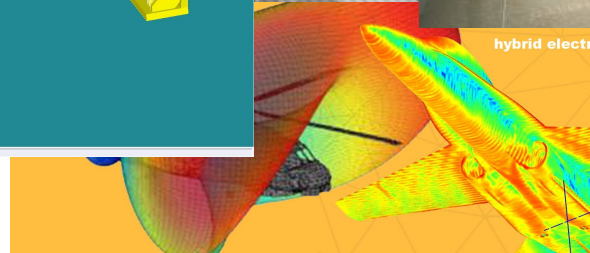
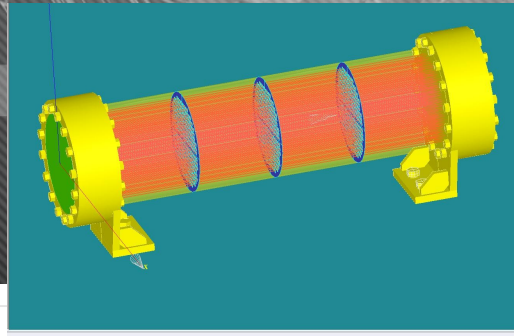


FINIS TERRAE: TOOLS & APPLICATIONS

Andrés Gómez

agomez@cesga.es

FINIS TERRAE



hybrid electro

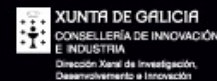
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CESGA FINISTERRAE
COMPUTATIONAL SCIENCE
CONFERENCE 2008

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GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN



APPLICATIONS SUPPORT

- ❑ INSTALL AND COMPILING SCIENTIFIC APPLICATIONS

- ❑ TECHNICAL SUPPORT
 - ✓ Parallelization
 - ✓ Libraries
 - ✓ Tools and scientific programming languages
 - ✓ Performance

- ❑ DEVELOPING VERY SMALL SCIENTIFIC APPLICATIONS

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APPLICATIONS SUPPORT (ii)

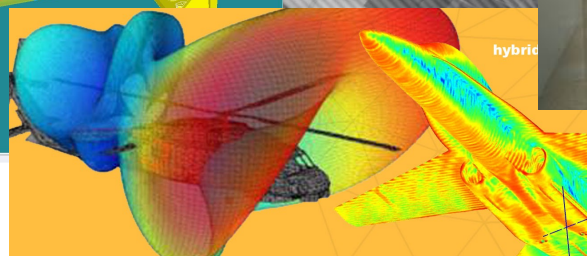
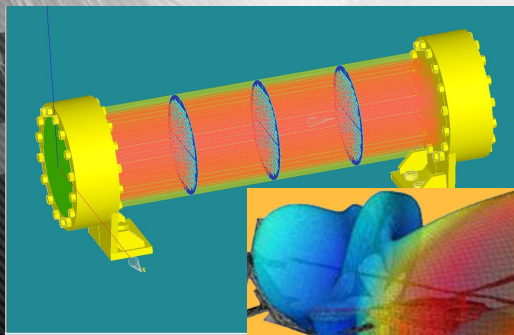
□ 3 + 1 TECHNICIANS

- ✓ PhD. on Physics (me)
- ✓ PhD. on Computational Chemistry
- ✓ PhD. on Computer Science
- ✓ Graduate on Mathematics (Applied, i-MATH)

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APPLICATIONS FOR FINIS TERRAE

FINISTERRAE



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INSTALLED APPLICATIONS ON APRIL 2008

Structural, Fluids and Magnetism Calculations

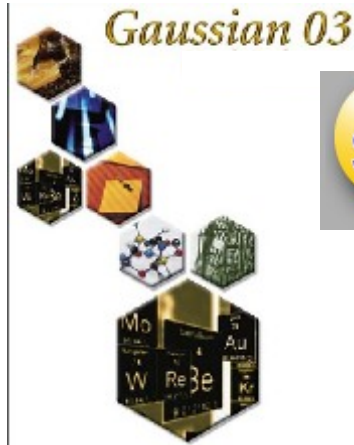
Elmer



Molecular Calculation



Amber



LAMMPS Molecular Dynamics Simulator

NAMD
Scalable Molecular Dynamics

LOOK AT CURRENT LIST ON
WWW.CESGA.ES OR MODULES

SANTIAGO, SPAIN, JUNE 2008

INSTALLED APPLICATIONS ON APRIL 2008

```
sd.cesga.es - PuTTY
----- /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      lammps/22Jan2008-impi
attach      icc/10.1.012      mkl/10.0.011
cmkl/10.0.011      icc/9.1.052 (default)      mkl/10.0.2.018
cmkl/9.1      idb/10.1.012      mkl/9.1 (default)
elmer      idb/9.1.052 (default)      namd/2.6 (default)
fftw/2.1.5      ifort/10.1.012      namd/2.6b1
fftw/3.0.1      ifort/9.1.052 (default)      netcdf/3.6.1
fftw/3.1.2 (default)      impi/3.0      netcdf/3.6.2 (default)
g03/c1      impi/3.1      numpy
g03/d2      impi/3.1.038 (default)      pyMPI
g03/e1 (default)      intel/10      siesta
grads      intel/9 (default)      stata/10.0 (default)
gromacs/3.3.1      itac/7.1/impi3      udunits
gromacs/3.3.2 (default)      lammps/22Jan2008 (default)
agomez@cn004:~>
```

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DEVELOPMENT TOOLS

COMPILERS AND TOOLS

Intel C++
Compiler

X

Intel Fortran
Compiler

X

Modules

X



HP Message Passing Interface library (HP-MPI)
Developer & Solution Partner Program (DSPP)

