

## THE SUPERCOMPUTING CENTER OF CATALONIA\*

The Supercomputing Center of Catalonia (CESCA) was inaugurated in October 1991 with the aim of offering high performance computing services to universities, research centers and enterprises. The *Fundació Catalana per a la Recerca* (FCR) promoted CESCA at the request of the *Departament de Presidència* of the Generalitat de Catalunya. The consortium was also made up of the –at those time– four public Catalan universities (Universitat de Barcelona, Universitat Autònoma de Barcelona, Universitat Politècnica de Catalunya and Universitat Pompeu Fabra). Later, Universitat de Girona, Universitat Rovira i Virgili, Universitat de Lleida and Universitat Oberta de Catalunya were also incorporated. To facilitate the access to its resources, since 1993 it manages the Anella Científica (Scientific Ring), sponsored by the FCR, the communications network that connects all the universities, research centers and several public institutions (libraries, hospitals, autonomous organizations of the Generalitat, etc.) and connects them with the statewide academic network RedIRIS.

Supercomputers have experimented a fast technological evolution from its creation. Thus, the performance of the new machines has increased significantly, while the ones have become obsolete quickly. Moreover, high performance computers based on standard processors are consolidated on the market and, for some applications, the rate cost/efficiency is better than for vector supercomputers. Therefore, nowadays, the division line between vector machines suitable for a service center like CESCA, and parallel machines for a research center like CEPBA has disappeared. Parallel computers used by researchers on parallelism may provide service to researchers in other fields, as it is shown by our acquisition of an IBM SP2 in 1995.

Consequently, it is natural to optimize the use of public resources, increasing the existing cooperation between both centers, with the purpose of facilitating the access to the hardware and software of each center to all the researchers in our community. The first cooperation between the two centers in 1993 let us be selected as a *Large-Scale Facility* by the EC, providing 1,7 mECU for European researchers coming to work to Barcelona. In order to formalize this cooperation, FCR, CIRIT and UPC signed an agreement in October 1995, to coordinate the activities of both centers

throughout the Computing and Communications Center of Catalonia (C<sup>4</sup>).

The C<sup>4</sup> was created in October 1995 by CIRIT, Catalan Research Foundation and Polytechnic University of Catalonia. The principal objectives are to coordinate the activities of both Catalan supercomputing centers, the Supercomputing Center of Catalonia (CESCA) and the European Center for Parallelism of Barcelona (CEPBA); to facilitate the access of their resources throughout the communications networks, specifically the Catalan Research Foundation's Scientific Ring; and to offer courses and seminars to divulgate and to promote the use and benefits of the new technologies to our community.

CESCA has dedicated its efforts to the vector computation using the high performance CRAY and IBM machines. Of all works carried out by CESCA, we remark some activity fields that show the diversity of the tasks undertaken: molecular modelling, design of new polyamides, conformation of metals, financial decisions, estimation of generic parameters in populations, arqueometria of archaeological ceramics, engineering of molecular crystals with technological interest, etc. One of the projects which has been developed with the participation of CIMNE was the aerodynamic and hydrodynamic study of the Spanish sailing ship for the American CUP 95. This project calculated the force exerted by the wind on the sail under several wind power conditions and the forces that the water bring to the keel under different sailing situations.

Since 1991, CEPBA has as a aim the parallel computing, an alternative to the vector one, based on the existence of a large number of processors that works simultaneously. CEPBA has leaded European initiatives of parallel technology transfer to companies. For example, on the European projec ESPRIT number 6753, CEPBA worked on a development of numerical methods applied to the fluid mechanics that was useful for the Catalan company INDO (that incorporated it to its own technology in the manufacture of lens) and also for the German company BMW to the design of cylinders formotors. In this case both companies profited by common computing tools to develop different final applications.

