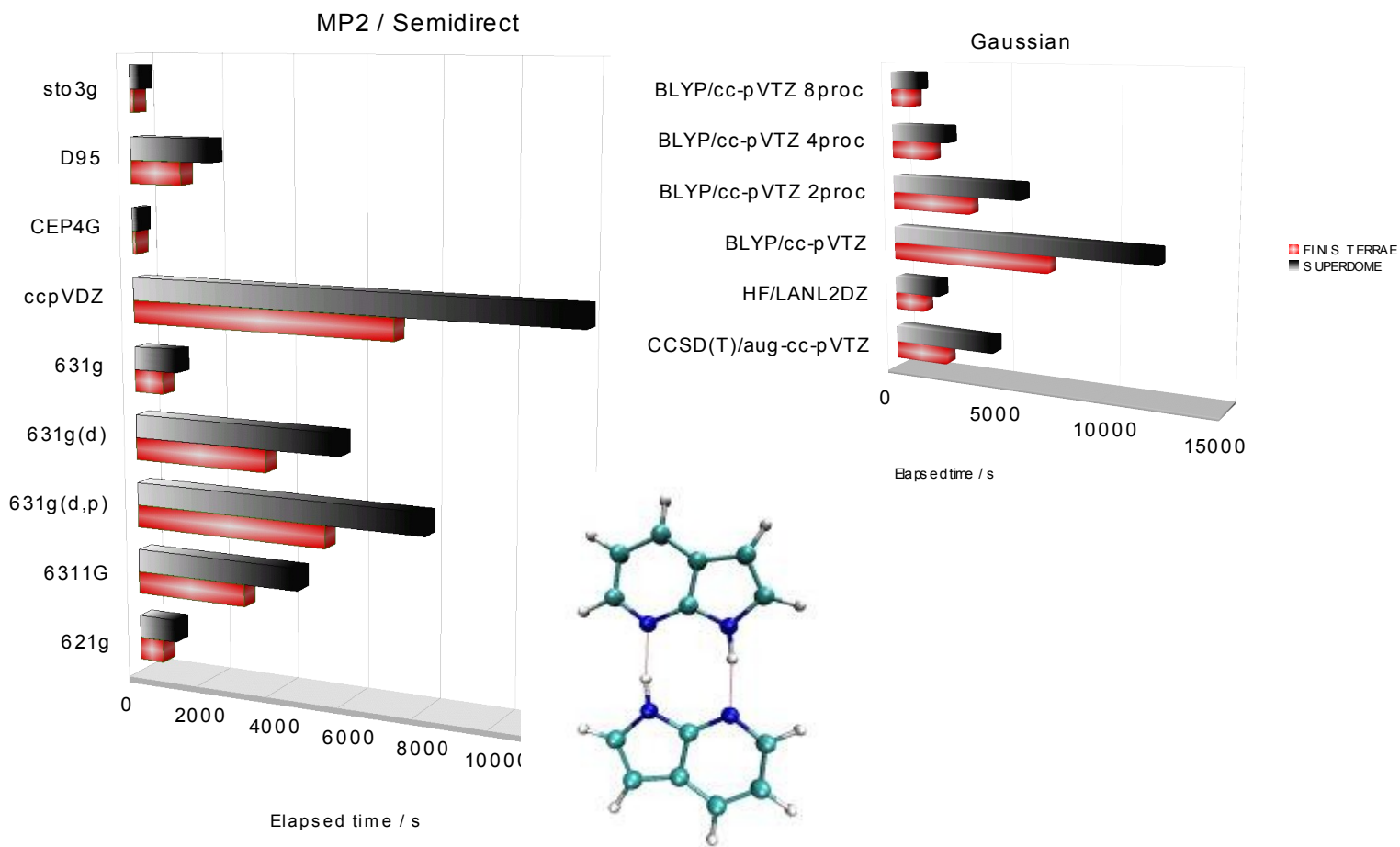
FINIS TERRAE – MKL Performance

DGEMV from MKL in FT



CSIC Madrid, SPAIN, June 2008

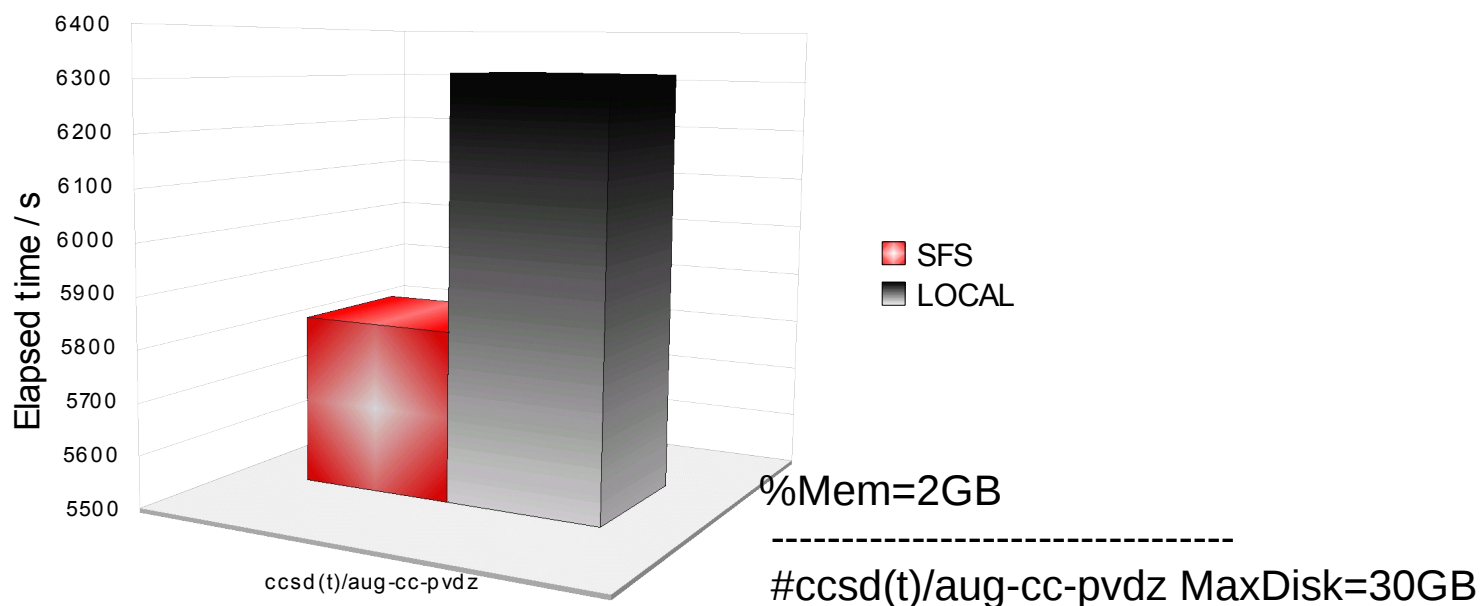
FINIS TERRAE – Gaussian Performance



CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – SFS: A Gaussian Test

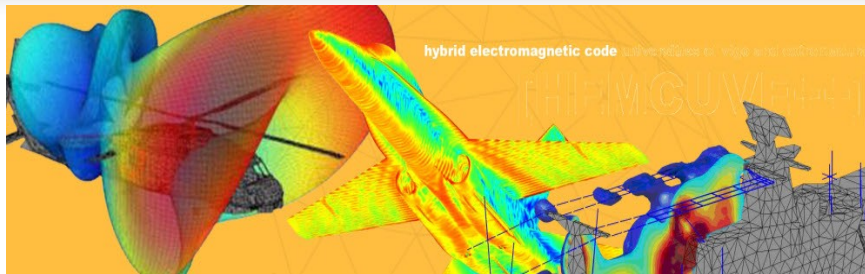
FULL OPTIMIZED FILESYSTEM



```
aurelio@fs001:~> df -H /sfs
S.ficheros          Tamaño Usado  Disp Uso% Montado en
84.21.168.199:/sfs  156T  5.8T  142T  4% /sfs
```