SOON



LIBRARIES

MKL

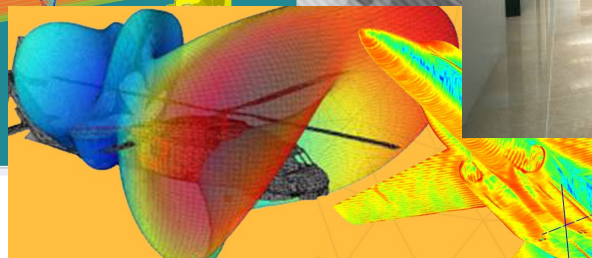
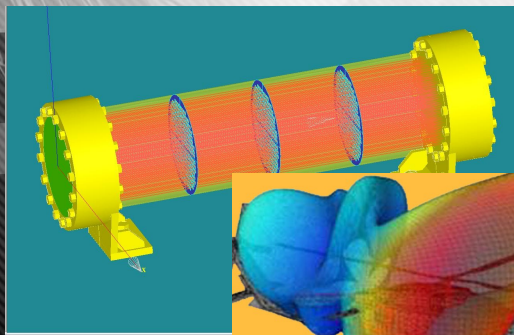
X

MPI	HP MPI	X
	Intel MPI Library	X

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APPLICATION PERFORMANCE

FINISTERRAE



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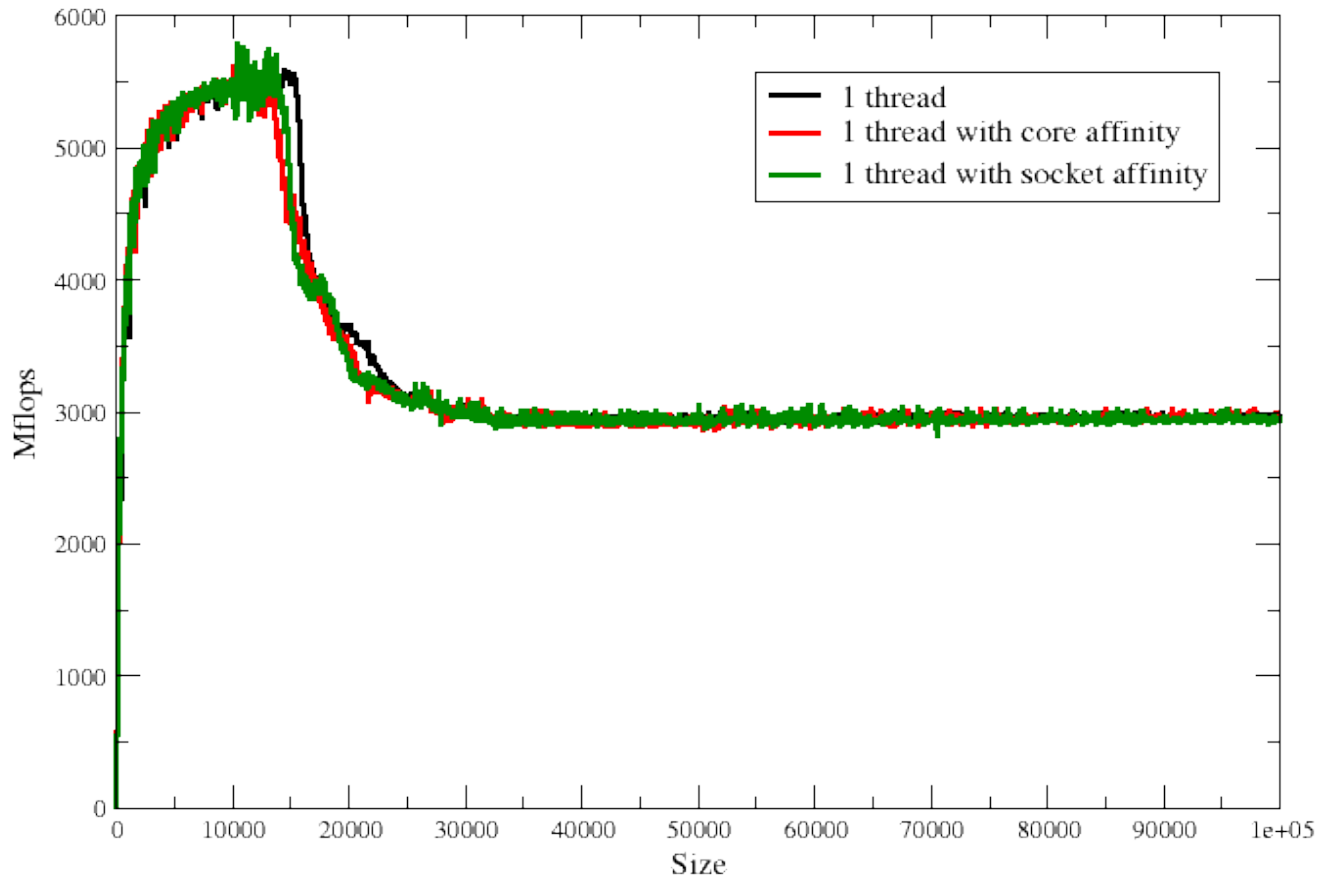


In collaboration with:



