Grid Open Days all'Universita' di Palermo

Abstracts book

Table of contents

Abstract ID : 0

Jet-induced stellar formation from AGNs: Simulating relativistic jets from central Black Holes

During the past months, we have performed a series of high resolution simulations of the propagation of relativistic jets into the Interstellar and Intergalactic Media (ISM/IGM). These jets are believed to be the final product of a complex accretion phenomenon of gas onto a Black Hole at the center of its host galaxy. Current cosmological models believe that virtually every galaxy in the Universe hosts a BH, and is affected by these relativistic jets for at least some fraction of its life. Until now, very little work has been aimed at studying how the jet affects stellar formation within the host galaxy. The simulations performed on TriGrid are the first which have addressed this specific problem, and provide quantitative information on the physical mechanism promoting BOTH the suppression of stellar formation within the diffuse IS/IGM (the so-called "negative" feedback) AND the induction of stellar formation within the shocked clouds.
We will present some of these findings, and how they help to model some observations, like those pertaining to the "Minkowski object", an extended region of stellar formation in an external galaxy associated with a powerful radio jet. Most of these results will be presented through a set of animations, showing the propagation of the jet and the dramatic effect it has on the ISM/IGM clouds already present.

Some preliminary results can be see on the website of the Marie Curie "COSMOCT" project:
http://web.ct.astro.it/cosmoct/web_group/research3/research3_jet.html

Primary authors : Dr. ANTONUCCIO, Vincenzo (INAF - Osservatorio Astrofisico di Catania)

Co-authors : Prof. SILK, J. (Astrophysics, Dept. of Physics, University of Oxford, United Kingdom) ; Dr. BECCIANI, Ugo (INAF - Osservatorio Astrofisico di Catania) ; Dr. ROMEO, Alessio (INAF - Osservatorio Astrofisico di Catania)

Presenter : Dr. ANTONUCCIO, Vincenzo (INAF - Osservatorio Astrofisico di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. ANTONUCCIO, Vincenzo

Submitted on Thursday 13 September 2007

Last modified on : Wednesday 28 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 1

The outer Oort cloud formation: Simulation of the first Gyr of its evolution.

We used the trigrid infrastructure to make a simulation of the dynamical evolution of comets during the first Gyr of the Solar System life. The project is a collaboration between Slovak, Polish, and Italian researchers. The whole set of calculations is performed by using the facilities available via both the "TriGrid " and
"VOCE" Virtual Organization (VO) facilities. VOCE is a central European VO which belongs to the "EGEE Computing Grid Project". The simulation starts with an initial proto-planetary disc model which is represented by 10038 test particles (theoretical cometary nuclei). The dynamical evolution of the particles/comets is followed taking into account the perturbations by four giant planets, Galactic tide, and stars passing the Solar System. The final product is the formation of a comet cloud in the outher region of the Solar System. This comet reservoir is known as the Oort cloud. We show that the population of the outer Oort cloud reaches its maximum at about 210 Myr. Then, it decreases down to an almost constant level, reached at about 500 Myr, which is followed by a very moderate population depletion. At 1 Gyr, the population decreases to about 40% of its maximum. The efficiency of the formation appears to be very low.
Only about 0.29% of all considered particles reside in the outer Oort cloud at 1 Gyr. From about 50 Myr to the end of the simulation, the orbits are not distributed randomly, but high galactic inclinations of the orbital planes are strongly dominant. We'll show the dynamical evolution of the particles by means of several animations created using the results of the calculated model.

Primary authors : Dr. LETO, Giuseppe (INAF - Osservatorio Astrofisico di Catania, Catania, Italy)

Co-authors : Dr. JAKUBIK, Marian (Astronomical Institute, Slovak Academy of Sciences, 05960 Tatranska Lomnica, Slovakia) ; Dr. NESLUSAN, Lubos (Astronomical Institute, Slovak Academy of Sciences, 05960 Tatranska Lomnica, Slovakia) ; Dr. DYBCZYNSKI, Piotr A. (Astronomical Observatory of the A. Mickiewicz University, Sloneczna 36, 60-286 Poznan, Poland) ; Dr. PAULECH, Tomas (Astronomical Institute, Slovak Academy of Sciences, Dubravska cesta 9, 84504 Bratislava, Slovakia)

Presenter : Dr. LETO, Giuseppe (INAF - Osservatorio Astrofisico di Catania, Catania, Italy)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. LETO, Giuseppe

Submitted on Saturday 20 October 2007

Last modified on : Saturday 20 October 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 3

Porting of CHIMERA multidetector and Constrained Molecular Dynamics model (CoMD) on a computational grid.

