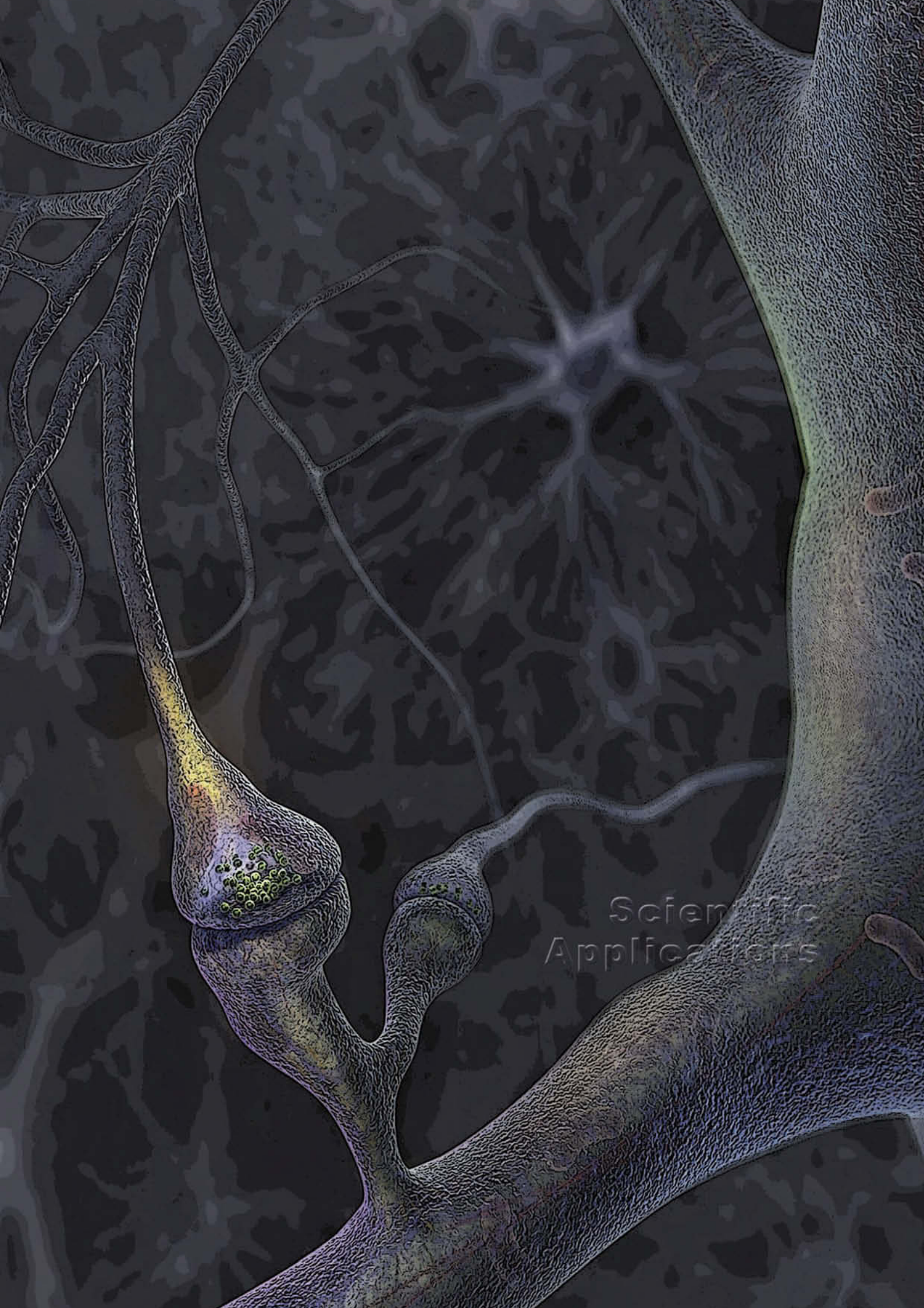


scientific computing applications

There was a significant increase in activity in the area of applications during 2008 due to the installation of the new supercomputer, Finis Terrae and the demonstration of its capacities in the execution of scientific challenges. Specifically, the following activities were performed in 2008.

- The execution of 6 scientific challenges, 4 in February and 2 during the rest of the year.
- A high number of support activities (241) during the year which represents an interannual increase of 96%.
- The installation of almost all the applications supported by CESGA in the Finis Terrae server, as well as other applications that users demand. This required the porting of several applications to Finis Terrae. A list of the ported elements is presented below.

Applications, such as:

- Amber version 9.0
- CHARMM version c34b2
- CPMD version 3.11.1
- Crystal version 06
- deMon2k version 2.3
- Elmer version 5.4.1
- FLEXPART version 8.0
- FLUENT version 6.3
- Gamess versions 24 MAR 2007 (R1) & 11 APR 2008 (R1)
- Gaussian 03 version E.01
- Grads version 2.0.a1
- Gromacs versions 3.3, 3.3.2, 3.3.3, 4.0 y 4.0.2
- LAMMPS versions 21May2008 & 22Jan2008
- Leadmix version 28-08-2005
- Macaulay 2 version 1.1
- Materials Studio version 4.3
- MOLCAS version 6.4
- Molden version 4.6
- molpro version 2006.1
- MrBayes version 3.1.2
- NAMD version 2.6
- NWChem version 5.1
- R versions 2.7.0 & 2.7.2
- SIESTA version 2.0.1
- Singular version 3.0.4
- Stata/MP version 10.0
- Turbomole version 5.10
- udunits version 1.12.4
- VASP version 4-6-28
- VMD version 1.8.6
- Wien2k version 08.1
- XcrySDen version 1.4