The activities of both centres have been complemented since their creation: CESCA has been providing services to the research groups and companies while CEPBA has been promoting the research and development of projects based on parallel computation. The experience of each center in its area benefits the other so that their users have a better service. The coordination between these two centers allows

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having the human and material resources more adequated at any moment.

The researchers use the combined power of both centers in order to work with vectorial and parallel processors with shared memory, superscalar processors with distributed memory, superscalar processors with shared memory and array processors from Convex, Cray, IBM, SGI and TMC. Their combined power is more than 50 Gflop/s.

The main objectives of the C<sup>4</sup> are:

- The evaluation and planning of the computational needs of the research groups to assign them the most adequate resources between the ones available in both centers, as well as to determine their necessities toward the combined acquisition of hardware and software.
- The sharing of the personal of both centers to provide a better service to the high performance computing community. For those who execute commercial programs the versions and platforms that gets the best performance will be evaluated, not only for vector processors, but also for parallel ones.
- The potentiation of the access to the high performance computing resources and to the comunicacion networks through the Scientific Ring. This is connected to RedIRIS and it is coordinated with the ATM National Host. All this infrastructure will facilitate the creation of consortia to realize projects using both supercomputing and communications technology, in the environment of the actual European programmes, as ESPRIT, ACTS and TELEMATICS.
- The preparation of courses and seminars to divulgate and to promote the use and benefits of the new technologies to our community.
- The creation of consortia between companies and research groups to participate in high performance computing R&D projects.
- The dissemination of the use and the benefits of these technologies throughout our documental data base (web) and the TERAFL0P magazine.

With C<sup>4</sup> it is expected to encourage the use of supercomputers with the coordinates of both existent centers, following the Research Guidelines of the Generalitat de Catalunya (1993 - 1996) which plans to agrupate related infrastructures and researchers activities.

In summary, among its functions C<sup>4</sup> has to support the research development activities of all the institutions that need high performance computing (mainly for scientific computation, but also for business environments that need large databases), to manage the Scientific Ring and the node of RedIRIS in Catalonia, and divulgate the use and benefits of these new technologies in our community.

## The projects

CESCA and CEPBA were selected in 1993 a Large-Scale

Facility, as part of the *Human Capital and Mobility* (HCM) program, to facilitate European researchers the access to the infrastructure of both centers and the collaboration in research projects to solve scientific and technological problems. In supercomputing, only the Scottish EPCC and the Italian CINECA share with Barcelona this category. Besides, during 1995 and 1996, CESCA and CEPBA took part in the PECO programme, similar to HCM but aimed to Eastern European countries. HCM has been extended with the TMR programme (Training and Mobility of Researchers), which will facilitate the access of European researchers to our installations till the end of 1998. These programmes have allowed up to now that 161 researchers have visited us in 196 stays invited by 47 local research groups. The Statistical Section shows some diagrams for these programs: the visitors by the visited institution, by speciality, by origin country...

TMR also involves Direct (*Development of an Interdisciplinary Round-table for Emerging Computer Technologies*; 11/97 to 10/00), a concerted action of the DGXII created as a round table which groups together computer centres, data centres and supercomputing users, aimed to address the role of emerging computer technologies, such as HPCN, defining the future direction of scientific computing and the impact on *Large Scale Facilities*. Direct also issues an on-line *newsletter*, Directions, which informs on the news of the participant centres.

CESCA has also taken part in the ESPRIT projects *HPCN Europe On-line Newsmagazine* (HOISe-NM), *Spanish Awareness Campaign* (SAC) and the *ACTS Information Window* (Infowin). HOISe-NM has created a virtual magazine (Primeur) on HPCN (1996-97), and has also compiled a list of all the Supercomputing Centres in Europe. The project has been continued as a consortium and, up to date, the tools for the virtual edition of the magazine are hosted at CESCA. The SAC project, coordinated by CEPBA, has spreaded the use of high performance technologies on three sectors: automotive, industrial machinery and financial (4/97 - 12/97). Infowin gave support to the ACTS project (*Advanced Communications Technologies and Services*) from 1/96 to 6/97. The project was aimed to settle a testing ground for the innovations on the communication and data transmission world, and has created several publications in paper and electronic format.