The goal of TriGrid Project is the creation of the first Sicilian regional computational grid. In particular, it aims to build various software-hardware interfaces between the infrastructure and some scientific and industrial applications. In this context, two projects carried out for the CHIMERA multidetector, have been integrated : ISOSPIN experiment and CoMD-II (Constrained Molecular Dynamics) model. This work will show how created porting applications are able to decrease the execution time of the analysis programs; to improve the accessibility to the data storage and to manage a lot of metadata for data processing.

Primary authors : Dr. LANZALONE, Gaetano (INFN Catania)

Co-authors : Dr. MUOIO, Annamaria (INFN Catania) ; Dr. IACONO MANNO, Marcello (Cometa)

Presenter : Dr. LANZALONE, Gaetano (INFN Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. MUOIO, Annamaria

Submitted on Monday 12 November 2007

Last modified on : Monday 12 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 4

GridVideo: a grid-based multimedia application

Grid Computing supports the shared and coordinated use of several resources in dynamic virtual Organizations that is the creation, from geographically distributed components belonging to distinct administrative domains, of virtual computing systems. Starting from 1990s and until now, Grid Computing has been mainly used in scientific laboratories. Only in the last few years it is evolving into a business innovating technology that is driving commercial adoption. The purpose of this paper is to show a real experience on enabling a non-scientific application using the Grid as underline technology. In particular, will be described the development of GridVideo, a multimedia application for the distributed tailoring and streaming of media files; its development has been carried out using the Grid testbed built within the Cometa project.
GridVideo, identifies two multimedia related activities: Multimedia Upload and Storage and Multimedia Streaming.
During the first activity, operators in each organization (the services providers for example) make a multimedia object available to the users by uploading the file in the system. During this activity we can distinguish the upload of the file to a grid node chosen where the file is splitted into many chunks, after that the files are encoded so as to store each piece of each file into a common high quality format.
The second activity is the Streaming activity, this activity deals with the end user requests and the media streaming. Users request a content with specified characteristics (in terms of resolution, color depth, audio reproduction and media format supported) using a GUI.
Once the first chapter has been tailored, the Streaming phase allows users to watch the entire stream in a transparent way over a set of plain HTTP connections.
Technical and practical problems encountered during the development are analyzed and a performance evaluation of the developed prototype will be presented.

Primary authors : Mr. IELLAMO, Giuseppe (University of Messina) ; Mr. MINUTOLI, Giuseppe (University of Messina) ; Dr. BRUNEO, Dario (University of Messina) ; Prof. PULIAFITO, Antonio (University of Messina)

Co-authors :

Presenter : Mr. IELLAMO, Giuseppe (University of Messina)

Track classification :

Contribution type : --not specified--

Submitted by : Mr. IELLAMO, Giuseppe

Submitted on Thursday 15 November 2007

Last modified on : Thursday 15 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 5

Grid-based analysis of simulated light curves to test planetary transit detection methods

The detection of extrasolar planets by means of the transit method is a rapidly growing field of modern astrophysics. The periodic light dim produced by the passage of a planet in front of its parent star can be used to reveal the presence of the planet itself, to measure its orbital period and relative radius, as well as to perform studies on the outer layers of the planet by analysing the light of the star passing through the planet's atmosphere. We have developed a new technique to detect transits by objects with a size comparable to that of our Earth in front of a solar-like star. Our technique exploits a physical model of solar-like variability to reduce the impact of stellar intrinsic flux variations on the detection of the transits. Tens of thousands of light curves have been simulated to test the performance of our method for different values of the radius and the orbital period of the planet and for different photometric accuracy, as expected for the space experiments CoRoT and Kepler. We shall briefly report on the use of the Grid to perform our assessment study and on the foreseen application for the CoRoT space experiment in which we are presently involved.