Libraries, such as:

- CGAL version 3.3.1
- FFTW versions 3.1.2 & 3.2alpha3
- HDF versions 4.2r3-ia64 & 5 1.8.1
- HP MPI 2.2.5.1
- Intel MPI Library 3.0 3.1 2 3.2.0.011
- Jrockit R27.5.0-jdk1.5.0_14
- MKL 10.0.011 10.0.2.018 9.1 10.1.0
- NumPy 1.0.4
- pyMPI 2.5b0
- Ncarg 5.0.0
- NetCDF 4.0 3.6.2

Compilers, such as:

- Intel C++ Compiler versions 9.1.052, 10.1.012 & 11.0.069
- Intel Fortran Compiler versions 9.1.052, 10.1.012 & 11.0.069

Software management utilities, such as:

- Modules version 3.1.6
- Subversion version 1.5.3

The installation of the majority of Intel development tools in the SVG server, thereby unifying the development tools supported by CESGA's servers.
The organisation of internal and external training courses on topics related to applications and tools.

Solely organised by CESGA:

- Free/Libre software tools for the debugging and the analysis of applications performance
- Parallel programming by means of OpenMP directives
- Fortran course (1st edition)
- Fortran course (2nd edition)
- Intel development tools

Organised by CESGA Node of the I-MATH project:

▪Introduction to MPI programming

▪COMPUTATIONAL MATHEMATICS: Compilation, execution and optimisation of programs

▪Intensive I-MATH course on Free/Libre Software oriented to sciences and engineering: Simulation in Multiphysics: ELMER (SMF)

The delivery of a training course for users:

▪Introduction to computational chemistry codes in CESGA (Gaussian, GAMESS, NWCHEM)

• The use of applications was made easier via the MODULES utility that permits the dynamic configuration of any number of software applications with their corresponding versions in a UNIX environment. MODULES is actually the method used to configure the environment used by default in CESGA's computing servers (SVG and Finis Terrae).

• A high number of requests for new installations or version updates (83) or for support for the compilation of user applications or user-licensed-applications.

• Ongoing collaboration with CSCS (Swiss National Supercomputing Centre) in the area of chemical visualisation by way of the COST GRIDCHEM network as reflected in a jointly published technical report: ".Quantum Chemistry common data format Q5COST and OpenBabel: A first answer to interoperability in Quantum Chemistry".

All the activity developed in the area of applications in 2008 can be summarised as follows.

▪59 applications or libraries of scientific computing in production,

▪83 versions of new applications installed or updated,

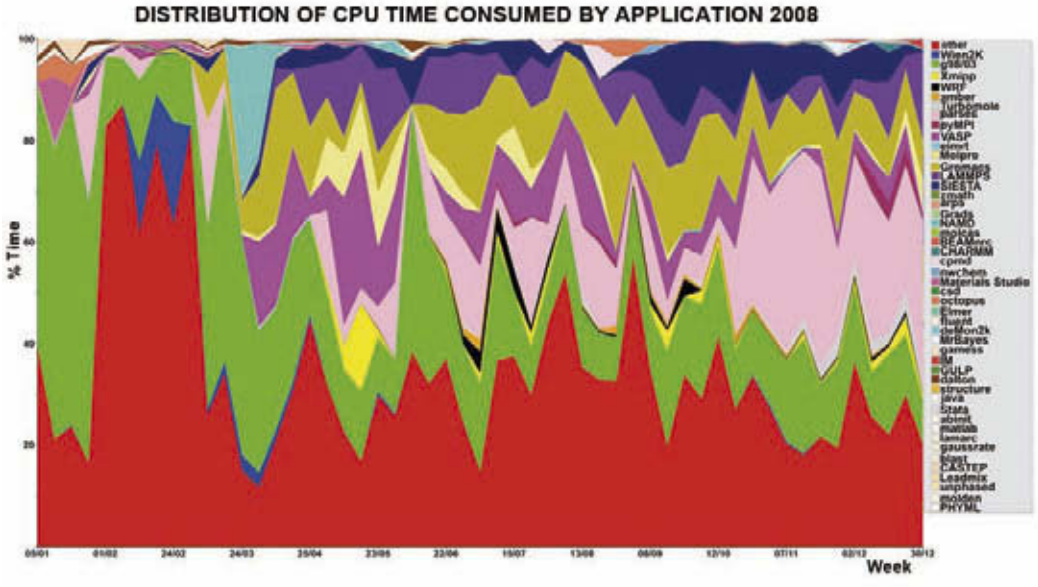
▪technical support was provided to 6 computing challenges which required the adaptation and modification of various applications,

▪the publication of one CESGA technical report,

▪241 user requests for technical assistance were attended.

statistics of applications use during 2008

These statistics summarise the use of applications from January 1, 2008 until December 31, 2008 and were extracted from the accounting records. Given that the information collected for the name of the executables in some systems is truncated, it is possible that a small error may exist in assigning same to an application (highly improbable). Data collected for accounting purposes include only those entries whose time of execution is greater than 30 seconds (including both system and user time) in order to avoid saturating the system, except in the CSD or in other explicitly marked applications in which the threshold is lower, since the time used on this sort of application is much lower. The 20 most used applications are presented in the Table ("others" means non-classified applications, fundamentally, those that are installed or developed by the users themselves).



Many new applications or libraries of utilities were incorporated in 2008 at the request of users or for the installation of new versions (see Table below).

