The S.Co.P.E. Project

L. Merola[1,2]
[1]Università degli Studi di Napoli Federico II, Napoli, Italy, leonardo.merola@na.infn.it
[2] *on behalf of the SCoPE project*

Abstract— **This paper describes the project SCoPE, which started at the beginning of the year 2006 and was completed in three years, with the construction and activation of a Data Center which is now perfectly integrated in the national and international GRID initiatives. The DataCenter hosts about 300 eight-core blade servers, 220 Terabyte of storage, and is already able to accommodate 500 more servers. The scientific applications which the Data Center is used for, in the areas of Astrophysics, Chemistry, Mathematics, Medicine, Engineering, Physics, are briefly described.**

***Index Terms*— SCoPE, GRID, scientific computing.**

Leonardo Merola is Full professor of *general physics* in the Faculty of Sciences, University of Naples Federico II, and is currently Director of the INFN section in Naples. He is working on the ATLAS project at CERN, and has been involved in many research projects in particle physics and in particular in data analysis projects.

I. INTRODUCTION

THE SCoPE project started in the year 2004 from an idea of a few researchers at the University of Naples *Federico II*, Italy, who recognized the need for a scientific Data Center, to be used in the framework of a more general GRID infrastructure. The acronym stands for "*Sistema Cooperativo per Elaborazioni Scientifiche Multidisciplinari*", that is a collaborative system for scientific applications in many areas of research. At the end of 2004 the group decided to submit a request for funding to the *Ministery of University and Research*, and the proposal, which gathered more than a hundred researchers from the University of Naples, was submitted in February 2005, receiving its final approval exactly a year later, in February 2006, when all activities started.

II. THE INFRASTRUCTURE

A. The need for a new infrastructure

THE University of Naples is a very large one, with more than 100,000 students and more than 3,000 professors and researchers. However, no significant scientific Data Center existed before the SCoPE project and most of the Departments in the Faculties of Sciences and of Engineering had their own small centers, with dedicated infrastructures.

With the SCoPE project, the proposing group, which had grown up to 128 people, agreed to build a new, single Data Center, in the Monte S. Angelo Campus, which already hosts the Faculty of Sciences, and is very near to the campus of the Faculty of Engineering. Excellent network infrastructures were already operational, with many kilometers of optical fibers, structured according to a multi-ring shape with multiple differentiated ways connecting all the departments; each fiber is operated at 1 Gbps or 2.5 Gbps, with several fiber pairs on each connection. The network infrastructure of the University *Federico II* is shown in the map below.

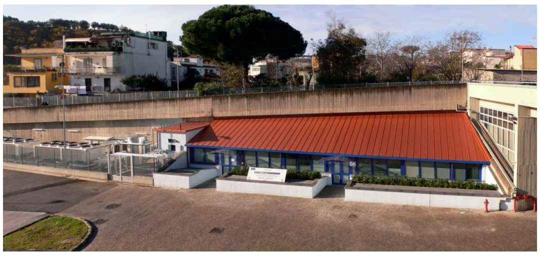
B. *The design of the Data Center*

The design of the Data Center was completed in a few months, according to the following constraints:

- Localization in the Monte S. Angelo Campus, in a small new building, max 150 square meters;
- New power plant, capable of delivering 1 Mwatt of electric power in a continuous mode;
- Efficient cooling system, capable of dissipating 2,000 watt per cubic meter, and 30,000 watt per rack;
- Standard (Gigabit Ethernet) networking infrastructure, with a high capacity switching fabric;
- Low latency (Infiniband) networking infrastructure, with a single switching fabric for each group of 256 servers;
- Large storage capacity, both NAS (Network Attached Storage) working with the iSCSI protocol, and SAN (Storage Area Network), working with a Fibre Channel Infrastructure;
- Open Source (Scientific Linux) for the operating system;
- Integrated monitoring system for all the devices of the Data Center, able to monitor the most relevant parameters of server, storage, networking, as well as all the environmental parameters (temperature, humidity, power consumption etc.)

C. *The realization of the Data Center*

The construction of the Data Center started at the end of 2007, after two European tender procedures were completed. The image below shows the Data Center after its completion.



The power plant, which is shown below, has three UPS’s for a total of 1 MWatt, and a diesel power generator of the same power, with 3,000 liters of gasoline.

A special effort was devoted to the cooling system, made by RITTAL: it is a liquid cooling system, with two redundant chillers (below, left) and a distribution system (below, right) which delivers cool water to each rack, equipped with redundants LCP units, and brings back the heated water to the chillers.

The interior of the Data Center accomodates as many as 33 racks, leaving plenty of space space for mantainance operations.

The racks are organized in three groups of "10+1", where the "1" is used for passive cabling, and the "10" are used for switchs, servers, storage.

All the hardware in the Data Center was given to a single general contractor, which was DELL. They provided the servers, the networking switches, the storage, the monitoring system.

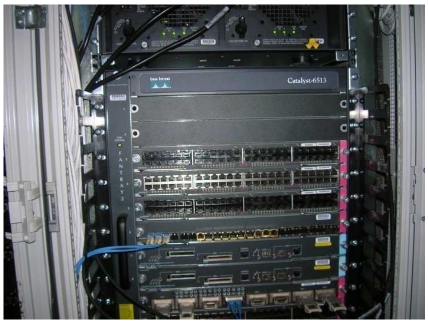
D. The servers in the Data Center

The servers are basically all blade servers, arranged in groups of 16 blade per chassis, as shown below; each blade has 2 quadcore CPU's by Intel, 8 or 16 Gbyte of memory per

blade. The chassis has pass-through switches for Gigabit Ethernet (copper) and for Infiniband (fibre).

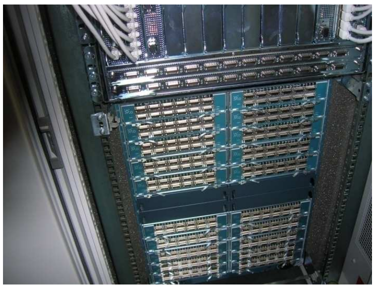
E. The network in the Data Center

The main gigabit network is based on Cisco 6513 switches. Each pairs of them provides full-wire-speed connectivity to all blade servers in the "10+1" group of racks, in a fully redundant architecture which guarantees that the switching matrix is unique for the whole group of servers, avoiding bottlenecks in transferring data from one switch to another. The switches, shown below, are however interconnected each other with a pair of 10 GbE lines for each switch.

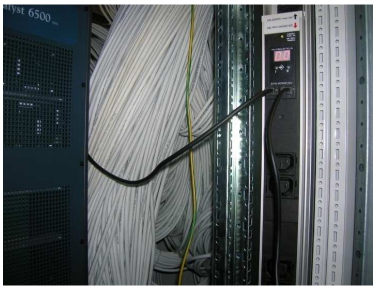


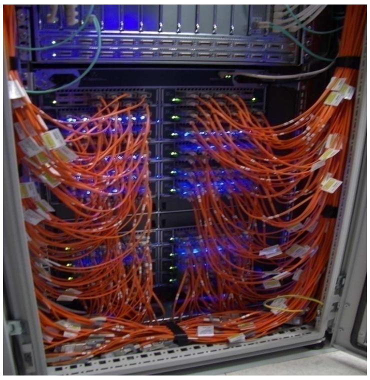
The same concept is applied for the

Infiniband switches, shown below, which are also made by Cisco. We used Fibre connections instead of the classical coax cable of Infiniband, to reduce the size of cabling and to increase in realiability because of the lack of interferences.