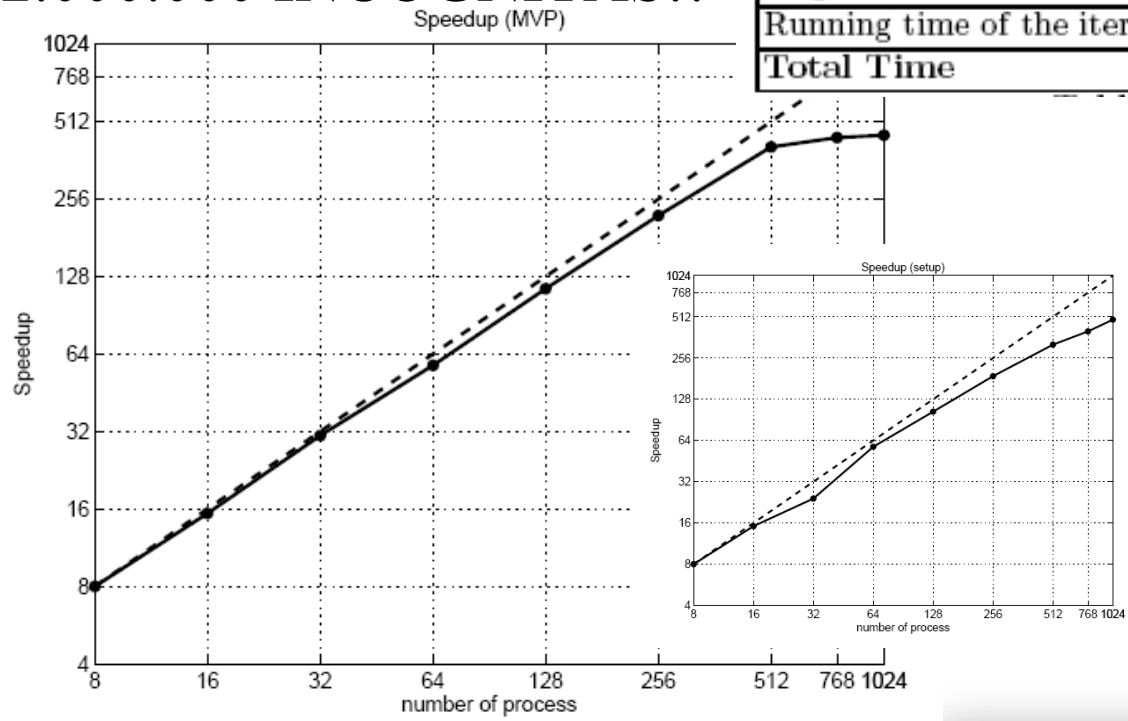
CSIC Madrid, SPAIN, June 2008

FINIS TERRAE – APLICACIONES PRUEBA



¡¡32.000.000 INCOGNITAS!!

RCS of a sphere with 200λ diameter.	
Unknowns number	32,411,106
Cell dimensions	2λ
Process number	512
Total Memory	7TB
Setup time	4h35m
Single MVP time	6m6s
Running time of the iterative process	10h35m
Total Time	15h10m



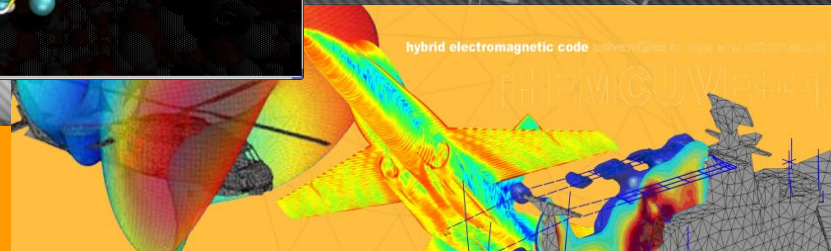
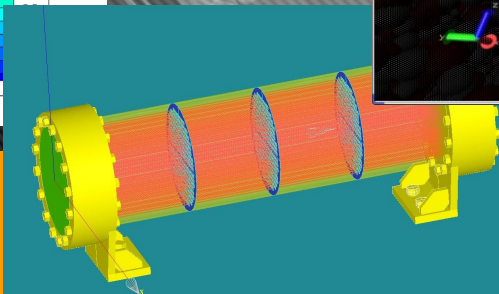
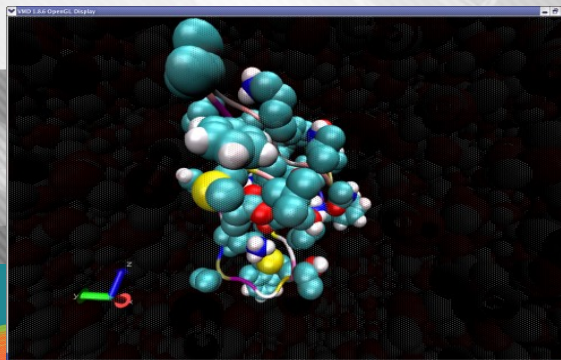
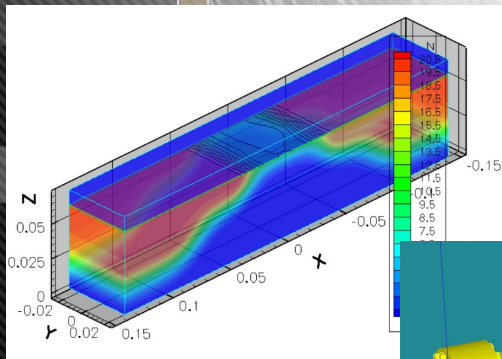
CSIC Madrid, SPAIN, June 2008