APPLICATION	TASK
SCIENTIFIC DATA BASES	
CSD (Migrated to the SVGD server; new version, V5.30 (2009) installed)	Cambridge Structural Database is a data base that collects bibliographic, chemical, and crystallographic information regarding organic and organometallic obtained by the diffraction of X-rays and the diffraction of neutrons. **http://www.ccdc.cam.ac.uk/products/csd**
MOLECULAR SIMULATION	
Amber (new installation, version 9.0, in Finis Terrae)	AMBER is a set of programs that allows the user to perform molecular dynamics simulations, fundamentally in biomolecules, based on theories of force fields. **http://ambermd.org**
CPMD (new installation, version 3.11.1, in Finis Terrae)	CPMD is an implementation of the theory of the functionality of density using plane waves/pseudopotentials that are particularly designed in order to carry out ab initio molecular dynamics studies. **http://www.cpmd.org**
Gamess (New installation, versions 11 APR 2008 (R1) and 24 MAR 2007 (R1), in Finis Terrae)	This is an analogue package for GAUSSIAN that incorporates ab initio methods, although it does offer specific solutions for the description of orbits and other methods of optimisation. **http://www.msg.chem.iastate.edu/gamess/gamess.html**
Gaussian 03 (new installation version E.01, in Finis Terrae)	Gaussian 03 is one of most used packages in Computational Chemistry that permits the prediction of properties (energies, frequencies of vibration, optimal geometry, etc.) of molecules and intermediates of reaction, fundamentally by means of theoretical ab initio methods. **http://www.gaussian.com**
Gromacs (New version, 3.3.2, in the SVG. New installation, versions 4.0.2, 4.0, 3.3, 3.3.3 y 3.3.2, in Finis Terrae)	GROMACS is versatile software for molecular dynamics calculations, i.e., it simulates the equations of Newton regarding movement for systems with hundreds of millions of particles. It is principally designed for the study of biochemical molecules such as proteins and lipids with a large number of complex bonding interactions. **http://www.gromacs.org**
LAMMPS (new installation, versions 21 May 2008 and 22 Jan 2008, in Finis Terrae)	LAMMPS is a molecular dynamics simulator. It runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain. The code is designed to be easy to modify or extend with new functionalityw. **http://lammps.sandia.gov**
Molden (new installation, version 4.6, in Finis Terrae)	Molden is a package for displaying Molecular Density from the Ab Initio packages GAMESS-UK , GAMESS-US and GAUSSIAN and the Semi-Empirical packages Mopac/Ampac, it also supports a number of other programs via the Molden Format. Molden reads all the required information from the GAMESS / GAUSSIAN outputfile. Molden is capable of displaying Molecular Orbitals, the electron density and the Molecular minus Atomic density. **http://www.cmbi.ru.nl/molden/molden.html**

APPLICATION	TASK
NAMD (new installation, version 2.6, in the SVG and in Finis Terrae)	NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on Charm++ parallel objects, NAMD scales to hundreds of processors on high-end parallel platforms and tens of processors on commodity clusters using gigabit ethernet. http://www.ks.uiuc.edu/Research/namd/
NWChem (new installation, version 5.1, in Finis Terrae)	NWChem is a computational chemistry package designed for execution on high performance parallel supercomputers as well as for conventional work station clusters. It is intended to be scalable in its capacity to deal with large problems in an efficient manner such as in its use of available parallel computational resources. **http://www.emsl.pnl.gov/docs/nwchem/nwchem.html**
SIESTA (new installation, version 2.0.1, in Finis Terrae)	SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and its computer program implementation, to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. **http://www.icmab.es/siesta**
Applications with limited licensing (User or single institution) **RESTRICTED TO SPECIFIC USERS**	
CHARMM (new installation, version c34b2, in Finis Terrae)	CHARMM (Chemistry at Harvard Macromolecular Mechanics) is a versatile and widely used program for molecular simulation that has many applications to multiparticle systems. **http://www.charmm.org**
Crystal (new installation, version 06, in Finis Terrae)	Crystal is a computational tool for simulations of solid state physics and chemistry. **http://www.crystal.unito.it/**
DeMon2k (new installation, version 2.3, in Finis Terrae)	deMon (density of Montréal) is a software package for density functional theory (DFT) calculations. It uses the linear combination of Gaussian-type orbital (LCGTO) approach for the self-consistent solution of the Kohn-Sham (KS) DFT equations. The calculation of the four-centre electron repulsion integrals is avoided by introducing an auxiliary function basis for the variational fitting of the Coulomb potential. **http://www.demon-software.com/public_html/program.html**
Materials Studio (new installation, version 4.3, in Finis Terrae)	Materials Studio is a modelling and simulation package that is easy to use for the study of chemical substances and materials. It provides tools for modelling crystal structure and crystallization processes, for the study of polymer properties, catalysis, and the study of structure-activity relationships. **http://accelrys.com/products/materials-studio**
MOLCAS (new installation, version 6.4, in Finis Terrae)	MOLCAS is a quantum chemistry software developed by scientists to be used by scientists. MOLCAS emphasizes the multiconfigurational approach for quantum chemical calculations, which allows studies of systems where a single configuration does not give a good representation of the electronic structure. Examples are excited states, transition states for chemical reactions, heavy element systems (transition metals, lanthanides, actinides), and much more. **http://www.teokem.lu.se/molcas**
MOLPRO (new installation, version 2006.1, in Finis Terrae)	Molpro is a complete system of ab initio programs for molecular electronic structure calculations. As distinct from other commonly used quantum chemistry packages, the emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem through the multiconfiguration-reference CI, coupled cluster and associated methods. **http://www.molpro.net**