The passive cabling was rather complicated, because of the thousands of cables which had to be deployed in the Data Center (see below for copper and fibre, respectively); most of the cabling is on aereal guides, and not under the pavement, in order to ease maintenance.





F. The storage in the Data Center

The storage system, shown below, is based on EMC^2 hardware, and in particular on the CX3-40 SAN system with 130 terabyte of storage, with a Fibre Channel infrastructure which connects each blade chassis, but we also use a couple of EqualLogic NAS (see below), based entirely on the iSCSI protocol, and with capacity of 16 terabytes for each system.

G. The Control Room

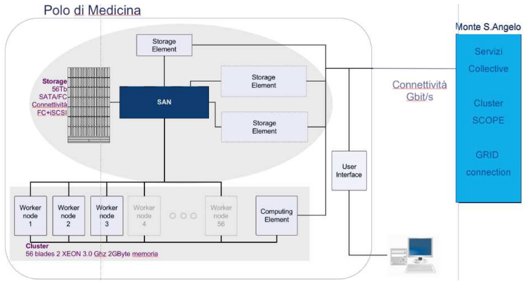
The small size of the Data Center (less than 150 square meters) does not allow for human presence inside; therefore we used the nearby open space, shown below, to accommodate all the operational people, involved in monitoring, troubleshooting, maintenance, and software development. More than 20 desktop PCs are connected via a dedicated (and redundant) fibre channel conncetion to the Data Center, which is however only 50 meters away. Large-size (58 inches) flat panel displays show in real time the status of the Data Center.

H. The remote sites

Three satellite installations ("remote sites") are present in the SCoPE infrastructure, namely at the Medicine Faculty (*site I*), at the Chemistry Dept. (*site II*) and at Applied Mathematics Dept. (*site III*). *Site I* hosts a 50 Terabyte storage system, which is connected to the SCoPE Data Center through a 5 km fiber optic link, using the fiber channel protocol, as well as through a similar link transporting TCP/IP at 2.4 Gbit/sec (packet over Sonet). *Site II* hosts a rack with 4 multi-processor servers, 32 cores per server, 2 Gbyte of memory per core, and is just 200 *m* away from the Data Center, to which is connected via 2 optical links operating at 1 Gbit/sec. *Site III* hosts a rack with 16 blade, 8 core per blade, 2 Gbyte of memory per core; also *site III* is just 200 *m* away from the Data Center and is connected in the same way.

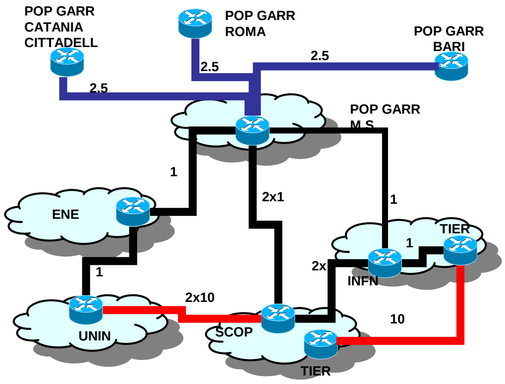
In addition the SCoPE Data Center is connected at 10 Gbit/sec to the INFN ATLAS Data Center which is located very close to it, inside the Physics Department building, which also hosts the Napoli Section of the INFN.

As an example of remote site, see the figure below, which is located within the area occupied by the Faculties of Medicine and Biotechnology. A 100 CPUs cluster provides computing resources mainly dedicated to support interactive computational requests in the field of bioinformatics, but its nodes are also connected to the university GRID through a local computing element that grants access to the nodes. The storage system based on EMC2 hardware, and in particular on theCX3-40 SAN system, consists of 60 terabytes dedicated to biological databases and bioinformatics tools. The storage system is directly connected to the local nodes, but also, via dedicated optical fibres, to the main plant nodes, which have fast access to the stored data. A custom developed fast scheduler takes care of distributing the computational requests to the local nodes, for interactive tasks or to the remote nodes, for less immediate, more complex and heavier jobs.



I. The wide area network connections

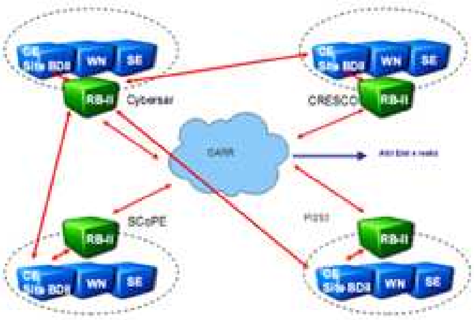
Starting from the Monte S. Angelo network exchange center, hosting the GARR (Italian NREN) GigaPOP the SCoPE Data Center is connected to the outside networks through 3 POS STM-16 (2.5 Gbps) fiber circuits reaching respectively the Roma, Catania and Bari GARR GigaPOPs. It is also connected with 2 10 Gbps Ethernet direct connections to the Napoli Metropolitan research Network, offering Giga-speed access to all the Universities and research institutes located in the Napoli urban Area (INFN, CNR, Enea, Unina, Orientale, Parthenope, SUN etc.).



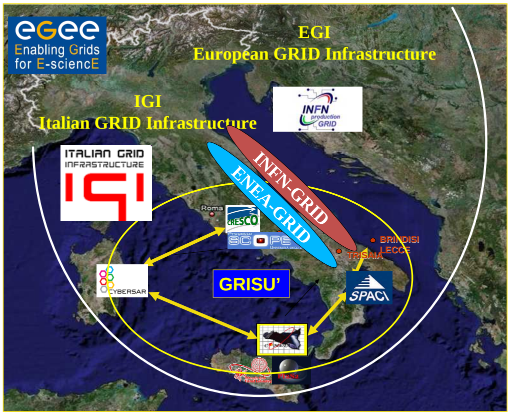
J. *Interoperability*

The Italian Ministry of University and Research has promoted the creation of an unified e-infrastructure and a new scientific-technical community [1], in the South of Italy by the synergy among the four e-infrastructures: CRESCO [2], CyberSar,[3] PI2S2 [4] and SCoPE. These projects have experienced a very successful cooperation since 2007, with the aim of sharing resources and knowledge, through a new interoperability model.

From a technical point of view, this approach provides an integrated production-quality service on four different e-Infrastructures based on the gLite middleware and the ENEA-Grid experience. Each e-infrastructure deploys a minimal subset of gLite collective services, called Primary Services (as shown in the picture below), in order to manage the access to resources and the membership of the authorized virtual organizations. This set of collective services, duplicated at each project infrastructure, avoids single points of failure.



This interregional experience, has been the basis for the new GRISU' e-infrastructure [5], which plans to extend the above interoperability model to other partners in the South of Italy, such as SPACI [6], and to be part of the planned Italian Grid Infrastructure (IGI) within the European Grid Infrastructure (EGI).