SOPORTE Y NUEVAS APLICACIONES



FLUJISTERRAE



SOPORTE

❑ FORMA DE CONTACTO

- ✓ E-CORREO: aplicaciones@cesga.es
- ✓ TELÉFONO: 981569810
- ✓ VISITA (PREFERIBLE PARA DESARROLLOS)

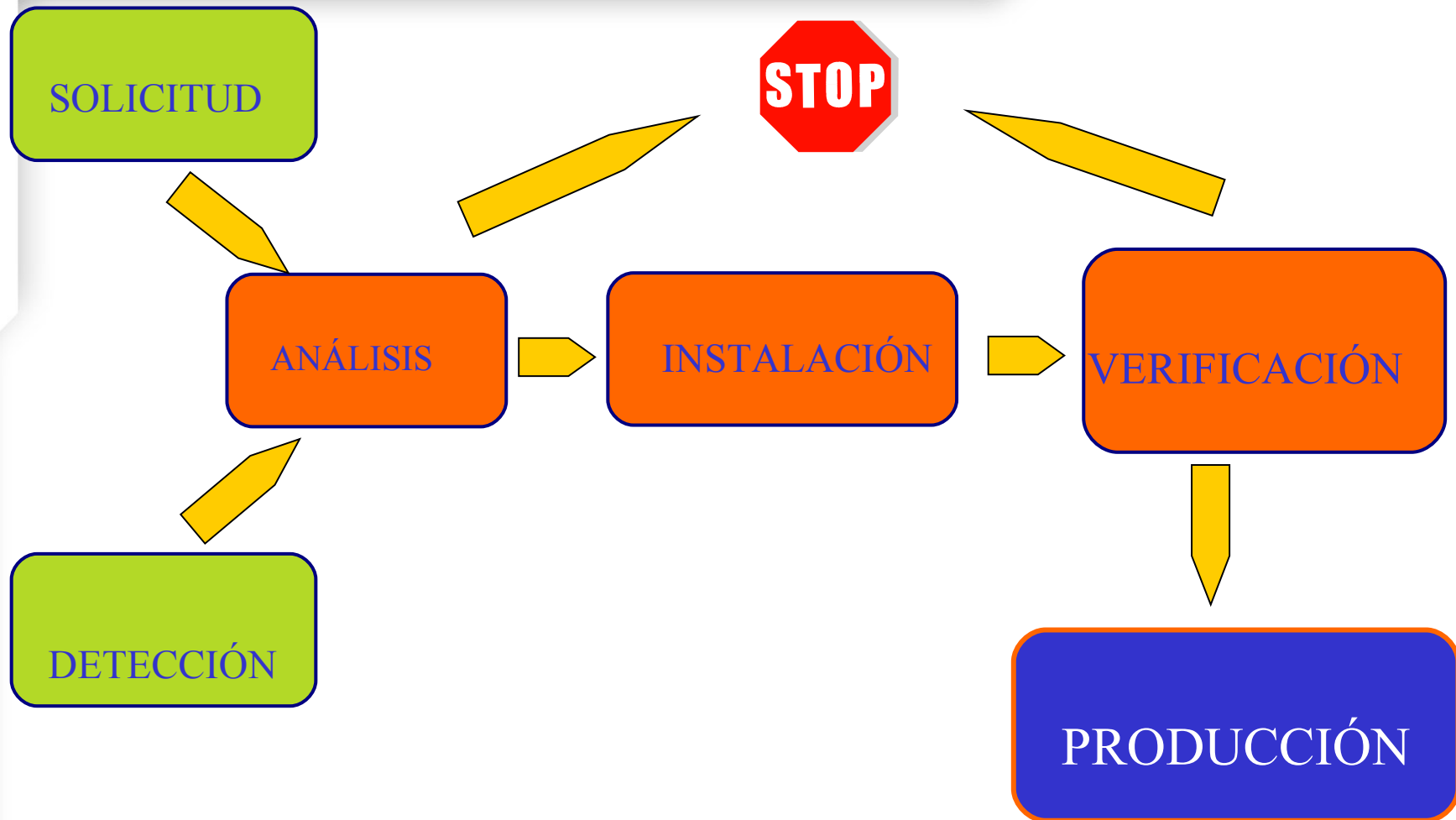
❑ SE ASIGNA TÉCNICO Y TICKET

❑ SERVICIOS

- ✓ ERRORES EN APLICACIONES
- ✓ INSTALACIÓN NUEVAS APLICACIONES Y LIBRERÍAS
- ✓ COMPILACIÓN APLICACIONES PROPIAS
- ✓ CONSULTAS SOBRE PARALELIZACIÓN, EJECUCIÓN, COMPILACIÓN
- ✓ DESARROLLOS DE APLICACIONES

CSIC Madrid, SPAIN, June 2008

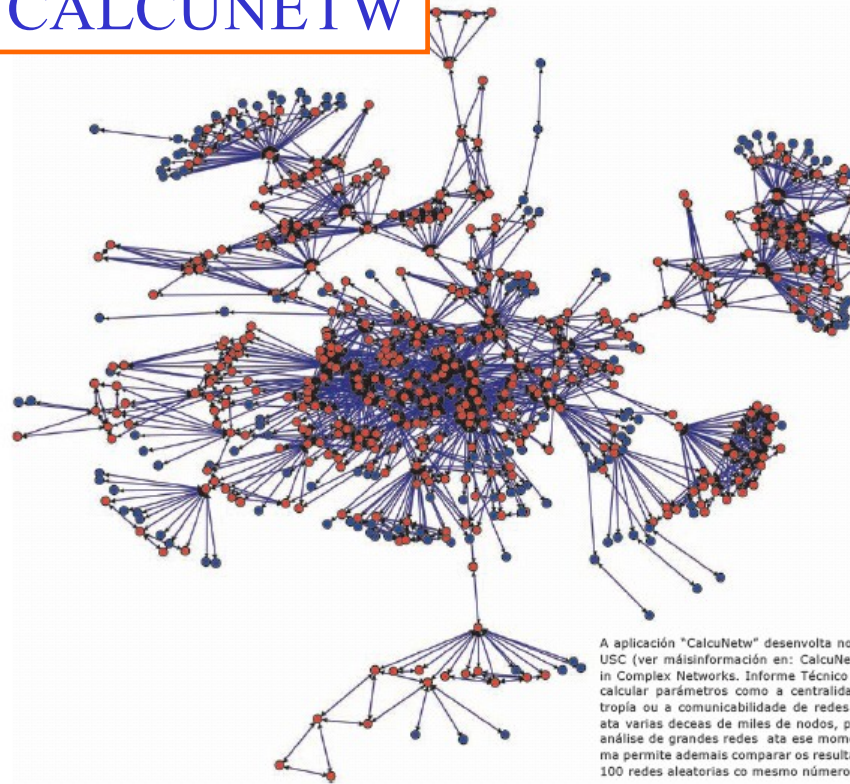
INSTALACIÓN APLICACIONES



CSIC Madrid, SPAIN, June 2008

EJEMPLOS APLICACIONES

CALCUNETW



WebBlast IIM Vigo - Mozilla Firefox

Explore the database

- WEBBLAST
 - SSH-Abeja_Perkinso-Hemocito-Directa