APPLICATION	TASK
Turbomole (new installation, version 5.10, in Finis Terrae)	TURBOMOLE is one of the fastest and most stable codes available for standard quantum chemical applications. Unlike many other programs, the main focus in the development of TURBOMOLE has not been to implement all new methods and functionals, but to provide a fast and stable code which is able to treat molecules of industrial relevance at reasonable time and memory requirements. **http://www.cosmologic.de/index.php?cosName=main_turbomole**
VASP (new installation, version 4-6-28, in Finis Terrae)	VAMP/VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. **http://cms.mpi.univie.ac.at/vasp**
WIEN2K (new installation, version 08.1, in Finis Terrae)	The program package WIEN2k allows users to perform electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. **http://www.wien2k.at**
BIOINFORMATICS	
IM (new version 3/2/2008 in the SVG)	IM is a program for the fitting of an isolation model with migration to haplotype data drawn from two closely related species or populations. IM is based on a method originally developed by Rasmus Nielsen and John Wakeley (Nielsen and Wakeley 2001 Genetics 158:885). Large numbers of loci can be studied simultaneously, and different mutation models can be used. **http://lifesci.rutgers.edu/~heylab/HeylabSoftware.htm#IM**
Lamarc (new installation, versions 2.1.2b and 2.1.3, in the SVG)	Lamarc is a program for doing Likelihood Analysis with Metropolis Algorithm using Random Coalescence. Lamarc estimates effective population sizes, population exponential growth rates, a recombination rate, and past migration rates for one to n populations assuming a migration matrix model with asymmetric migration rates and different subpopulation sizes. **http://evolution.genetics.washington.edu/lamarc/lamarc_prog.html**
Leadmix (new installation, version 28-08-2005, in the SVG and Finis Terrae)	LEADMIX is a Fortran program to estimate the admixture proportions and genetic drift using data on genetic markers, based on the likelihood method **http://www.zoo.cam.ac.uk/ioz/software.htm#LEADMIX**
MrBayes (new installation, version 3.1.2, in Finis Terrae)	Mrbayes is a program for the Bayesian phylogenesis estimation based on a simulation technique known as Markov chain Monte Carlo (or MCMC). **http://mrbayes.csit.fsu.edu/index.php**
Structure (new installation, version 2.2.3, in the SVG)	The program structure is a free software package for using multi-locus genotype data to investigate population structure. Its uses include inferring the presence of distinct populations, assigning individuals to populations, studying hybrid zones, identifying migrants and admixed individuals, and estimating population allele frequencies in situations where many individuals are migrants or admixed. **http://pritch.bsd.uchicago.edu/structure.html**
Unphased (new installation, version 3.0.13, in thel SVG)	UNPHASED is a versatile application for performing genetic association analysis. **http://www.mrc-bsu.cam.ac.uk/personal/frank/software/unphased**

APPLICATION	TASK
METEOROLOGICAL SIMULATION	
ECBILT/CLIO (new installation, version 3, in the SVG)	The ECBilt-Clio model is an 'intermediate-complexity', three-dimensional coupled atmosphere-ocean-sea ice General Circulation Model. **http://www.knmi.nl/onderzk/CKO/ecbilt.html**
Field (new installation, version 1.2 in the SVG)	The Field library provides high-level access to gridded data fields in a data format independent manner. This library is required for models such as ECBILT. **http://www.knmi.nl/onderzk/CKO/tools.html**
STRUCTURAL MODELLING, FLUIDS, AND MAGNETISM	
Elmer (new installation, version 5.4.1, in Finis Terrae)	Elmer is an open source multiphysical simulation software developed by CSC. Elmer includes physical models of fluid dynamics, structural mechanics, electromagnetism, heat transfer and acoustics, for example. These are described by partial differential equations which Elmer solves by the Finite Element Method (FEM). **http://www.csc.fi/english/pages/elmer**
OpenFOAM (new version, 1.4.1, in the SVG)	The OpenFOAM® (Open Field Operation and Manipulation) CFD Toolbox can simulate anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics, electromagnetism and the pricing of financial options. OpenFOAM is produced by OpenCFD Ltd and is freely available and open source, licensed under the GNU General Public Licence. **http://www.opencfd.co.uk/openfoam**
Applications with limited licensing (User or sole institution) **RESTRICTED TO SPECIFIC USERS**	
FLUENT (new installation, version 6.3, in Finis Terrae)	FLUENT software is a powerful and flexible general-purpose computational fluid dynamics (CFD) package used for engineering simulations of all levels of complexity. It offers a comprehensive range of physical models that can be applied to a broad range of industries and applications. **http://www.fluent.com**
SIMULATION	
FLEXPART(new installation, version 8.0, in Finis Terrae)	FLEXPART is a model of particle dispersion that is used more and more every day. **http://transport.nilu.no/flexpart**
Macaulay 2 (new installation, version 1.1, in Finis Terrae)	Macaulay 2 is a software system devoted to supporting research in algebraic geometry and commutative algebra. **http://www.math.uiuc.edu/Macaulay2**
MATLAB (new versions, R2007b and R2008b, in the SVG)	MATLAB® is a high-level language and interactive environment that enables you to perform computationally intensive tasks faster than with traditional programming languages such as C, C++, and Fortran. It is possible to use MATLAB in a wide range of applications, including signal and image processing, communications, control design, test and measurement, financial modeling and analysis, and computational biology. **http://www.mathworks.com/products/matlab**
SCIENTIFIC VISUALISATION AND ANIMATION	