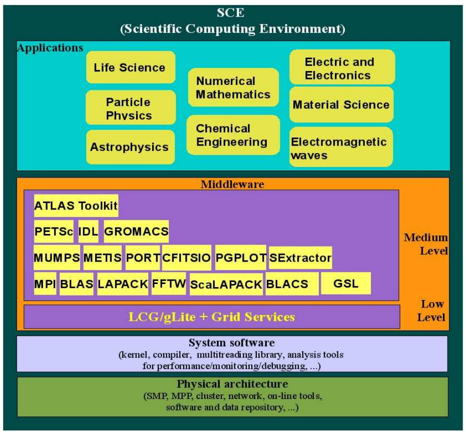


The new interoperable GRISU' Grid infrastructure provides more than 10.000 logical CPU, 500 TB of raw disk to support a large scientific community with hundreds of applications. GRISU' is now ready to export this experience in other national and international research and industrial frameworks.

III. The Software

THE SCoPE Grid solution is based on the INFN-GRID release, realizing a structured architecture built on a customization of the LCG storage and computing infrastructure projected for the high-energy physics community using the Large Hadron Collider (LHC) and the gLite middleware developed within the EGEE project context. It offers a computational and storage environment where the Resource Framework Layer (RFL), the Information System Framework (IS) and the Information Data Model encompass semantic and interaction models for all the available resources. The actual implementation provides the creation of a central Virtual Organization (VO) named *unina.it* managed by a local Virtual Organization Membership Service (VOMS) which collects all the users of the project and is enabled in each shared resource. Other VOs, are enabled respectively on the resources used in explicit local groups associated to specific experiments. The centralized collective services offer Services Discovery, Resource Brokering, File Catalog, Grid Monitoring and graphical user interface facilities. The site gLite component provides two Computing Element (CE) in High availability, batch execution systems, with 304 associated Worker Nodes (WN) offering computing power, together with 10 Storage Element (SE) servers based on the Disk Pool Manager (DPM).

A *localized* medium level middleware, named SCOPE Toolkit, including all the mathematical packages, software and libraries needed to the Unina researchers, has been designed and realized [7]. The architecture of a such scientific computing environment is depicted below.



For what concerns the operating system, all machines use the freely available Scientific Linux 5.2; in general, only public domain software is used in the project, apart from a few commercial applications, like IDL from Research Systems, inc.

The monitoring system is based on proprietary, but free, tools from the vendors (DELL, RITTAL, CISCO), and on NAGIOS for the network monitoring. Higher level monitoring is provided by the gridICE utility.

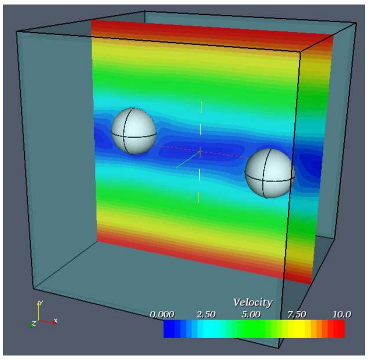
IV. The Scientific Activities

A. *The area of material sciences*

Several applications have been studied within SCoPE, among these, very promising is the study of the behavior of suspended particles in liquids. Suspensions of particles in liquids are a class of materials relevant in a huge variety of applications, e.g.: i) polymer melts with fillers; ii) biomedical materials; iii) food; iv) cosmetics; v) detergents. This variegate spectrum is due to the differences in particle concentration, mechanical properties, shape, and size. Particles suspended in viscoelastic media are known to develop structures when sheared at sufficiently high shear rates. Jefri and Zahed [8] experimentally analyzed suspensions in planar Poiseuille flow, with the following three results: a) in Newtonian suspensions the particles were uniformly distributed in both the transverse and axial directions; b) in the shear thinning fluid migration of particle toward the upper and lower plates was observed followed by string formation close to walls; c) in the constant viscosity elastic fluid the particles were found along the tube axis with very few particles on the upper and lower plates.

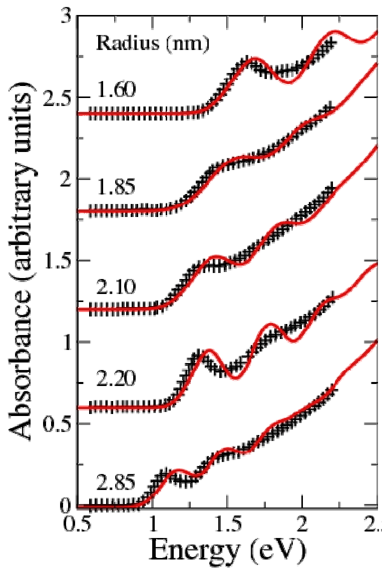
The aim of these studies in the SCoPE project is to characterize the flow behavior of dilute and semidilute suspensions of rigid spheres in viscoelastic media in confined geometries (e.g. [9-10]). We considered: i) dilute and semidilute suspensions; ii) rigid; iii) spherical; iv) nonBrownian inclusions; v) confined geometries. We used intensive numerical simulations in 2D and 3D FEM. This code uses the following libraries: a) BLAS/LAPACK; b) METIS. The code is in Fortran 95, and the SCoPE group used the Intel Fortran Compiler v 9.1.043 and the G95 Fortran Compiler. Moreover, the following solvers were used: a)

HSL library; b) MKL Gmres; c) Sparsekit; d) Pardiso; e) Mumps; f) Petsc. PARDISO gave the best results in terms of efficiency. A simulation is given below [11].

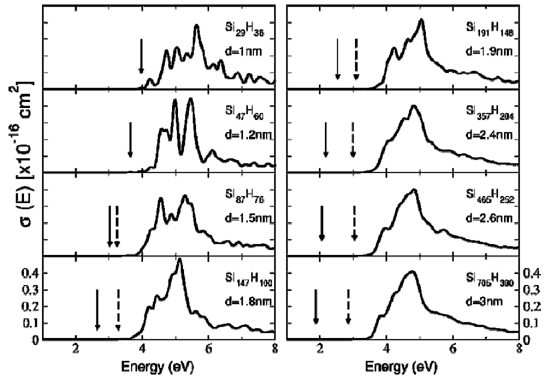


Another research area is related to emerging fields of nanotechnology which is believed to be the basis for innovative materials and devices in the near future. In a nutshell, Nanotechnology is the ability to engineer materials and devices on a length scale as small as several nanometers. The optical and transport properties of such nanostructures cannot be described in terms of macroscopic parameters and therefore a microscopic or atomistic viewpoint is called for. There is the need of developing computational methods that, given the complex nature of a nanostructure, must be tailored on massively parallel supercomputers in order to reduce the code execution time. In this respect, the SCOPE project has offered a tremendous opportunity for studying the optical properties of large silicon and InAs nanocrystals. It has been, indeed, developed an efficient computer code based on the tight-binding method which is able to work out both the nanocrystal electronic structure and the optical absorption spectrum $\alpha(\omega)$ using two level of description. In the first level, the polarization induced on the nanocrystal surface by the external field is ignored (this approximation is known as RPA) while in the second this surface contribution is fully taken into account. Comparing the numerical results with experimental data it turned out that for a nanocrystal the surface polarization plays a fundamental role while, for a bulk material; it only gives a marginal contribution. In the following figure a direct comparison between numerical [12,13] (red lines) and experimental (crosses) data [14] is shown for the case of colloidal InAs nanocrystals with a spherical shape and with different dimensions. As it is seen, the agreement is very good.