 - Bandoo-Larño-Fanta
 - SSH-Zebrafish-Directa
 - Eucariotas-Impresión-IV
 - SSH-Abeja-Perkinso-branquia-reversa
 - Eucariotas-ImpresiónII
 - SSH-Abeja_Bacteri
 - Abeja_Bacteri
 - 10-24-188.1
 - 10-25-188.1
 - 10-26-188.1
 - SSH-Abeja-Perki
 - test
 - test1
 - 2-22-197.1
 - test2
 - Eucariotas-Impresión-III
 - Eucariotas-Impresión-I
 - SSH-Abeja_Perkinso-Branquia-Directa-II
 - SSH-Abeja-Perkinso-Hemocito-Reversa-II
 - Abeja-Perkinso-Hemocito-Reversa-II
 - 11-22-188.1
 - ESTs-SSH-LUBINA-RINON-NODA
 - Cepas_Deg_Arena_IL_07
 - 2-24-197.1
 - prueba
 - SSH-Abeja-Perkinso-Hemocito-Reversa
 - Perkinso-Hemocito-Reversa
 - 11-22-188.1
 - ESTs-SSH-Lubina-Cerebro-Noda-Directa
 - SSH-Lubina-Cerebro-Noda-Directa
 - 11-22-188.1

Sequencias IRS corregidas.