FINIS TERRAE – MKL Performance

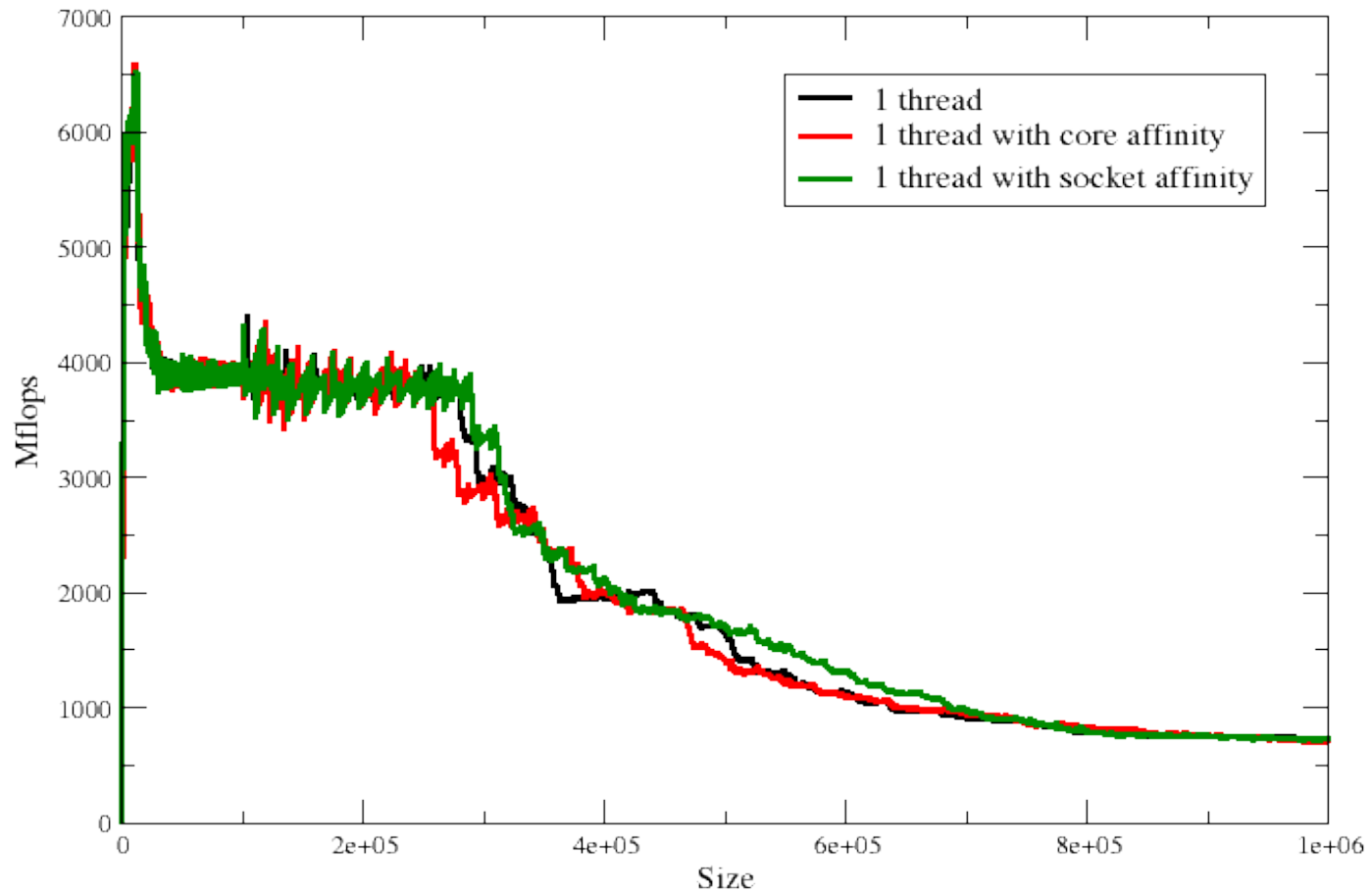
DAXPY from MKL in FINIS TERRAE



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FINIS TERRAE – MKL Performance