Primary authors : Dr. LANZA, Antonino Francesco (INAF-Osservatorio Astrofisico di Catania)

Co-authors : Dr. BONOMO, Aldo Stefano (Dipartimento di Fisica e Astronomia, Università degli Studi di Catania)

Presenter : Dr. LANZA, Antonino Francesco (INAF-Osservatorio Astrofisico di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. LANZA, Antonino Francesco

Submitted on Friday 16 November 2007

Last modified on : Friday 16 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 6

Looking for Class Records in the 3x+1 problem by means of the Cometa grid

The design of a parallel algorithm for the subject search on the Cometa grid is presented. Known optimization techniques of the basic algorithm are supplemented with novel ones. These, and especially the higher performance enabled by the 64-bit architecture, outperform current implementations on 32-bit machines by a rough 2.7 speed-up factor. This work introduces the basic algorithm, its optimization techniques and their mathematical underpinnings. The most novel aspect of this contribution relates to the optimal integration of a new optimization technique for delay computation, called Acceleration, with known ones, such as Head cut-off, that stop delay computation at an early stage, under appropriate conditions. The performance gain delivered by each of these techniques depends on user-defined parameters, easily amenable to empirical optimization. Seemingly, the two kinds of techniques work on orthogonal aspects of the computation, since Acceleration decreases the delay computation time for any given trajectory, whereas Head cut-off decreases the number of trajectories whose delay is eventually computed. So, one might expect that optimal integration of these techniques ought to result from their combination with parameter values that are respectively optimal for each technique considered in isolation. At a closer look, however, this expectation proves ill-founded, because of actual interference between the techniques in question. A key idea to obtain near-optimal integration of Acceleration with Head cut-off is that of appropriately smoothing the former in order to prevent the loss of information that would harm the effectiveness of the latter. This is exposed in detail in this work, where a more general applicability of this idea is argued as well. The software is open source, written in standard C++, but for a few scripts, mostly meant for job monitoring and control on the Cometa grid, and is going to be made freely available on the PI2S2 Web in the GRID CT Wiki.

summary :

Primary authors : Prof. SCOLLO, Giuseppe (Dipartimento di Matematica e Informatica, Università di Catania)

Co-authors :

Presenter : Prof. SCOLLO, Giuseppe (Dipartimento di Matematica e Informatica, Università di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. SCOLLO, Giuseppe

Submitted on Saturday 17 November 2007

Last modified on : Saturday 17 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 7

Structural properties of methanol and carbon tetrachloride mixtures: A molecular dynamics study

I report preliminary results of an extended molecular dynamics (MD) investigation of the structural properties of fluid mixtures composed by methanol and carbon tetrachloride, at ambient conditions and over a wide range of relative compositions.

Interests in this mixture stem from the modification in the associating properties of the methanol induced by the presence of an apolar solvent like the CCl4 molecule. Methanol is in fact
the smallest organic compound able to exhibit an hydrogen bond, and is largely used as solvent in experimental setups. Its liquid structure is well characterized by winding chains of hydrogen-bonded
monomers with a rather low fraction of branching points. Upon dilution, the degree of cross links among different chains progressively diminishes and a significant fraction of such chains closes to form cyclic structures. The purpose of this study is twofold: on the one hand, a comparison is planned between the MD results and the light-scattering data generated in the laboratory of one of the co-authors (FS), in order to elucidate at the molecular level the progressive modifications of the hydrogen bond properties. On the other hand, simulations will provide the necessary benchmark to gauge the accuracy of the liquid state theories for molecular fluids currently adopted in our group.

I will discuss how important properties of the mixture can be accessed thanks to the large scale computing facilities provided by the Consorzio COMETA through the PI2S2 project. In particular, the use of large sample sizes (of the order of 10000 interaction centres) allows one the accurate determination of the structure of the fluid over a wide spatial range, with a refined calculation of the compressibility of the mixture, and of the equation of state in turn. Another important isuue concerns the possibility to characterize the local order of the methanol at the molecular scale with confident statistical accuracy, also in the high dilution regime.

Primary authors : COSTA, Dino (Consorzio COMETA and Dipartimento di Fisica, Università di Messina - ITALY)

Co-authors : SAIJA, Franz (CNR - Istituto per i Processi Chimico-Fisici, Sede di Messina - ITALY) ; MUNAò, Gianmarco (Dipartimento di Fisica, Università di Messina - ITALY) ; CACCAMO, Carlo (Dipartimento di Fisica, Università di Messina - ITALY)

Presenter : COSTA, Dino (Consorzio COMETA and Dipartimento di Fisica, Università di Messina - ITALY)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. COSTA, Dino

Submitted on Monday 19 November 2007

Last modified on : Monday 19 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 8

Grid-K: A Grid Service for Compression-Based Classification of Biological Sequences and Structures