WebBlast

 - Explore the database
 - Report
 - UPLOAD
 - Upload a trace file
 - Batch Submission
 - Change Status
 - Change History
 - ADMIN
 - New Project
 - Remove Project
 - HELP
 - Explore the database
 - Project
 - New Project
 - Upload a trace file
 - Batch Submission

Results for Clon2BPlasid_A4-01PJY

Clon2BPlasid

Sequence analysis report

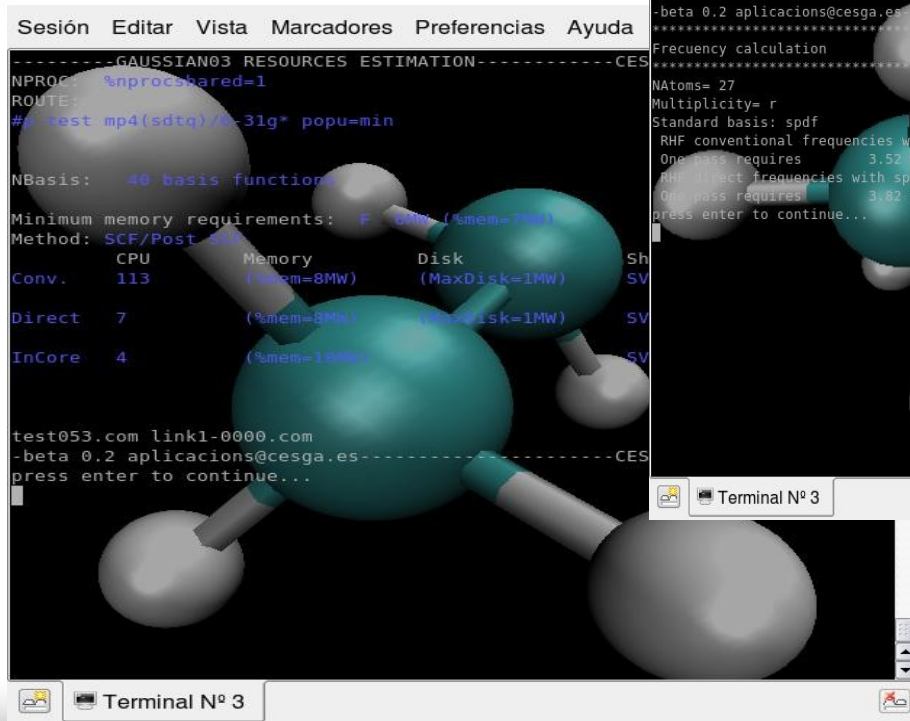
Clon2BPlasid

Sequence analysis report

CSIC Madrid, SPAIN, June 2008

EJEMPLOS APLICACIONES

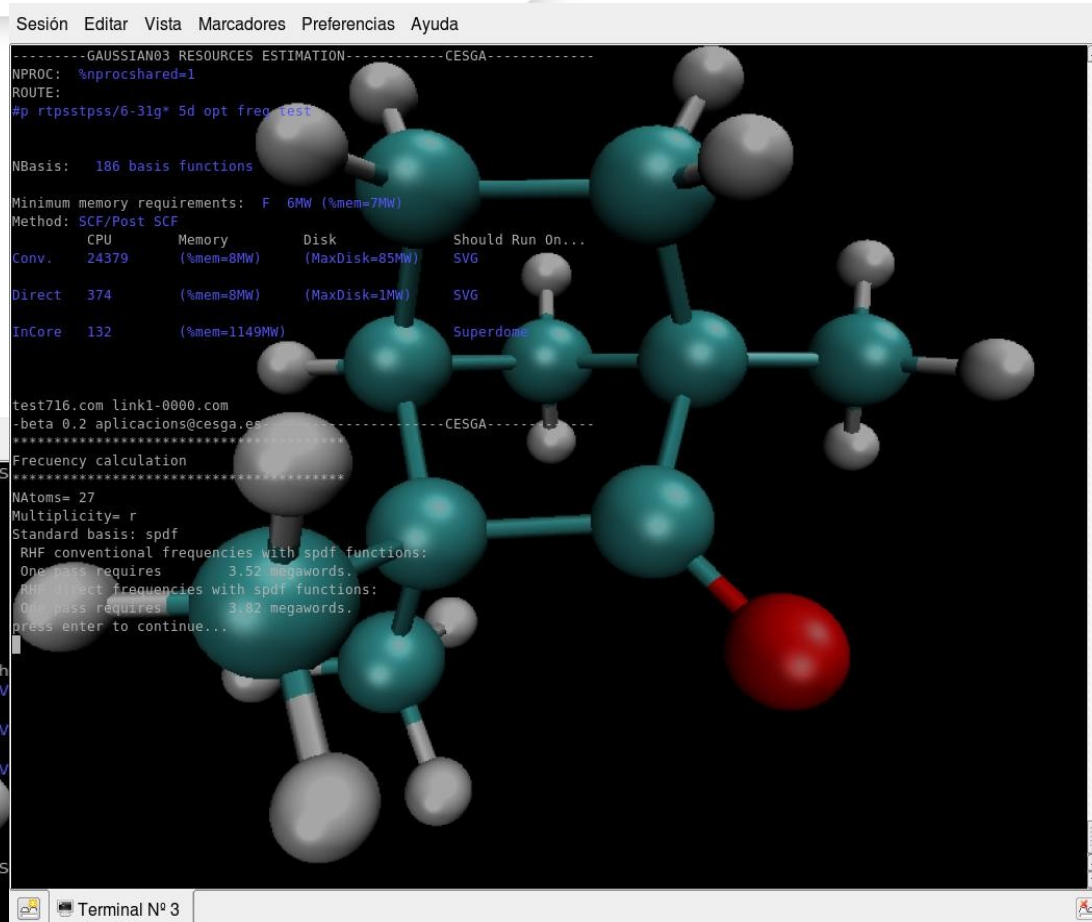
G03MEM Gaussian03 Resources Estimation



```
Sesión Editar Vista Marcadores Preferencias Ayuda
-----GAUSSIAN03 RESOURCES ESTIMATION-----CES
NPROC: %nprocshared=1
ROUTE:
# test mp4(sdtq)/0-31g* popu=min

NBasis: 40 basis functions
Minimum memory requirements: F 6MW (%mem=7MW)
Method: SCF/Post SCF
CPU      Memory      Disk      Sh
Conv.    113          (%mem=8MW) (MaxDisk=1MW) SV
Direct   7            (%mem=8MW) (MaxDisk=1MW) SV
InCore   4            (%mem=1149MW)

test053.com link1-0000.com
-beta 0.2 aplicaciones@cesga.es