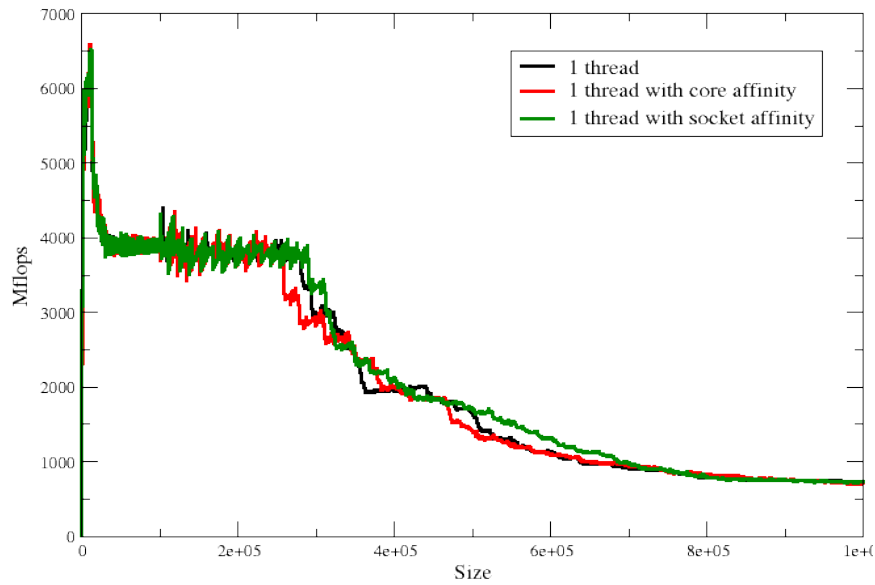
DDOT from MKL in FINIS TERRAE



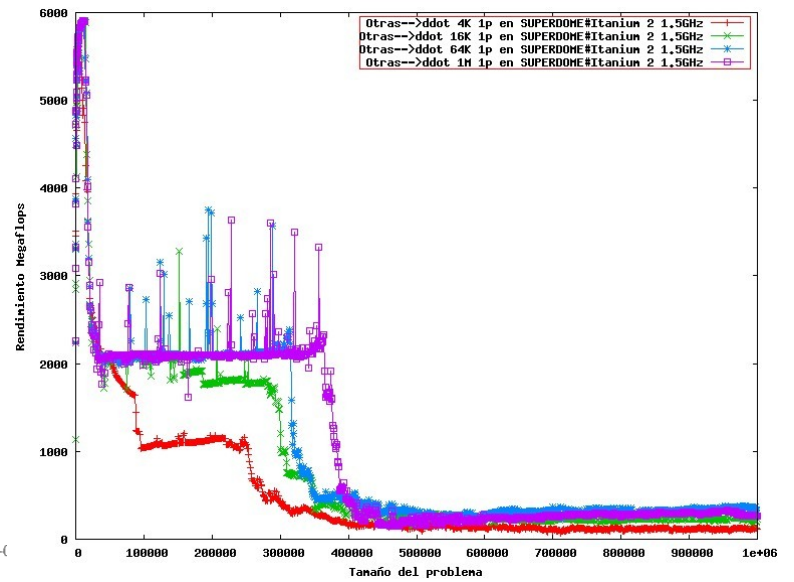
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FINIS TERRAE – SUPERDOME

DDOT from MKL in FINIS TERRAE



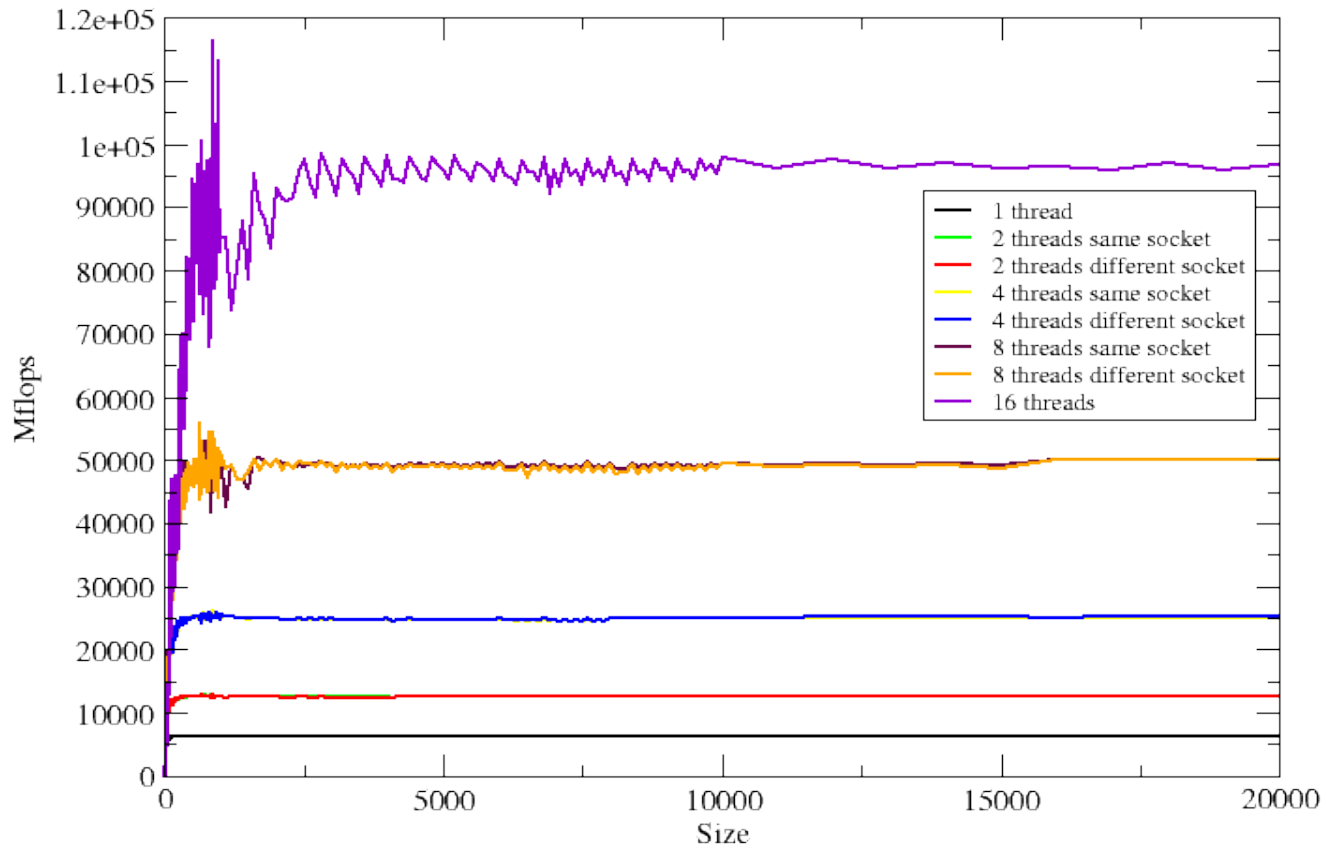
SUPERDOME HP-UX -MLIB



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FINIS TERRAE – MKL Performance