APPLICATION	TASK
Grads (new installation, version 2.0.a1, in Finis Terrae)	The Grid Analysis and Display System (GrADS) is an interactive desktop tool that is used for easy access, manipulation, and visualization of earth science data. The format of the data may be either binary, GRIB, NetCDF, or HDF-SDS (Scientific Data Sets). **http://www.iges.org/grads**
HDF (new installation, version 4.2r3-ia64, in FinisTerrae)	At its lowest level, HDF is a physical file format for storing scientific data. At its highest level, HDF is a collection of utilities and applications for manipulating, viewing, and analyzing data in HDF files. Between these levels, HDF is a software library that provides high-level APIs and a low-level data interface. **http://www.hdfgroup.org/products/hdf4**
HDF5(new installation, version 1.8.1, in Finis Terrae)	HDF5 is a unique technology suite that makes possible the management of extremely large and complex data collections. **http://www.hdfgroup.org/HDF5**
JASPER(new installation, version 1.900.1, in Finis Terrae)	The JasPer Project is an open-source initiative to provide a free software-based reference implementation of the codec specified in the JPEG-2000 Part-1 standard (i.e., ISO/IEC 15444-1). **http://www.ece.uvic.ca/~mdadams/jasper**
Ncarg(new installation, version 5.0.0, in Finis Terrae)	NCAR Graphics is a Fortran and C based software package for scientific visualization. **http://ngwww.ucar.edu/**
NCO (new installation, version 3.9.3, in the SVG)	The netCDF Operators, or NCO, are a suite of programs known as operators. Each operator is a standalone, command line program which is executed at the UNIX shell-level. The operators take netCDF files as input, then perform a set of operations (e.g., deriving new data, averaging, hyperslabbing, or metadata manipulation) and produce a netCDF file as output. **http://nco.sourceforge.net**
NetCDF (new installation, versines 3.6.2 and 4.0, in Finis Terrae. New version, 3.6.2, in the SVG)	NetCDF (network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data. **http://www.unidata.ucar.edu/software/netcdf**
Udunits (New installation, version 1.12.4, in Finis Terrae)	The UDUNITS package supports units of physical quantities (e.g., meters, seconds). Specifically, it supports conversion between string and binary representations of units, arithmetic manipulation of units, and conversion of numeric values between compatible units. **http://www.unidata.ucar.edu/software/udunits**
VMD (new installation, version 1.8.6, in Finis Terrae)	VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. **http://www.ks.uiuc.edu/Research/vmd**
XcrySDen (new installation, version 1.4.1, in Finis Terrae)	XCrySDen is a crystalline and molecular structure visualisation program, which aims at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. **http://www.xcrysden.org**

APPLICATION	TASK
MATHEMATICAL LIBRARIES	
CGAL (new installation, version 3.3.1, in Finis Terrae)	The goal of the CGAL Open Source Project is to provide easy access to efficient and reliable geometric algorithms in the form of a C++ library. CGAL is used in various areas needing geometric computation, such as: computer graphics, scientific visualization, computer aided design and modeling, geographic information systems, molecular biology, medical imaging, robotics and motion planning, mesh generation, numerical methods... **http://www.cgal.org**
FFTW (new installation, versions 3.1.2 and 3.2alpha3, in Finis Terrae)	FFTW is a C subroutine library for computing the discrete Fourier transform (DFT) in one or more dimensions, of arbitrary input size, and of both real and complex data (as well as of even/odd data, i.e. the discrete cosine/sine transforms or DCT/DST). FFTW, which is free software, should become the FFT library of choice for most applications. The benchmarks, performed on a variety of platforms show that FFTW's performance is typically superior to that of other publicly available FFT software, and is even competitive with vendor-tuned codes. In contrast to vendor-tuned codes, FFTW's performance is portable: the same program will perform well on most architectures without modification. **http://www.fftw.org**
Libmcrypt (new installation, version 2.5.8, in the SVG)	Libmcrypt is the library which implements all the algorithms and modes found in mcrypt and facilitates a standard mechanism of access to them. **http://mcrypt.hellug.gr/lib/index.html**
Mcrypt (new installation, version 2.6.7, in the SVG)	Mcrypt allows developers to use a wide range of encryption functions, without making drastic changes to their code. It allows users to encrypt files or data streams without the necessity of advanced knowledge of cryptography. **http://mcrypt.sourceforge.net**
MKL (new installation, versions 9.1, 10.0.011, 10.0.2.018 and 10.1.0, in Finis Terrae. New versions, 9.1.023 and 10.0.3.020, in the SVG)	Intel® Math Kernel Library (Intel® MKL) is a library of highly optimized, extensively threaded math routines for science, engineering, and financial applications that require maximum performance. Core math functions include BLAS, LAPACK, ScaLAPACK, Sparse Solvers, Fast Fourier Transforms, Vector Math, and more. Offering performance optimizations for Intel next-generation microarchitecture, it includes improved integration with Microsoft Visual Studio*, Eclipse*, and XCode*. Intel MKL allows for full integration of the Intel Compatability OpenMP* run-time library for greater Windows*/Linux* cross-platform compatibility. **http://software.intel.com/en-us/intel-mkl**
NumPy (new installation, version 1.0.4, in Finis Terrae)	NumPy is the fundamental package needed for scientific computing with Python. It contains a powerful N-dimensional array object, sophisticated broadcasting functions, basic linear algebra functions, basic Fourier transforms, sophisticated random number capabilities and tools for integrating Fortran and C/C++ code. **http://numpy.scipy.org**
SCIENTIFIC ANALYSIS	
R (new installation, versions 2.6.1, 2.7.0 and 2.7.2, in Finis Terrae)	R is a language and environment for statistical computing and graphics. It is a GNU project that provides a wide variety of statistical (linear and nonlinear modelling, classical statistical tests, time-series analysis, classification, clustering, ...) and graphical techniques, and is highly extensible. **http://www.r-project.org**

