



# The Computerworld Honors Program

Honoring those who use Information Technology to benefit society

## Final Copy of Case Study

**LOCATION:**  
*Trujillo, Caceres,  
Spain*

**YEAR:**  
*2011*

**STATUS:**  
*Laureate*

**CATEGORY:**  
*Innovation*

**ORGANIZATION:**  
COMPUTAEX

**ORGANIZATION URL:**  
<http://www.computaex.es>

**PROJECT NAME:**  
CenitS

### PROJECT OVERVIEW

CénitS is a R&D&TI Supercomputing center located in Extremadura aiming to promote, disseminate and offer services on intensive computation and advanced communications to research groups, companies or institutions requesting them. Through technology improvement and innovation, we make businesses more competitive. The COMPUTAEX Foundation (Extremadura Computation and Advanced Technologies Foundation) intends to develop several fundamental activities such as the following: - Encourage, implement and manage the Extremadura Supercomputing Center (CénitS). - Promote research and technology development projects. - Provide processing power, communications and technical support to users through equipments available at the Foundation. - Collaborate to the exchange of processing-based research results between public centres and companies. - Operate and transfer technologies developed by the Foundation. - Promote and provide cooperation among companies and institutions. - Promote and collaborate in the organization of courses, seminars and meetings. - Develop and publish books, journals, audiovisual and multimedia material related to the Foundation's aims. - Search and find resources to develop activities. - Contribute to the development and strengthening of competitive abilities by the research groups and the business sector in Extremadura. - Consider supercomputing-based technology requirements of entities and companies asking for support. The traditional way in which researchers solve problems with a computer is based on the execution of serial operations. Those calculations were usually executed on single processor computers; their instructions were processed in a sequential way, i.e. one after another and only one instruction at the same time. With our Itanium-based solution the greatest challenge was to teach them how to parallelize their source codes in order to achieve better performance. Another challenge was to port already parallelized distributed applications to a shared-memory approach to exploit the memory management benefits of this architecture. Distributed and parallel programming consists of using several resources simultaneously to solve specific problems. Instructions are executed on multi-core computers, the problem is divided into independent parts which are executed in parallel on each processing unit. Parallel programming is frequently mistaken with

distributed programming because they have similar philosophies. Despite that they both are based on the simultaneous use of several resources, parallel programming is distinct from distributed programming in the sense that the problem is solved in the same computer. In a distributed environment, it is not necessary to use the same hardware with the same architecture or even the same programming language. One of the most important advantages of our shared memory Itanium-based computer is that it is easier to program than distributed memory computers. It is also very quick when sharing data between processes or threads and researchers have been taught to exploit all the benefits of our Itanium-based computer (work-load balancing, data locality, memory footprint and quick communications). We overcame those challenges by instructing researchers in the use of big shared-memory nodes, they were taught how to combine OpenMP code with MPI to get the maximum from the Itanium processors. MPI for internode process communications and OpenMP for loop and thread parallelization. Thus, we nominate the Supercomputing Center project (CéniS) for this valuable award.

## **SOCIETAL BENEFITS**

Thanks to CéniS, Supercomputing has become a very accessible well for companies, technological centers and researchers that want to reduce costs, increase productivity, innovate, to be more efficient and competitive.

## **PROJECT BENEFIT EXAMPLE**

We are currently executing projects like: - SIATDECO (Information System to Aid in the Decision-Making process in the field of green energy). This project is a collaboration project between a University, three technological centers and a public science&technology foundation. Green energies share a key feature, the direct dependence on weather conditions. It is therefore important to analyze the location of production plants. However, in recent years we are facing climate change, that seems to be recognized as the cause of the variations that occur in weather forecasts. A number of climate models and their correlation with renewable energies are being prosecuted in LUSITANIA supercomputer, those will provide an information system for decision-making predictions and should consider the short, medium and long term not only to analyze and predict productivity, but in order to identify gaps, needs and other factors that may be useful for investment planning, infrastructure and logistics. - A Unified Mechanistic View on the Morita-Baylis-Hillman Reaction: Computational and Experimental Investigations. The thermodynamic properties and reaction mechanism of the Morita-Baylis-Hillman (MBH) reaction have been investigated through experimental and computational techniques. The impossibility to accelerate this synthetically valuable transformation by increasing the reaction temperature has been rationalized by variable-temperature experiments and MP2 theoretical calculations of the reaction thermodynamics. An increase in temperature results in a switching of the equilibrium to the reactants occurring at even moderate temperature levels. The complex reaction mechanism for the MBH reaction has been investigated through an in-depth analysis of the suggested alternative pathways, using the M06-2X computational method. The results provided by this theoretical approach are in agreement with all the experimental/kinetic evidence such as reaction order, acceleration by protic species (methanol, phenol), and autocatalysis. In particular, the existing controversy about the character of the key proton transfer in the MBH reaction (Aggarwal versus McQuade pathways) has been resolved. - WACCM (Whole Atmosphere Community Climate Model): The Whole-Atmosphere Community Climate Model (WACCM) is a comprehensive numerical model, spanning the range of altitude from the Earth's surface to the thermosphere. Projected applications of the model for scientific studies include the following: Investigate interactions between stratospheric