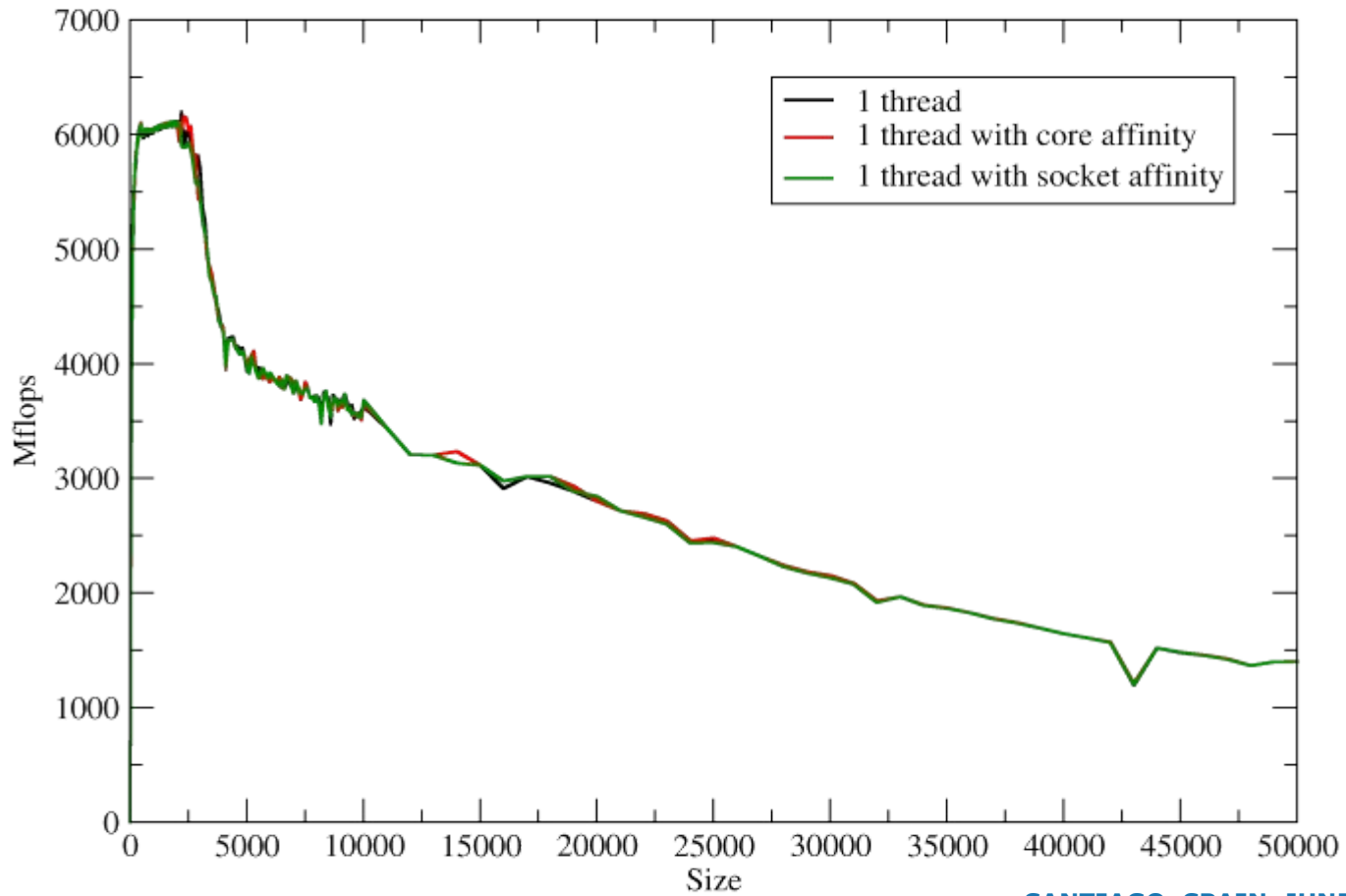
DGMM from MKL in FT



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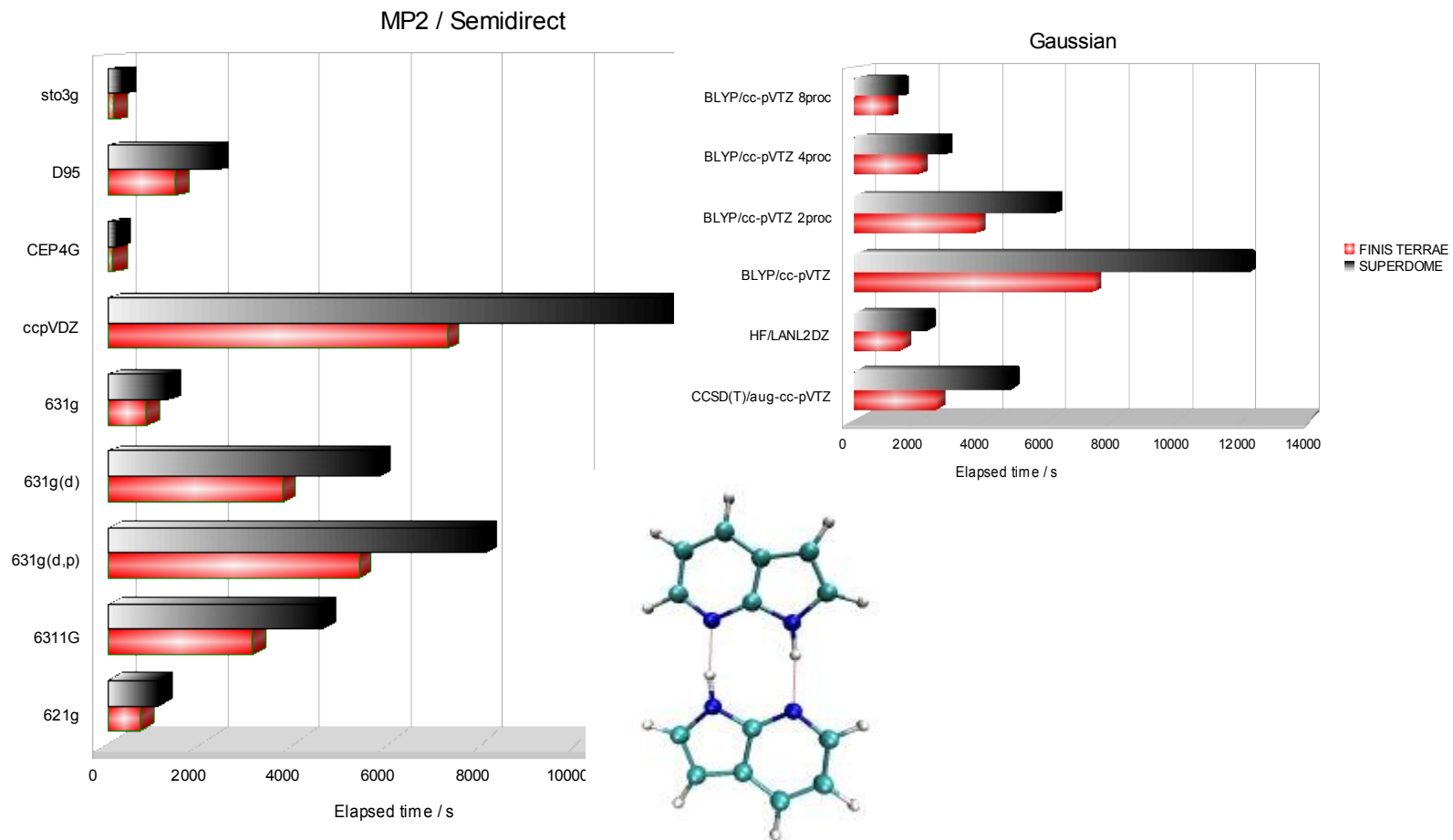