APPLICATION	TASK
Singular (new installation, version 3.0.4, in Finis Terrae)	SINGULAR is a Computer Algebra System for polynomial computations with special emphasis on the needs of commutative algebra, algebraic geometry, and singularity theory. **http://www.singular.uni-kl.de**
Applications with limited licensing (User or sole institution) **RESTRICTED TO SPECIFIC USERS**	
Stata/MP (new installation, version 10.0, in Finis Terrae)	Stata is a complete, integrated statistical package that provides everything you need for data analysis, data management, and graphics. Stata/MP is a version of Stata/SE that runs on multiprocessor and multicore computers. **http://www.stata.com/statamp/index.html**
JAVA	
JROCKIT(new installation, version R27.5.0-jdk1.5.0_14, in Finis Terrae)	The Oracle JRockit JDK provides tools, utilities, and a complete runtime environment for developing and running applications using the Java programming language. The JRockit JDK includes the Oracle JRockit Java Virtual Machine (JVM). The Oracle JRockit JVM is developed and optimized for Intel architectures to ensure reliability, scalability, and manageability for Java applications. **http://www.oracle.com/technology/products/jrockit/index.html**
PARALLEL LIBRARIES	
HP MPI (New installation, version 2.2.5.1, in Finis Terrae)	HP-MPI for Linux is a high performance and production quality implementation of the Message-Passing Interface (MPI) standard for HP servers and workstations. HP-MPI uses enhancements whenever appropriate to provide low latency and high bandwidth point-to-point and collective communication routines. It supports multi-protocol execution of MPI applications on clusters of shared-memory servers so that applications can take advantage of the shared memory for intra-node communications. **http://www.hp.com/go/mpi**
Intel MPI Library (New Installation, versions 3.0, 3.1 3.2.0.011, in Finis Terrae)	Intel® MPI Library focuses on making applications perform better on IA-based clusters—implementing the high performance MPI-2 specification on multiple fabrics. It enables you to quickly deliver maximum end user performance even if you change or upgrade to new interconnects, without requiring major changes to the software or operating environment. Use this high-performance message-passing interface library to develop applications that can run on multiple cluster fabric interconnects chosen by the user at runtime. **http://software.intel.com/en-us/intel-mpi-library**
PyMPI (new installation, version 2.5b0, in Finis Terrae)	pyMPI is a fully functional Python interpreter that just happens to include a large subset of MPI functions. pyMPI has extensive support for running parallel Python scripts and has been tested on a number of clusters and other scientific machines. **http://pympi.sourceforge.net**
COMPILERS	
Intel C++ Compiler (new installation, versions 9.1.052, 10.1.012 y 11.0.069, in Finis Terrae. New installation, version 10.1.017, in the SVG)	Intel® C++ Compiler offers the best support for creating multi-threaded applications. It offers the breadth of advanced optimization, multi-threading, and processor support that includes automatic processor dispatch, vectorization, auto-parallelization, OpenMP*, data prefetching, and loop unrolling, along with highly optimized C++ templates for parallelism, math processing, and multimedia libraries. **http://software.intel.com/en-us/intel-compilers**

APPLICATION	TASK
Intel Fortran Compiler (new installation, versions 9.1.052, 10.1.012 and 11.0.069, in Finis Terrae. New installation, version 10.1.017, in the SVG)	The Intel Fortran Compiler for Linux delivers rapid development and winning performance for the full range of Intel® processor-based platforms. It is a full-language Fortran 95 compiler with many features from the Fortran 2003 standard, plus a wide range of popular extensions. It automatically optimizes and parallelizes software to take best advantage of multi-core Intel processors, including dual-core mobile, desktop, and enterprise platforms. **http://software.intel.com/en-us/intel-compilers**
PGI Fortran Workstation (New version, 8.0.1, in the SVG)	The PGI Fortran Workstation Fortran compilers deliver outstanding performance on 64-bit x64 and 32-bit x86 processor-based workstations and servers, and enable simple portable parallel programming for both shared-memory and clustered computing systems. **http://www.pgroup.com/products/workpghpf.htm**
SOFTWARE MANAGEMENT	
Modules (new installation, version 3.1.6, in Finis Terrae. New installation, version 3.2.6, in the SVG)	The Environment Modules package provides for the dynamic modification of a user's environment via modulefiles. Modules abstracts the details about a software package's installation, environment, and software dependencies so that from a user's perspective, all software is accessed in the same way. **http://modules.sourceforge.net**
Subversion (new installation, version 1.5.3, in Finis Terrae)	Subversion is an open source version control system. It is used to maintain current and historical versions of files such as source code, web pages, and documentation. Its goal is to be a mostly-compatible successor to the widely used Concurrent Versions System (CVS). **http://subversion.tigris.org**

computing challenges on FINISTERRAE

During its first year of operation, Finis Terrae executed 6 computing challenges, that is, large computational problems that either had not been proposed until that moment or that could now be executed thanks to the excellent computing potential that this equipment offers.

Three problems were first approached during Finis Terrae's test period with a dual intent. First, to take advantage of the fact that the machine was not occupied, and second, to measure the capacity of the machine itself and to detect possible bottlenecks, hardware errors, or missconfigurations. Following the success obtained with the first 3 computing challenges, 3 additional challenges were selected from those proposed by CSIC researchers. The six challenges executed are described below.

Fekete

The VARIDIS group of the Department of Applied Mathematics III in the Universitat Politècnica de Catalunya has tested a new robust, effective and versatile algorithm, the Forces Method, for the solution of the Fekete problem. This problem consists in minimising under general constraints a potential functional energy depending on the relative distances between N particle points. The Fekete points are the optimal configurations obtained in these types of problems. Finding an efficient algorithm for the search of good estimations of such optimal points for the logarithmic energy in the 2-sphere is the centre of S. Smale's "7th 'Mathematical problem for the 21st century". More precisely, Smale asks for a real number algorithm which computes these optimal points in polynomial time in N.