An important conceptual point in the physics of semiconductor nanocrystals is the evolution of the optical response with the dimension. Since the number of atoms making the structure increases very rapidly with the nanocrystal diameter, this type of study require significant computational resources. In the other figure, the absorption cross section of hydrogenated spherical silicon nanocrystals is shown as a function of their diameter within the RPA approximation [15].



The two arrows in each panel indicate the HOMO-LUMO (full line) gap and the absorption onset (dashed line). The important piece of information coming from that figure is that the absorption evolves rapidly to that of bulk silicon. About 700 silicon atom (2 nm in diameter) are almost enough for reproducing the typical bulk silicon absorption. This finding is relevant for silicon optoelectronic applications.

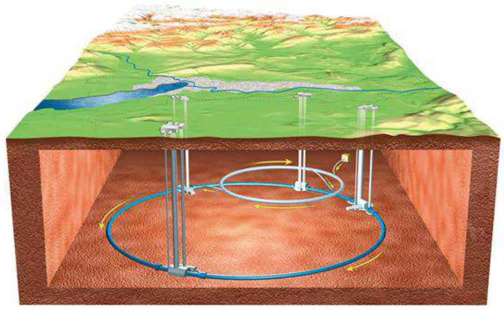


There are some other areas which have been touched during the SCOPE project. It is worth mentioning the problem of screening studied with both the tight-binding and ab initio methods [13,16,17], the role of oxygen vacancies on SnO_2 nanobelts [18] and some questions related to the physics of carbon nanotubes [19]. In the latter case the work has been done in collaboration with STMicroelectronics.

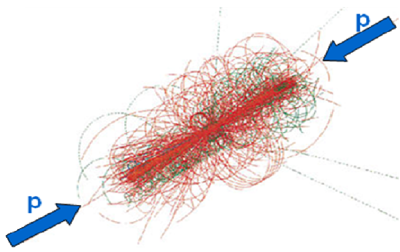
B. *The area of particle physics*

Nowadays, most of the particle physics activities are devoted to the search for the Higgs boson. Higgs boson is the particle whose existence has been postulated [20-22] by the Scottish physicist Higgs, to explain the difference in mass between *photons* and *vector boson W* and *Z*; Higgs boson should interact with all other particles, thus fixing their mass value.

The Large Hadron Collider (LHC) at CERN [23] (photos below) will allow collisions at very high energy, between protons and protons, thus freeing energy that will create other particles, among which physicists expect to reveal also the Higgs boson.

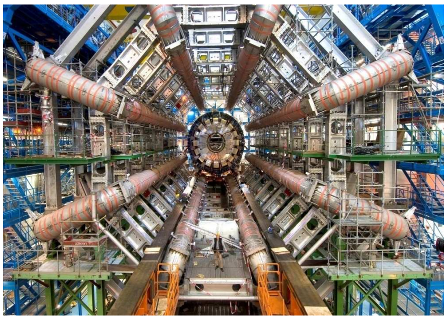


This particle cannot be seen directly, but through the decay products, such as 4 high-energy muons (see below).

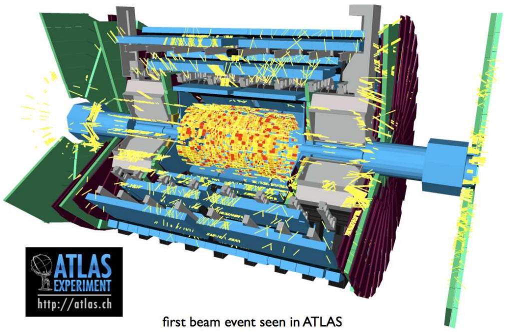


The scientific analysis of the huge amount of LHC data is possible only in Data Centers which adopt the computational Grid model [24,25], but a lot of effort is still needed to optimize the use of the systems and to completely analyse the data.

ATLAS [26], whose main apparatus is shown below, is one of the two main experiments at LHC. Naples, and the SCoPE project, has its role in ATLAS, as a Tier-2 site [27] for the experiment.



A reconstruction of the first beam event seen in ATLAS in September 2008 is shown below.



first beam event seen in ATLAS

C. The area of life sciences [28-30]

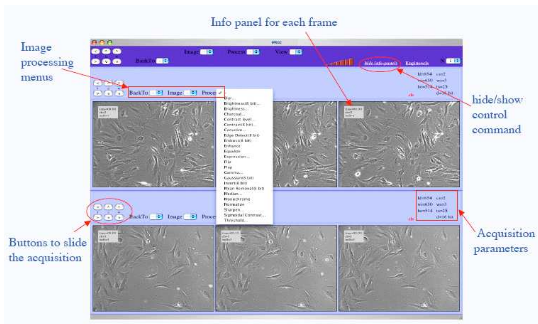
The goal of the life science team in the SCoPE project is twofold and consists of: building a system able to provide a large number of users with general purpose bioinformatics resources, and using them in a number of specific applications. Bioinformatics tools are designed to take advantage of high performance hardware and are easily accessed through a web interface for quick operations, performed by the vast majority of users, but are also available via Unix level access in the form of an integrated problem solving environment. Most commonly used programs have been made available to the users, including software for sequence analysis and alignment, structure prediction and fast sequence search, among others.

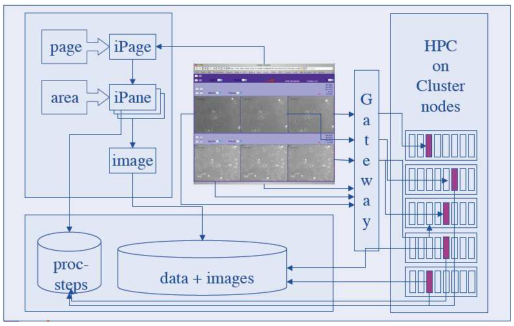
A large number of public databases are mirrored locally, and include most DNA and protein sequence collections, such as EMBL or UNIPROT databases, annotated genome sequences for human as well as mouse, ape, dog, cow and many more eukaryotic and prokaryotic sequences, EST collections and other expression data collections. Databases are accessible through the SRS web interface, but data bank have also been made available to SCoPE users, both in fastA and in BLAST format.

By using these resources, an automatic annotation system has been set up and used in specific computational or experimental projects, to provide analysis of conserved sequences (CST) obtained by comparative genomic analysis. Systematic analysis of human genes allowed to identify and study protein variants as well as gene changes associated with genetically transmitted diseases, such as CFTR. Genome data mining has been used to identify regulatory RNA sequences within completely sequenced bacterial genomes.

Computational analysis of biological images has been used in projects aimed to model the behaviour of cell populations in culture. Large amounts of image data are acquired in 3D observations and in time-lapse studies, and analyzed within the project. A web-based application, IPROC, has been adapted to work in a distributed environment, where image processing is executed in parallel by taking advantage of the available computational resources.