dynamics and chemistry to elucidate the role of natural and anthropogenic variability in ozone depletion during the last 20 years and into the 21st century. Investigate the effects of solar variability on the middle and upper atmosphere on time scales ranging from the solar rotation period to the 11-year solar cycle. Study processes controlling the stratosphere/troposphere exchange of mass and minor constituents. Our Supercomputer is also executing more than 30 projects, including: - Stellarator TJ-II: Calculations of bootstrap current. - Neutronic dose calculations for radiotherapy patients. - 3-D Heisenberg spin glass model simulation with external electromagnetics fields. - Parallel heterogeneous algorithms for multichannel image processing. - AzequiaMPI evaluation. - Supercomputing and GRID development. - Supercomputing and e-Science. - SheliOS 2009 expedition. - com.info.com: Communication infrastructure predictability by using supercomputing for MIPv6/FTTx network deployment. - Optic Communication System Design and Simulation.

## **IS THIS PROJECT AN INNOVATION, BEST PRACTICE?** Yes

### **ADDITIONAL PROJECT INFORMATION**

To understand the situation of Extremadura, it is necessary to remark that Extremadura is one of the less developed Spanish regions with an unemployment rate of more than 22%. The regional economy has improved in recent years, being the Spanish Region which has been converging at a faster pace with other economies within the European Union, in the 1985-1999 period. Extremadura has benefited from the European Union Cohesion Funds and has used them to implement several projects regarding research, education, social issues and businesses. These projects, in order to make the Region catch up with the Information and Communication Technology Revolution, are favoring its development on the basis of equality and freedom, and are preparing it to firmly face all the changes the Knowledge Revolution will spark. In 1997 the regional government of Extremadura started working in the articulation of a Regional Strategy of Information Society for Extremadura with the creation of the Infodex European Project, an organization financed in equal parts by the regional government of Extremadura and the Structural Funds under the Regional Information Society Initiative (RISI). Infodex studied the pressing challenges of Extremadura to identify all the requirements that could be met with a cohesive IT strategy. In the 21st century, innovation has become a fundamental value in our society to achieve progress and development levels in a world in constant evolution. The central importance of innovation in improving the performance of the Extremadura economy was recognized from the original launch of the 1st Extremadura Regional Research and Technological Development Plan (I PRI+DT) in 1998. The aim, in a global and more competitive economy than ever, was to help Extremadura move up the value chain and, in particular, to exploit the opportunities offered by the growing knowledge economy. For these reasons, and bearing in mind the Europe 2020 strategy objectives in terms of innovation. This strategy was to create an "Innovation Union" to improve infrastructure and access to finance for research and innovation. This would ensure that innovative ideas could be turned into products and services that create growth and jobs. The Regional Government of Extremadura has strongly promoted the creation of the Extremadura Supercomputing, Technological Innovation and Research Center (CénitS), and the establishment of the LUSITANIA Supercomputer to strengthen the innovative process in our region. The availability of a fully functional data center helps to overcome economic barriers that prevent great projects from accessing great technology. Therefore, the Supercomputing Center of Extremadura was not born by chance or spontaneously, but rather by the need to fulfill a double goal; on one hand, to



provide methodologies and tools for research and technological centers of Extremadura, and to help small and medium technological based businesses. It should be noted that, despite its short existence, CénitS has achieved some important milestones such as the World Record in computational electromagnetics (solving a problem of 600 million unknowns) and the international recognition of the Itanium Solutions Alliance (Humanitarian Impact winner and computationally Intensive Applications finalist).