CESCA's hardware is used by a large number of academic research projects in the fields of:

- Astrophysics, Meteorology and Climate.
- Applied Physics.
- Theoretical Physics.
- Computer Science.
- Numerical Methods in Engineering.
- Molecular Modelling.
- Theoretical Chemistry.
- Telecommunications.
- Others.

In addition to facilitating high performance computing

services to research groups, the Centre allows that institutions and enterprises experiment with the use and benefits of these technologies, specially in the environment of parallel data bases and data mining.

CESCA also collaborates in two projects with CIRIT financing. These projects support the molecular design research infrastructure in Catalonia and reaffirm the intention to integrate the pharmaceutical companies in the *I Pla de Recerca de la Generalitat de Catalunya*. One is the creation of the SCF, the pharmacophore search service in databases of 3D compounds with biological interest, with the *Catalyst* program. The second is the *Xarxa Temàtica de Model·lització Molecular* that has been created to coordinate all Catalan researchers in this field.

## Communications

Communications are very important for high performance scientific computation, because they let users access to remote resources. Communications are also useful to facilitate the development of research projects shared among people in geographically dispersed groups.

The Centre manages the Anella Científica (Scientific Ring), sponsored by the Fundació Catalana per a la Recerca, the node of RedIRIS in Catalonia, sponsored by the CICYT and the *Punt Neutre d'Internet a Catalunya* (CAT-NIX), sponsored by the *Comissionat per a la Societat de la Informació*. It also manages some technical resources, such as ISDN and leased lines.

Moreover, it offers some additional services to the members of the Scientific Network (Secondary server of the .es domain, MBone, news, proxy-cache, mirror ftp, Remote Access, Direct Access and S24x7) and housing and hosting servers.

## The Scientific ring

With the aim of creating a high performance communications network to connect the most important research centers of Catalonia with CESCA, the Fundació Catalana per a

la Recerca signed on April 1993 an agreement with Telefónica to install a network, which was called *Anella Científica* (Scientific Ring). The network was entirely operative in December 1993 and the transmission of information among the different originally installed points started immediately.

Physically, the Scientific ring is based on a fiber-optic cable spread over the areas of Barcelona and Vallès by Telefónica with a transmission capability of 34 Mbps.

*Catalana de Telecomunicacions Societat Operadora de Xarxes, S.A.* is the technological supplier of the Scientific Ring, which is going to connect the institutions mentioned above, from May 1st 1998. Telefónica has been in charge of the installation and maintenance of the Ring for the last 5 years and until the previously mentioned date, and gently accepted to share the management with the CTGC for one more month in order to make the change as smooth as possible for the users.

The new Scientific Ring, instead, is based in ATM technology upon an SDH transportation network. The switching capacity available is 6,4 Gbps and 2, 34 and 155 Mbps in the accesses. The services that will be provided in future are: Frame Relay at 2 Mbps, and ATM at 34 Mbps and 155 Mbps. Interworking ATM/Frame Relay will also be offered. This network has been designed with a high MTBF, and it is electrically protected with batteries, electric generators, and APS and PPS protection.

The physical structure of optical fibre that supports the new Ring is more than 90 kilometres long. Over this physical infrastructure a transport network based on SDH technology has been implemented. This network has 2 rings at 622 Mbps (main and secondary) with different layouts. The main advantage this double ring offers is that it provides an alternative way in case of failure of the main ring, thus giving high availability to the accesses to the Ring. The network has been designed to optimize the bandwidth available, avoiding the creation of predetermined paths.

A big effort has been made to integrate equipment from different vendors (for example, Fore, CISCO, Lucent Technologies, etc.) because several connected institutions had already bought their own devices.