The Forces Method has been used to perform a massive computation program with the objective of producing significative statistical information in order to extract conclusions about Smale's 7th problem. In total, we consumed approximately 350,000 hours of computation in FinisTerrae in about two weeks of real time and using 50% of its capacity (which is equivalent to 40 years using only one CPU).

The obtained results confirmed all the predictions about the behaviour of the Forces Method, overcoming the uncertainty related to convergence conditions or cpu-time estimations which emerge in other optimisation algorithms.

As a result of this challenge, more than 50 million local minima for the logarithmic energy in the 2-sphere are obtained. This is the greatest sample ever obtained for the Fekete problem and for Smale's 7th problem. From the statistical analysis of this sample information, a positive answer to the probabilistic Smale's 7th problem could be concluded. Furthermore, this analysis allows the identification of the master lines of a possible proof.

The results of this challenge are reported in the following scientific publications:

- E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto, A. Gómez, C. Mouriño, M.T. Sánchez, Computational cost of the Fekete problem I: the Forces Method on the 2-sphere, Journal of Computational Physics 228 (2009), 3288 -- 3306.

- J.M. Gesto, Estimation of Fekete points, Dissertation, Departament de Matemàtica Aplicada III, Universitat Politècnica de Catalunya, 2008.

Hemcuve:

A mixed group of researchers in computational electromagnetism from the Universities of Vigo and Extremadura, along with CESGA staff, have implemented a code in order to perform electromagnetic calculations. That code is in constant development and it is based on an algorithm that is now out of date for these kinds of problems, considerably surpassed by more recent multilevel algorithms, but it has the particularity that it is more scalable. Multilevel algorithms are very efficient with only a few processors but they present scalability problems. The developed monolevel approximation which in principal is much more computationally intensive, scales almost linearly above 100 CPUs, and allows dealing with larger problems.

The first challenge attempted a problem of 35 million unknowns, close to the world record of 42 million. This challenge was finally achieved after multiple adaptations of the application to the platform, using 512 CPUs and 8 TB of RAM memory (64 full nodes of FT). After this execution, some unbalancing and bottlenecks were detected, limiting the scalability.

A new improved version of the code was developed and a challenge of 150 million unknowns was executed during the summer using 1024 CPUs and 5.4 Tb of memory, the biggest run at that moment in the world.

Note that the new problem, 5 times larger, consumes less memory than the previous one, due to the optimisations performed in the code. A new improved version of the code is under development and we plan to execute a problem with more than 500 million unknowns during January 2009.

For the execution of these challenges, a hybrid parallelization was implemented and half of FT was fully occupied, using MPI for inter-node communications and OpenMP within the nodes. This demonstrates that FT is perfect for these kinds of problems due to its great amount of memory per CPU.

This project is applicable for the solution of electromagnetic problems in large structures equipped with radio systems, such as ships, planes, or satellites. In that manner, the electromagnetic behaviour of the structures in their stage of design can be simulated, in order to verify and guarantee the electromagnetic requirements and to minimise later problems during the manufacturing process.

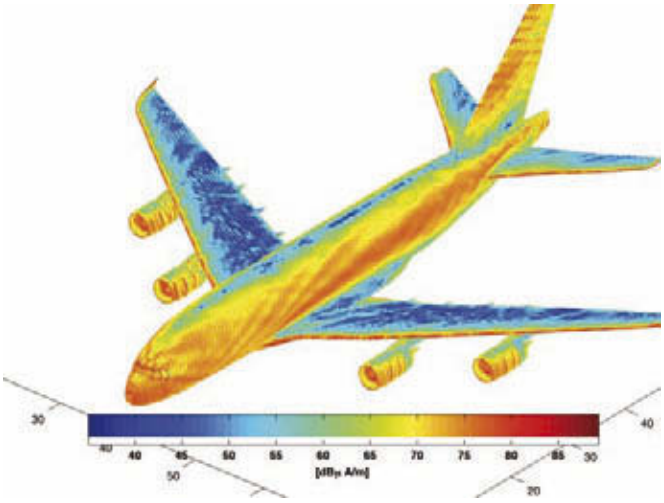
The following scientific publications were produced as a result of this challenge.

• L. Landesa, J.M. Taboada, F. Obelleiro, J.L. Rodríguez, J.C. Mouriño, A. Gómez, "FMM in electromagnetic problems with tens of millions of unknowns", XXIII National Symposium of the International Scientific Radio Union (URSI 2008), Madrid, September 22-24, 2008.

• L. Landesa, J.M. Taboada, F. Obelleiro, J.L. Rodríguez, J.C. Mouriño, A. Gómez, "Fast Multipole Method in Supercomputers", VI Iberian Meeting of Computational Electromagnetism, Chiclana de la Frontera, Cádiz, October 21, 2008.

• J.C. Mouriño, A. Gómez, L. Landesa, J. M. Taboada, F. Obelleiro, J. L. Rodríguez, "High Performance Computing Electromagnetics Challenge: solving tens of millions of unknowns." Proceedings of IBERGRID 2008, Oporto (Portugal), May 12-14, 2008.