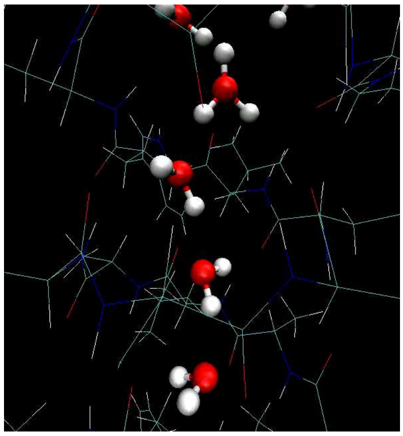
An example of application portal is shown below.





D. The area of computational chemistry [31-45]

Computational modeling of molecular and supra-molecular systems is carried out by the chemistry group in the SCoPE project. Recent developments at the level of theoretical descriptions (e.g. advanced solvent models suitable for dynamical simulations, improved density functionals and basis sets), coupled with efficient algorithms (e.g. linear-scaling implementations) are allowing to achieve good results for small to medium sized structures, and for periodic systems. However, computational descriptions of large, non-periodic structures still represent a challenge. The SCoPE group is focusing on the development and application of integrated computational tools based on hierarchical models, and capable of providing accurate yet computationally feasible descriptions of "difficult" systems such as "soft matter" systems. Crucial elements of the scheme are: a general and powerful electronic model (obtained through the development of original and effective approaches in the framework of the density functional theory); an accurate description of solute-solvent interactions (through mixed discrete-continuum models: see figure below), and the inclusion of the most important effects of nuclear motions (vibrational averaging of physico-chemical observables, reaction rates).

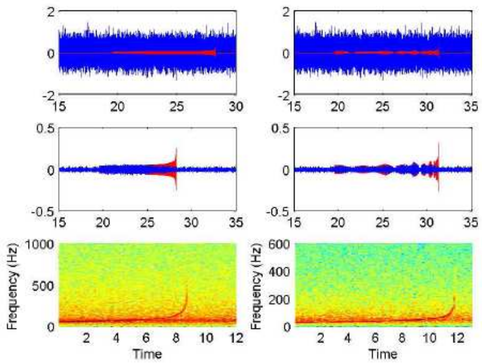


E. The area of gravitational physics [46-48]

Another research area is that of gravitational waves: these are waves due to the presence of a gravitational field, and are predicted by Einstein's General Relativity theory, although nobody has yet observed them. To allow their detection in the frequency interval from 10 to 6000 Hz, Italy and France have built near Pisa, a dedicated observatory, with an instrument, named VIRGO, which is a Michelson interferometer with 3 km arms (see below).

This instrument will be able to detect the effects of gravitational waves coming from supernovae and from coalescing binaries in the Virgo cluster (see simulation below).

The direct measurement of gravitational waves, very small distortion of the space-time, is one of the most important area of research of modern science.



The figure shows examples of inspiralling gravitational waveforms detection at sampling frequency f =4096 Hz. Top left: classical Neutron Star-Neutron Star binary 1.4 Ms + 1.4 Ms in normalized units with starting frequency 60 Hz, embedded in white noise (SNR=24.5). Middle left: in red theoretical waveform and in blue detected waveform by IIR Ale. Top right: Neutron star+ Black Hole binary 1.4 Ms+10 Ms with maximally spinning BH; Spin=0.99; starting frequency 30 Hz, embedded in white noise (SNR=20). Middle right: theoretical waveform(red) and detected waveform(blue). Bottom right: time – frequency behaviour of the detected waveform by IIR Ale.

Their direct detection of gravitational waves will allow a complete new vision of our universe, including the very first moments of its creation, which are not visible through the investigation of electromagnetic waves. The data which the VIRGO experiment will collect are temporal series at very high frequency, characterized by a very small signal-to-noise ratio; the large number of templates necessary for data analysis using matched- filtering techniques poses problems due to the great computing power needed to perform this task on-line. In fact, as a consequence of the large band of these detectors (some kHz), sampling rates of the order of 20 kHz are foreseen, resulting in a huge amount of data/day to be analyzed on-line (of the order of 10 GByte/day). Of course, the analysis of such a large amount of information could be made on-line, but it would be better to select on-line all the data frames which may contain a GW signal. The computational cost depends on the number of parameters considered in the approximation of the phase, on the accuracy of the sampling of the likelihood function (connected with the ability to recover weak signals) and on the actual frequency band to be considered, taking into account the VIRGO sensitivity . Actually, the direct application of the matched-filtering technique to the VIRGO antenna requires a computing power of at least 3 Teraflops starting from a minimum mass of 0.25 M_Θ with a SNR recovery of 90% including the computing power necessary for the production of the templates. So these data require computing resources, such as those available in the SCoPE Data Center; but they also require a comparison with similar data from other instruments, such as LIGO in the USA and GEO6000 in Germany. For all these aspect, the Grid model will allow results on a short time frame.

F. *The area of astrophysics* [49-53]

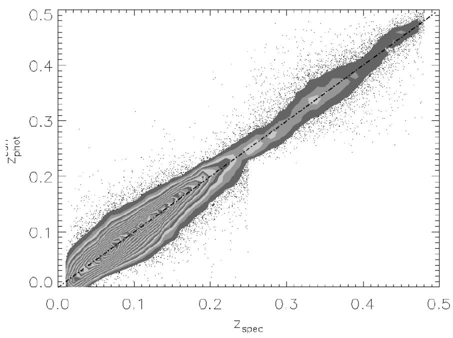
An area of astrophysics research in which GRID infrastructures are essential is that of the so called "Virtual Observatory or VObs". The VObs aims at federating and ensuring the interoperability of all existing data archives (of either observed or simulated data) as well as of data reduction and data analysis methods. Since modern instruments and numerical simulations produce data sets in the range of several hundreds of terabytes or petabytes, the VObs poses outstanding computational challenges which find their natural answer in the distributed computing paradigm. At a difference with what happens in other domains, the use of the VObs infrastructure is open to the community as a whole, and therefore poses peculiar security and scalability problems which can be used as a test bed for more general applications.

In this context, the main activity has developed along three research lines: i) the implementation of a procedure based on the use of e-Token robot certificates to allow everyone (even someone who does not possess a personal certificate) to launch specific tasks on the GRID; ii) the implementation of a WEB application for data mining and exploration in Massive Data Sets (In collaboration with the

California Institute of Technology) and, iii) the implementation of several specific scientific problems which effectively show-case the potentialities of the GRID in an astrophysical environment.

The DAME/VOneural platform [49] is a flexible Data Mining and exploration web based framework which allows a generic user to access a large number of machine learning and statistical methods and to run them on the SCOPE-GRID. For its generality the DAME framework is being used also for applications outside of astronomy (such as, bioinformatics and social sciences). The framework interfaces to the distributed computing environment through GRID – Launcher which associates each individual method to a specific robot-certificate.

Among the many science cases produced so far, we wish to emphasize two which have recently been published.



The figure shows the spectroscopic vs photometric redhifts trend for a sample of 3x10^5 galaxies extracted from the SDSS (rms =0.0186).

Photometric redshifts are one of the most effective ways to estimate the distances of large samples of extragalactic objects. Within the DAME platform it was implemented a specific sub tasks which allows the generic user to derive the phot-z estimate for large samples of objects. The method makes use of an ensemble of machine learning methods trained on a base of knowledge consisting of almost 10^6 spectroscopic redshifts extracted from the Sloan Digital Sky Survey. The resulting catalogue contains photometric redshifts for more than 30 million galaxies derived with unprecedented accuracy (D'Abrusco et al. 2007; Laurino et al. these proceedings).