FINIS TERRAE – MKL Performance

DGEMV from MKL in FT



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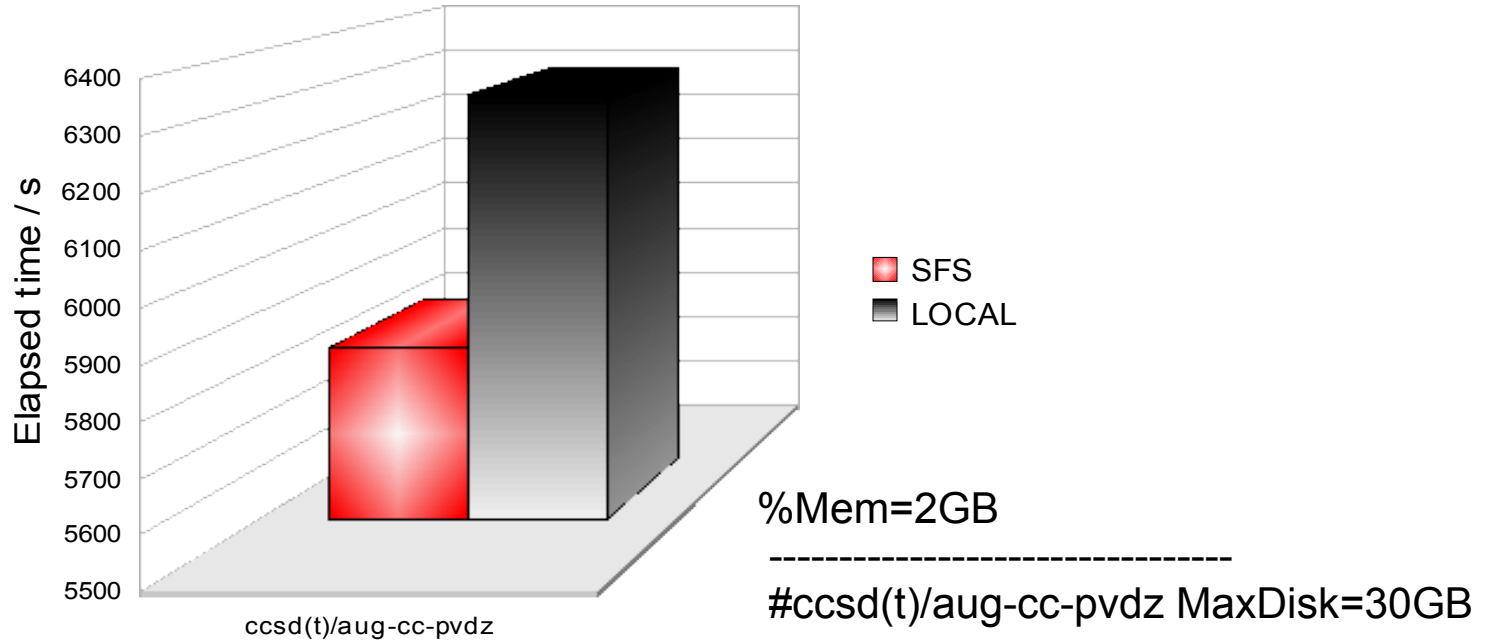
FINIS TERRAE – Gaussian Performance