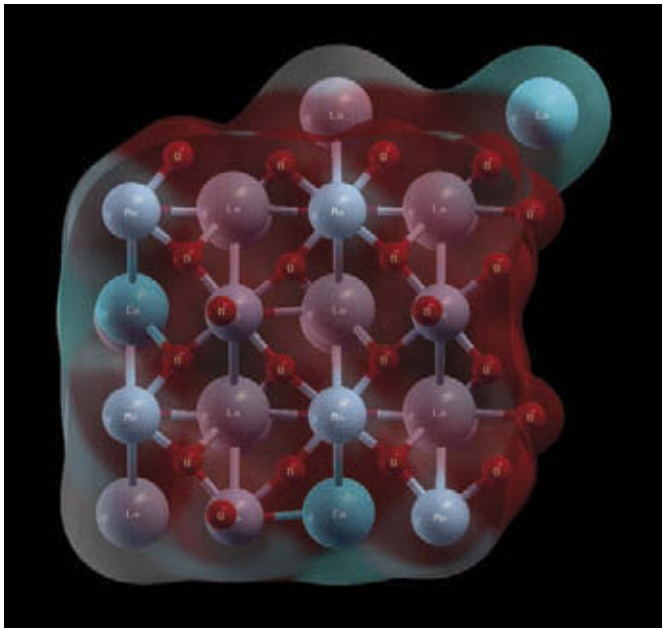
Other scientific articles have been presented for review but, at this moment, none have been published nor completely accepted.



Phase Transitions

A group of researchers from the Department of Applied Physics of the University of Santiago de Compostela, coordinated by Professor Daniel Baldomir along with CESGA staff, intend to solve the 3rd/4th most important physics problems of the decade according to the American Institute of Physics. The problem consists of discovering how exactly the phenomenon called "phase transition" is produced. This deals with the critical point in which a material acquires effective magnetic properties as a result of human intervention, concretely, adding other compounds or varying the temperature. Until now, the manipulation of the magnetic characteristics of a compound have been common, although we could only understand the dynamics in an approximate way. Due to the exhaustive understanding yielded by this discovery, it will be able to be controlled and, as a consequence, its applications can be refined.

To carry out the problem, 24 of all 142 computation nodes of Finis Terrae (which adds up to a total of 384 cores) were used, during an accumulated time of almost 68,000 hours, using 100 GB of memory and approximately 300 GB of disk space. These challenge results can open up many research lines. Some of those are the optimisation of battery technology for mobile telephones, a qualitative improvement in the memories of portable computers, or the optimisation of the sensors used to detect very small magnetic fields, and other multiple applications. At this moment, none of the obtained results have been published but work is in progress.



Genetic Algorithm for the Astrophysics of Massive Stars

This challenge was proposed by Francisco Najarro, a researcher in the Department of Infrared Molecular Astrophysics (DAMIR) of the Institute of the Structure of Material (IEM) at CSIC.

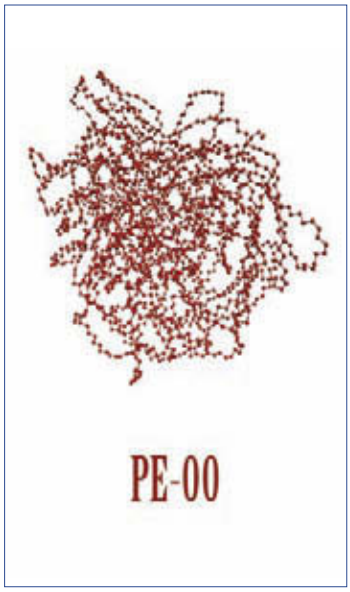
They have proposed genetic algorithms as an alternative method to obtain the stellar parameters that are generated by observations of astrophysical models of the atmosphere of massive stars.

The precision and efficiency of the genetic algorithms depend in great part on the fine tuning of the genetic parameters to the problem of optimisation. This work has consisted of the adequation of the necessary diagnostics, the spectral lines, the genetic parameters, the codification, and the number of parameters in order to approach the astrophysical problem in a realistic manner.

In this challenge, the quantitative study of massive stars was initially based on infrared observations. Until now, these methods were only used in the stellar optical spectrum. Infrared is important because it permits the study of regions, such as the centre of our galaxy, that are optically dark and cannot be observed.

The studies, still in course, are revealing the enormous potential of this method. Actually, we are adapting our observation for later automatic analysis using the genetic algorithm implanted in Finis Terrae.

The typical resources used in the method correspond to the computation of about 20,000 to 40,000 models with an average time of 15 minutes per model. The method is highly parallel and scales linearly with the number of processors available. The tests are performed with a maximum of 80 cores. Work is underway to publish results of these computations.



Mathematical Sciences

The researcher Ana María Mancho from the Institute of Mathematical Science in CSIC used Finis Terrae to carry out her research.

The objective was to justify a new definition of Distinguished Trajectory (DT) which generalises the concepts of fixed point and periodic orbit to aperiodic flows. Finis Terrae made possible the exploration of this definition in an incredibly short period of time while, before the FT era, the work was progressing slowly, dragging through months. The required computational resources were between approximately 10000 and 15000 hours.

The obtained results are collected in the following publications:

- J. A. Jiménez Madrid, Ana M. Mancho. Distinguished trajectories in time- dependent vector fields. Accepted in Chaos.
- A. M. Mancho. Numerical studies on the self-similar collapse of the α-patches problem. In preparation.

Crystallization process of macromolecular systems

CSIC Researchers from the Macromolecular Physics Department of the Institute of Material Structure have proposed a problem concerning the crystallization process of macromolecular systems to be solved by means of molecular dynamics techniques using the public domain, massively parallel program, LAMMPS.

At this time, 16 computation nodes of Finis Terrae (256 cores) have been used during an accumulated time of more than half a million CPU hours. Preliminary results derived from molecular dynamics simulations of polyethylene models containing short chain branches concerning the molecular mechanisms involved in the formation of ordered structures during the early stages of crystallization have been obtained.