A second application concerns the physical classification of Active Galactic Nuclei (AGN) using both MLPs and an implementation of Support Vector Machines on the SCoPE Grid. Also in this case the machine learning methods were trained on an extensive spectroscopic base of knowledge and applied to the SDSS photometric catalogues. The results (Cavuoti et al 2009 in preparation) seem capable to open a new era in the exploitation of multiband digital surveys. Preliminary results show in fact that different types of AGN can be disentangled with an accuracy close to 92 %.

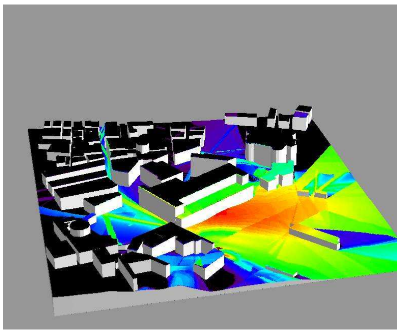
An additional result, concerning the simulation of the signatures left by cosmic strings on the Cosmic Microwave Background is presented in Riccio et al. (these proceedings).

G. The area of electromagnetic waves

Several research activities are being carried out in this area, and one of particular interest concerns the determination of the radio coverage of telecommunication networks (e.g. GSM/UMTS signals) within a city, in order to measure the impact on the environment.

Propagation of electromagnetic waves in the urban environment is in principle a well-posed problem: the electromagnetic field radiated by the sources, for example a single antenna, must fulfill Maxwell equations in the open space, with boundary conditions determined by the buildings walls. But a solution to this apparently simple problem must face the complication of the scattering scenario.

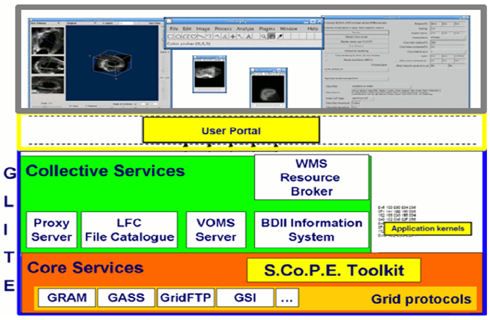
The cities distribution may be considered as a stochastic process, each city being an element of this ensemble. Accordingly, the study of electromagnetic propagation and scattering in the city becomes the problem of searching the solution of Maxwell equations in a stochastic environment. This task may be pursued on along essentially two lines of thought, either a deterministic or a stochastic one: the former makes reference to an element of the ensemble, the latter exploits the statistical properties of the distribution [54]. In the deterministic approach, an element of the cities ensemble is chosen, namely the particular city of interest. Then, each building is schematized in terms of a parallepipedic structure with plane walls and sharp edges, see figure below, topped with a (usually) flat roof; in addition, average electromagnetic properties of the buildings' walls are either known or postulated.



By accepting this model, ray tracing procedures have been implemented to compute the electromagnetic field everywhere in the open space surrounding the buildings, i.e., in the streets and squares of the city [55-59].
All these studies will allow to plan correctly the implementation and distribution of antennas in the city: the use of the computer grid provided by SCoPE is very convenient for speeding-up the computations and improving the accuracy of the results [60-64] Furthermore, the developed software may be used to interpolate the field values in-between their sampled ones, measured by a limited number of sensors scattered in the city area. In such a way it is possible to evaluate and control the overall exposure level of the population in all points of the city, with a continuous checking of compliance with the Norms, thus reassuring the population in the spirit of the International Health Institute stating that *Health is a state of complete physical, mental, and social well-being and not merely the absence of disease or infirmity.* Concerning this last application, the use of the computer grid provided by SCoPE is fundamental, due to the very large number of electromagnetic sources involved and the convenience of real-time operations.

H. The area of the high level middleware

Special efforts have been devoted to the development of (high level) middleware. It is needed to know, for example, how the new multicore computing platforms affects the efficiency of the underlying numerical kernels [68,69]. Another example of the results obtained is the MedIGrid framework. It is concerned with improvements and enhancements of a medical imaging grid-enabled framework, oriented to the transparent use of resource-intensive applications for managing, processing and visualizing biomedical images. In particular the group has realized an implementation of the MedIGrid PSE, based on the integration of the LCG/gLite and SCOPE-toolkit middlewares, obtaining more efficiency in data management and job submission (see below for software architecture).



The applications allowed by MedIGrid are denoising of 3D echocardiographic images sequence and segmentation of 2D echocardiograph images [65]. Both applications are based on the *Portable, Extensible Toolkit for Scientific Computation* (**PETSc**) library, a suite of data structures and routines that provide the building blocks for the implementation of large-scale codes concerning the scalable parallel solution of scientific applications modelled by partial differential equations. The group has focused its attention to avoid:

- bottlenecks due to multiple and unuseful Resource Broker (WMS) transits;
- bound to data sizes, imposed by WMS.

Furthermore, the group worked to modify, extend and improve the underlying numerical components to introduce, at the application level, mechanisms to sustain a given level of performance and to survive to a fault during execution flow [66,67].

ACKNOWLEDGMENTS

This work has been funded by the Ministery of University and Research, Italy, under grant no.255/RIC dated 14.02.2006.

The author wishes to thank all the colleagues of the SCoPE project, which have collaborated for the success of the project, as well as to the realization of this paper. Special thanks to the project leader prof. Giuseppe Marrucci.

The realization of the SCoPE infrastructure has been possible thanks to the precious efforts of a number of people, among which Guido Russo, Elena Cesaro (administrative officer), Giovanni Battista Barone (head of the technical staff), Francesco Palmieri (leader of the networking group) and of many young people (among which Silvio Pardi who coordinated the interoperability technical group of the four projects of the PON 200-2006 Avviso 1575/2004) who significantly contributed to the scientific and technical efforts.

The SCoPE group also wishes to thank the staff from DELL, leaded by M. De Leo, who generously devoted most of his time during 2008 to complete the infrastructure in due time.

REFERENCES

[1] The Grid Community at the MIUR web site www.ponricerca.it/Public/grid/F1737/F1737.aspx

[2] The CRESCO e-infrastructure we bsite http://www.cresco.enea.it/

[3] The CyberSar e-infrastructure web site: http://www.cybersar.com/

[4] The PI2S2 e-infrastructure web site: http://www.pi2s2.it

[5] The GRISU web site http://www.grisu-org.it/

[6] The SPACI e-infrastructure website: http://www.spaci.it

[7] Barone G.B., D.Bottalico, V.Boccia, L. Carracciuolo, S.Pardi, M.Scognamiglio, F.Serio, *Middleware applicativo: lo SCOPE Toolkit*, Italian Nat. Conference e-Science2008, 2008.

[8] M.A. Jefri and A.H. Zahed. Elastic and viscous effects on particle migratrion in plane-poiseuille flow. J. Rheol., 33:691, 1989.

[9] D'Avino G, Hulsen MA, Snijkers F, Vermant J, Greco F, Maffettone PL "Rotation of a sphere in a viscoelastic liquid subjected to shear flow. Part I: Simulation results" J. Rheol. 52, 1331-1346, 2008-

[10] G. D'Avino, G. Cicale, M.A. Hulsen, F. Greco, P.L. Maffettone, "Effects of confinement on the motion of a single sphere in a sheared viscoelastic liquid", J. nonNewt. Fluid Mech., 157, 101-107, 2009.