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FINIS TERRAE – SFS: A Gaussian Test

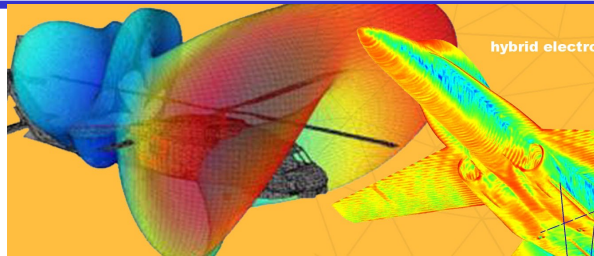
FULL OPTIMIZED FILESYSTEM



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

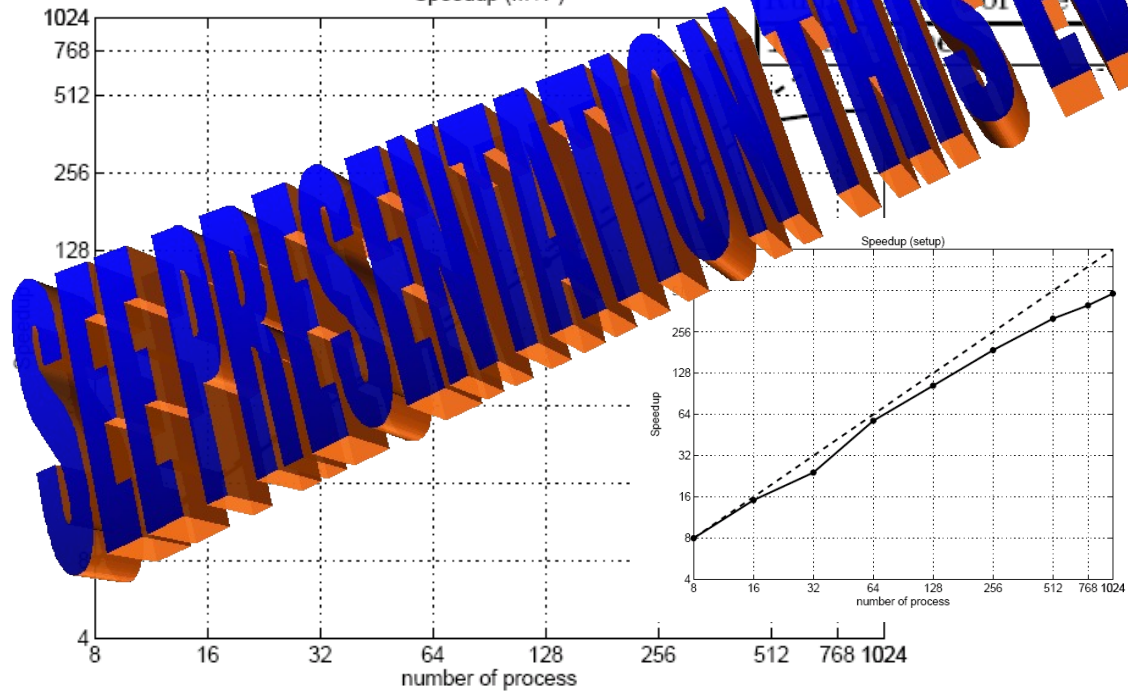
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FINIS TERRAE – FIRST CHALLENGES