press enter to continue...
```



```
Sesión Editar Vista Marcadores Preferencias Ayuda
-----GAUSSIAN03 RESOURCES ESTIMATION-----CESGA-----
NPROC: %nprocshared=1
ROUTE:
# rtpsstpss/6-31g* 5d opt freq test

NBasis: 186 basis functions
Minimum memory requirements: F 6MW (%mem=7MW)
Method: SCF/Post SCF
CPU      Memory      Disk      Should Run On...
Conv.    24379       (%mem=8MW) (MaxDisk=85MW) SVG
Direct   374        (%mem=8MW) (MaxDisk=1MW)  SVG
InCore   132        (%mem=1149MW) Superdome

test716.com link1-0000.com
-beta 0.2 aplicaciones@cesga.es
-----CESGA-----
Frequency calculation
*****
NAtoms= 27
Multiplicity= r
Standard basis: spdf
RHF conventional frequencies with spdf functions:
One pass requires 3.52 megawords.
RHF direct frequencies with spdf functions:
One pass requires 3.82 megawords.
press enter to continue...
```

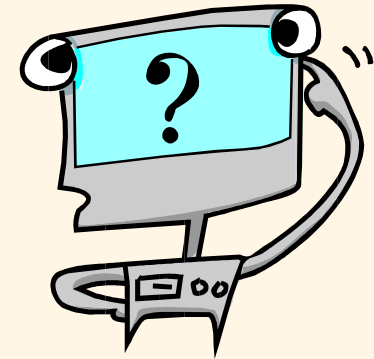
CSIC Madrid, SPAIN, June 2008

END



THANK YOU!

QUESTIONS



CONTACT:

Aurelio Rodríguez

aurelio@cesga.es

<http://www.cesga.es>

CSIC Madrid, SPAIN, June 2008