[11] Carracciuolo L., D. Casaburi, L. D'Amore, G. D'Avino, P.L. Maffettone, A. Murli, *Computational simulations of 3D fluido-dynamic processes in High Performance Computing Environment*, 2009, this volume.

[12] F. Trani, D. Ninno, G. Iadonisi, *Tight-binding formulation of the dielectric response in semiconductor nanocrystals*, Physical Review B 76 , 085326 (2007).

[13] F. Trani, D. Ninno, G. Iadonisi, *Role of local fields in the optical properties of silicon nanocrystals using the tight binding approach*, Physical Review B 75, 33312 (2007).

[14] Yu et al., *Absorption Cross-Section and Related Optical Properties of Colloidal InAs Quantum Dots*, Journal of Physical Chemistry B 109, 7084 (2005).

[15] F. Trani, G, Cantele, D. Ninno, G. Iadonisi, *Tight-binding calculation of the optical absorption cross section of spherical and ellipsoidal silicon nanocrystals*, Phys. Rev. B 72, 75423 (2005).

[16] D. Ninno, F. Trani, G. Cantele, K. J. Hameeuw, G. Iadonisi, E. Degoli, S. Ossicini, *Thomas-Fermi model of electronic screening in semiconductor nanocrystals*, Europhysics Letters 74, 519 (2006).

[17] F. Trani, D. Ninno, G. Cantele, G. Iadonisi, K. Hameeuw, E. Degoli, S. Ossicini, *Screening in semiconductor nanocrystals: ab initio results and Thomas-Fermi theory*, Physical Review B 73, 245430 (2006).

[18] F. Trani, M. Causà, D. Ninno, G. Cantele, and V. Barone, *Density functional study of oxygen vacancies at the SnO_2 surface and subsurface sites*, Physical Review B 77, 245410 (2008).

[19] F. Buonocore, F. Trani, D. Ninno, A. Di Matteo, G. Cantele, G. Iadonisi, *Ab initio calculations of electron affinity and ionization potential of carbon nanotubes*, Nanotechnology 19, 025711 (2008).

[20] P. W. Higgs, *Broken Symmetries, Massless Particles and Gauge Fields*, Phys. Lett. **12**:132, (1964).

[21] P. W. Higgs, *Broken Symmetries and the Masses of Gauge Bosons*, Phys. Rev. Lett. **13**:508 (1964).
[22] P. W. Higgs, *Spontaneous Symmetry Breakdown without Massless Bosons*, Phys. Rev. Lett. **145**:1156 (1966).
[23] O.Brüning et al., *LHC Design Report Volume I: the LHC Main Ring*, CERN-2004-003-V-1, http://cdsweb.cern.ch/record/782076 (2004).
[24] ATLAS Collaboration, *ATLAS: technical proposal for a general-purpose pp experiment at the Large Hadron Collider at CERN*, CERN-LHCC-94-43, http://cdsweb.cern.ch/record/290968 (1994).
[25] L. Perini et al., *Overview of the contributions of the LHC experiments in INFN GRID for bringing the Grid to production quality*, these proceedings (2009).
[26] ATLAS Computing Group, *ATLAS computing: Technical Design Report*, CERN-LHCC-2005-022, http://cdsweb.cern.ch/record/837738 (2005).
[27] G. Carlino et al., *Distributed analysis for the ATLAS Experiment in the SCoPE Project*, these proceedings (2009).
[28] Boccia A, Busiello G, Milanesi L, Paolella G. , *A fast job scheduling system for a wide range of bioinformatic applications*, IEEE Trans Nanobioscience. 2007 Jun;6(2):149-54.
[29] Ausilia Elce, Angelo Boccia, Giuseppe Cardillo, Sonia Giordano, Rossella Tomaiuolo, Giovanni Paolella, Giuseppe Castaldo, *Three novel CFTR polymorphic repeats improve segregation analysis for cystic fibrosis*, Clinical Chemistry, In Press.
[30] Luca Cozzuto, Mauro Petrillo, Giustina Silvestro, Pier Paolo Di Nocera and Giovanni Paolella, *Systematic identification of stem-loop containing sequence families in bacterial genomes*, BMC Genomics. 2008 Jan 17;9:20.
[31] G. Brancato, N. Rega, V. Barone, *A discrete/continuum QM/MM MD study of the triplet state of acetone in aqueous solution*, Chem. Phys. Lett. 453, 202-206 (2008).
[32] V. Barone, M. Biczysko, M. Pavone, *The role of dispersion correction to DFT for modeling weakly bound molecular complexes in the ground and excited electronic states*, Chem. Phys. 346, 247 (2008).
[33] G. Brancato, N. Rega, V. Barone, *A hybrid explicit/implicit solvation method for first-principle molecular dynamics simulations*, J. Chem. Phys. 128, 144501 (2008).
[34] F. Trani, M. Causà, D. Ninno, G. Cantele, V. Barone, *Density functional study of oxygen vacancies at the SnO2 surface and subsurface sites*, Phys. Rev. B 77, 245410 (2008).
[35] M. d'Ischia, O. Crescenzi, A. Pezzella, M. Arzillo, L. Panzella, A. Napolitano, V. Barone, *Structural Effects on the Electronic Absorption Properties of 5,6-Dihydroxyindole Oligomers: The Potential of an Integrated Experimental and DFT Approach to Model Eumelanin Optical Properties*, Photochem. Photobiol. 84, 600–607 (2008).
[36] M. Di Valentin, S. Ceola, G. Agostini, G.M. Giacometti, A. Angerhofer, O. Crescenzi, V. Barone, D. Carbonera, *Pulse ENDOR and density functional theory on the peridinin triplet state involved in the photo-protective mechanism in the peridinin-chlorophyll a-protein from Amphidinium carterae*, Biochim. Biophys. Acta - Bioenergetics 1777, 295-307 (2008).
[37] G. Brancato, N. Rega, V. Barone, *Accurate density functional calculations of near-edge X-ray and optical absorption spectra of liquid water using nonperiodic boundary conditions: The role of self-interaction and long-range effects*, Phys. Rev. Lett. 100, 107401 (2008).
[38] V. Barone, R. Improta, N. Rega, *Quantum mechanical computations and spectroscopy: From small rigid molecules in the gas phase to large flexible molecules in solution*, Acc. Chem. Res. 41, 605-616 (2008).
[39] J. Bloino, M. Biczysko, O. Crescenzi, V. Barone, *Integrated computational approach to vibrationally resolved electronic spectra: Anisole as a test case*, J. Chem. Phys. 128, 244105 (2008).
[40] V. Barone, P. Cimino, O. Crescenzi, M. Pavone, *Ab initio computation of spectroscopic parameters as a tool for the structural elucidation of organic systems*, Theochem 811, 323-335 (2007).
[41] G. Brancato, V. Barone, N. Rega, *Theoretical modeling of spectroscopic properties of molecules in solution: toward an effective dynamical discrete/continuum approach*, Theor. Chem. Acc. 117, 1001-1015 (2007).
[42] A. Pezzella, O. Crescenzi, A. Natangelo, L. Panzella, A. Napolitano, S. Navaratnam, R. Edge, E.J. Land, V. Barone, M. d'Ischia, Chemical, *Pulse Radiolysis and Density Functional Studies of a New, Labile 5,6-Indolequinone and Its Semiquinone*, J. Org. Chem. 72, 1595-1603 (2007).
[43] R. Improta, V. Barone, F. Santoro, *Ab Initio Calculations of Absorption Spectra of Large Molecules in Solution: Coumarin C153*, Angew. Chem. Int. Edit. 46, 405-408 (2007).
[44] M. Pavone, P. Cimino, O. Crescenzi, A. Sillanpaa, V. Barone, *Interplay of Intrinsic, Environmental, and Dynamic Effects in Tuning the EPR Parameters of Nitroxides: Further Insights from an Integrated Computational Approach*, J. Phys. Chem. B 111, 8928-8939 (2007).
[45] I. Borriello, G. Cantele, D. Ninno, G. Iadonisi, M. Cossi, V. Barone, *Ab initio study of electron affinity variation induced by organic molecule adsorption on the silicon (001) surface*, Phys. Rev. B 76, 035430 (2007).
[46] C. Bradaschia, et al., *VIRGO: Proposal for the construction of the very large baseline interferometric antenna for gravitational wave detection*, Proposal to the INFN (Italy) and CNRS (France) (1989, 1992, 1995).
[47] P. Bender, I. Ciufolini, J. Cornelisse, K. Danzmann, W. Folkner, F. Hechler, J. Hough, Y.Jafry, R. Reinhard, D. Robertson, A. Rudiger, M. Sandford, R.