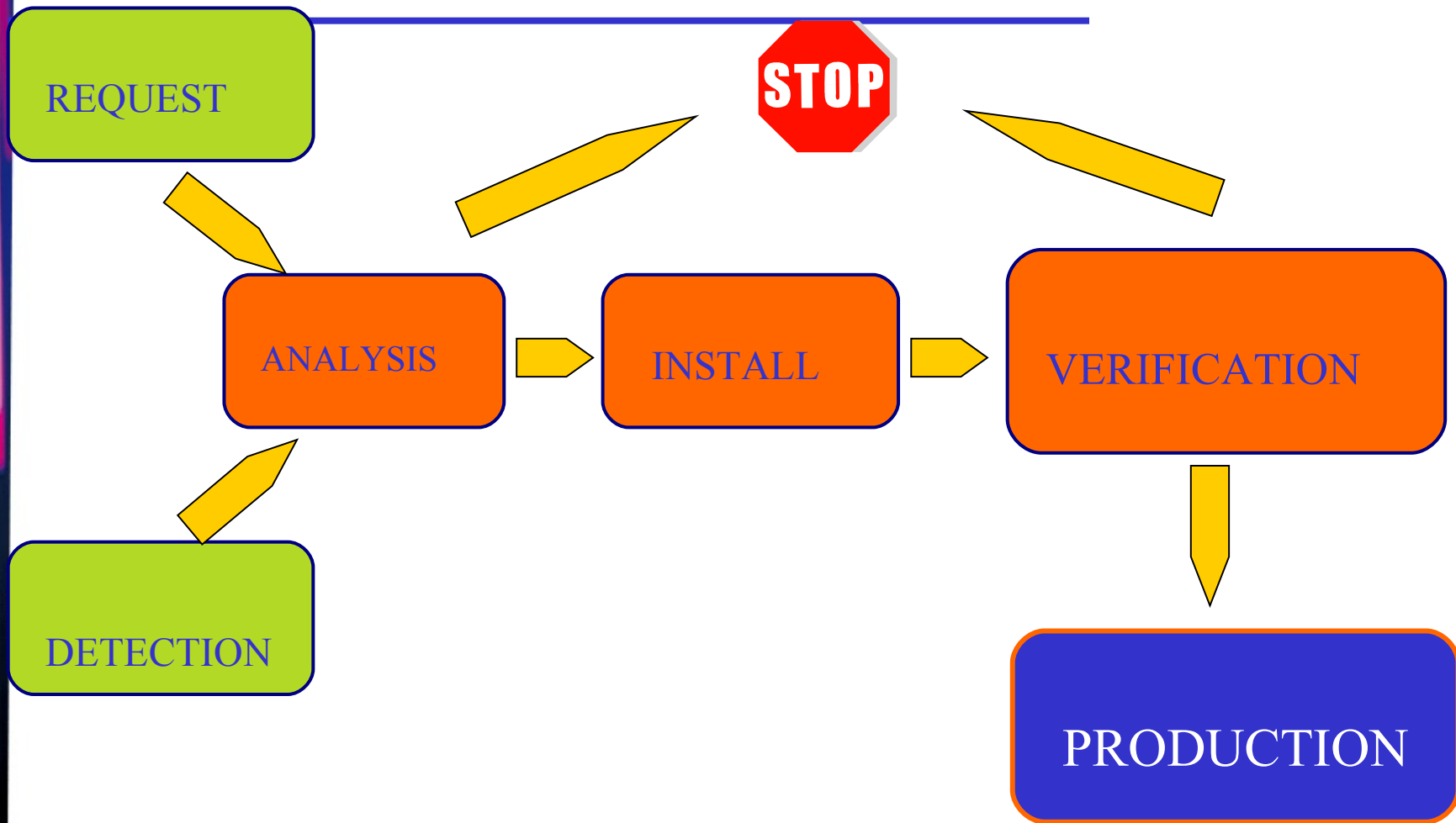
RCS of a sphere with 200λ diameter.	
Unknowns number	32 411,106
Cell dimensions	2λ
Process number	512
Total Memory	1 TB
Setup time	6m
Single iteration	6m6s
Time of execution	10h35m
	15h10m

¡¡32.000.000 UNKNOWNNS!!



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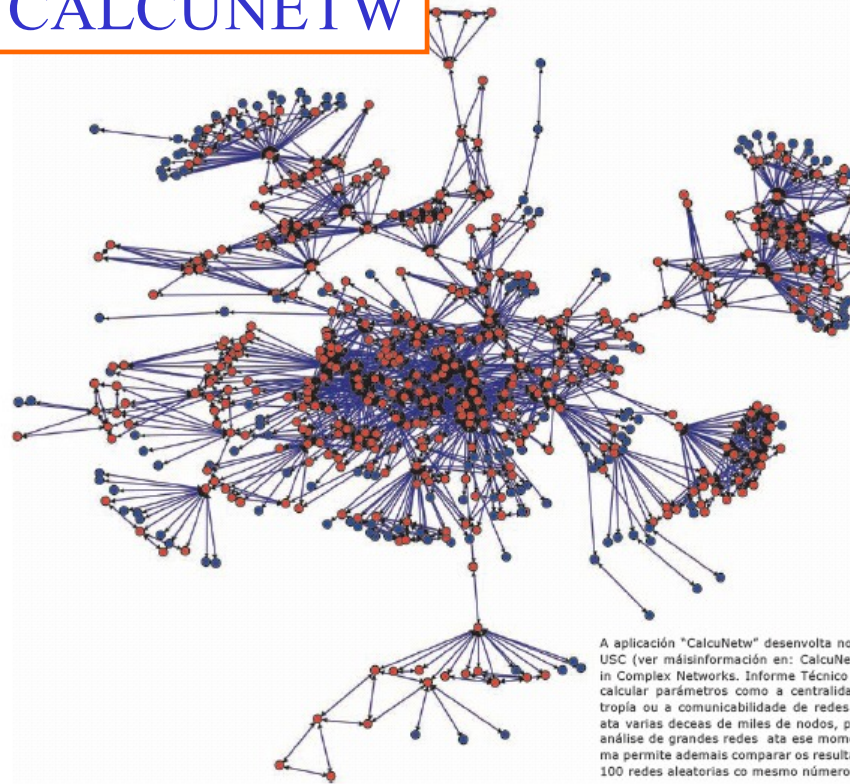
INSTALL APPLICATIONS



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EXAMPLE SMALL APPLICATIONS

CALCUNETW



The image shows two overlapping browser windows. The top window is titled "WebBlast IIM Vigo" and displays a search interface with a tree view of databases on the left, a search input field, and a "WebBlast" button. The bottom window shows the "Results for ClustalW" page, which includes a sequence alignment visualization and a table of results.

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SUPPORT

CONTACT

- ✓ E-MAIL: APLICACIONES AT CESGA.ES
- ✓ PHONE: +34 981569810
- ✓ VISIT (WE LIKE IT!)

TICKETS

SERVICES

- ✓ ERRORS IN APPLICATIONS
- ✓ INSTALL NEW APPLICATIONS AND LIBRARIES
- ✓ COMPILE PRIVATE CODES
- ✓ QUESTIONS ABOUT PARALLELIZATION, EXECUTION AND COMPILING
- ✓ DEVELOPMENT (VERY) SMALL SCIENTIFIC APPLICATIONS

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