Schilling, B. Schutz, R. Stebbins, T. Summer, P. Toubol, S. Vitale, H. Ward, W. Winkler, *LISA: Laser Interferometer Space Antenna for the detection and the observation of gravitational waves*, ESA Pre-Phase A Report, MPQ 208, Max Planck Institut fur Quantenoptik, Munich, Germany (February 1996).

[48] A. Eleuteri, L. Milano, S. Pardi et al., *Adaptive filters for detection of gravitational waves from coalescing binaries*, Phys. Rev. D 73, (2006).

[49] M. Brescia et al., *The DAME/VO-Neural infrastructure: an integrated data mining system support for the science community*, these proceedings (2009).

[50] R. D'Abrusco, et al., *Mining the SDSS data. I. Photometric redshifts for the nearby universe*, ApJ., 663, 752-764 (2007).

[51] O. Laurino et al., *Photometric Redshifts of QSO's*, these proceedings (2009).

[52] S. Cavuoti 2009, Laurea Thesis, University of Napoli.

[53] G. Riccio et al., *Simulations of cosmic string signatures in the CMB*, these proceedings (2009)

[54] G. Franceschetti, R. Marano, F. Palmieri *Wave propagation without wave equation. Toward an urban area model*, IEEE Trans. Antennas Propagat., 1999, 47, 1393-1404 (Vincitore del Premio Schelkunoff per il miglior lavoro su IEEE-AP per l'anno 1999).

[55] M.Franceschetti, D.Riccio, *Wireless Channel Model*, in Wireless Networks: from the Physical Layer to Communication, Computing, Sensing and Control, G.Franceschetti, S.Stornelli, eds., Academic Press, 2006, 161-185.

[56] G.Franceschetti, A.Iodice, D.Riccio, G.Ruello, *A Tool for Planning Electromagnetic Field Levels in Urban Areas*, Proceedings of the Antennas and Propagation Society International Symposium, Monterey, 2004, 2211-2214.

[57] G.Franceschetti, A.Iodice, D.Riccio, G.Ruello, *Pianificazione dei Livelli di Campo Elettromagnetico*, Atti della XIV Riunione Nazionale di Elettromagnetismo, Ancona, 2002, 226-229.

[58] G.Franceschetti, A.Iodice, D.Riccio, G.Ruello, *Determinazione della Radiocopertura per Reti di Telecomunicazioni*, Atti della XV Riunione Nazionale di Elettromagnetismo, Cagliari, 2004, 477-480.

[59] G.Franceschetti, R.Guida, A.Iodice, D.Riccio, G.Ruello, *Verifica di un Software per la Previsione della Radiocopertura*, Atti della XVI Riunione Nazionale di Elettromagnetismo, Genova, 2006, 170-173.

[60] P. Imperatore, F. Moscato, R. Guida, G. Ruello, A. Iodice, D. Riccio, N. Mazzocca, G. Franceschetti, *Strumento su Piattaforma GRID per la Predizione del Campo Elettromagnetico in Aree Urbane*, Conferenza Nazionale Italian e-Science, Napoli, 2008, 117-118.

[61] F. Moscato, N. Mazzocca, P. Imperatore, G. Franceschetti, R. Guida, *COSCA: Una Architettura per l'Analisi di Campi Elettromagnetici su Scala Geografica in Ambienti E-Science Basati su GRID*, Conferenza Nazionale Italian e-Science 2008 - IES08, Napoli, 2008, 148-149.

[62] G. Franceschetti, R. Guida, P. Imperatore, A. Iodice, N. Mazzocca, F. Moscato, D. Riccio, G. Ruello, *Previsione e Controllo della Radiocopertura in Aree Urbane: Un Modello Computazionale Parallelo*, Atti della XVIII Riunione Nazionale di Elettromagnetismo, Lecce, 2008.

[63] G. Franceschetti, P. Imperatore, A. Iodice, D. Riccio, *Radio-Coverage Parallel Computation on Multi-Processor Platforms*, 39th European Microwave Conference, Rome, 2009 (submitted).

[64] G. Franceschetti, P. Imperatore, A.Iodice, D.Riccio, *Computation of the Electromagnetic Field Levels in Urban Environment: a Parallel Model*, to be submitted to IEEE Trans. Antennas Propag.

[65] Carracciuolo L., L. D'Amore, and A. Murli. *Towards a parallel component for imaging in PETSc programming environment: A case study in 3-D echocardiography*. Parallel Computing, 32, 2006, pag. 67-83.

[66] Murli A., V. Boccia, L. Carracciuolo, L. D'Amore, G. Laccetti, and M. Lapegna, *Monitoring and Migration of a PETSc-based Parallel Application for Medical Imaging in a Grid computing PSE*. In P. Gaffney and J. Pool, editors, Grid-Based Problem Solving Environments, Springer Verlag, 2007, pag. 421-432.

[67] Boccia V. , L. Carracciuolo, L. D'Amore, G. Laccetti, M. Lapegna and A. Murli, *Recent advances of MedIGrid PSE in an LCG/gLite environment*, 2009, this volume.

[68] Carracciuolo L., G. Laccetti and M. Lapegna, *Implementation of effective data management policies in distributed and grid computing environments,in Parallel Processing and Applied Mathematics 2007* (R. Wyrzykowski, J. Dongarra, N. Meyer, J. Wasniewski, editors), Lecture Notes in Computer Science 4967, 2007, pag. 902-911.

[69] Laccetti G., M. Lapegna, D. Romano, V. Mele, *Multilevel Algorithms for Multidimensional Integration in High Performance Computing Environment*, 2009, this volume.