As an increasing number of full genomic sequences and protein structures become available, the need for efficient and reliable algorithms for their classification becomes more and more important. For many reasons alignment-free similarity measures are actively pursued. In this scenario, prominence has been gained by a new notion of similarity among sequences: the Universal Similarity Metric (USM). It is based on the deep theory of Kolmogorov Complexity and universality is its most novel and striking feature. Unfortunately, it can only be approximated via data compression. In our prior work, it has been established that the USM methodology is worth using because of its robustness, flexibility, scalabity and competitiveness with existing techniques. However, because of the large amount of data usually involved in classification, the method is very slow on conventional computers, in particular when the workload is substancial. Fortunately, the method is also so well structured to lend itself to a natural parallelization in terms of independent jobs, being ideal for a highly efficient implementation on Grid. Indeed, from a preliminary analysis, Grid computing allows great flexibility in providing computational resources to the application, on demand. Apart from computational speed-ups, the GRID paradigma offers an ideal setting for the massive use of GRID-K for Bioinformatic classification tasks. Indeed, a prototype of a Grid-aware Web service has been set up on the Genius Portal (https://infn-ui-01.ct.pi2s2.it/). The service includes also visualization tools for display and navigation in phylogenetic trees.

Primary authors : Dr. GRECO, Valentina Greco (Contrattista Cometa) ; Prof. GIANCARLO, Raffaele (Dipartimento di Matematica ed Applicazioni, Università di Palermo)

Co-authors :

Presenter : Dr. GRECO, Valentina Greco (Contrattista Cometa)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. GRECO, Valentina Greco

Submitted on Tuesday 20 November 2007

Last modified on : Thursday 22 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 9

Analysis of the systematic error in direct simulation Monte Carlo

Charge transport phenomena in submicrometric semiconductor devices can be investigated by mean of the Direct Simulation Monte Carlo (DSMC). It provides an accurate description of carrier transport phenomena because the various scattering mechanisms and band structure models are taken into account.

However, in exchange for this advantage, significantly longer computer execution time are required, and the results are affected by discretization and stochastic errors, which influence dramatically their accuracy and efficiency.

In this work we have analysed the systematic error introduced in DSMC, with respect to the particles number and to the time step, in the case of a simple n+ n n+ silicon diode. The efficiency of the algorithm has been studied, with respect to the precision of the results.

Primary authors : Prof. MUSCATO, Orazio (Dipartimento di Matematica e Informatica)

Co-authors : Dr. WAGNER, Wolfgang (Weierstrass Institute fro Applied Analysys and Stochastics , Berlin)

Presenter : Prof. MUSCATO, Orazio (Dipartimento di Matematica e Informatica)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. MUSCATO, Orazio

Submitted on Tuesday 20 November 2007

Last modified on : Tuesday 20 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 10

Theoretical Physics use cases in the PI2S2 Project

Modern studies of the properties of ground state and excited states of many body systems require more and more powerful computer resources. The grid infrastructure is thus a particularly well suited tool for their implementation. In the present work we will discuss two different lines of investigation. The first one is directed to the analysis of electronic properties of Metal Clusters within the Random Phase Approximation (RPA) and an improved RPA approach. RPA calculations are usually carried out in order to improve the standard mean field description of a physical system. However, RPA presents some limits and many efforts are still done by the scientific community in order to overcome them by improving the RPA description of ground state correlations. We have thus developed an improved RPA approach in order to take into account correlations in a self-consistent way. In particular we have analysed dipole plasmon modes in Metal Clusters and we have found a good agreement with experimental results, better than standard RPA does. With the use of grid technology, it has been possible to carry out a systematic study of several Metal Clusters.
In the second line of investigation we have studied, in a schematic physical model, some features of SLEPC, a free software library for the solution of large sparse eigenvalue problems. The eigenvalue problem is one of the most recurring numerical task in scientific disciplines. The critical points in the diagonalization methods are the amount of needed memory and the time spent in the diagonalization process. Standard methods are often not suited and alternative approaches have to be used. SLEPC library allows to choose different algorithm of diagonalization and to use parallel distributed-memory strategies, where the data of the problem are distributed across the available processors. Particular attention has been directed to its parallel efficiency and good results have been obtained.

summary :

An analysis of electronic properties of Metal Clusters within RPA-like approaches is carried out.
Furthermore, an application of SLEPC parallel eigensolvers to a schematic physical model is presented and their performance is studied.

Primary authors : GAMBACURTA, Danilo (Consorzio Cometa)

Co-authors :

Presenter : GAMBACURTA, Danilo (Consorzio Cometa)

Track classification :

Contribution type : --not specified--

Submitted by : GAMBACURTA, Danilo

Submitted on Wednesday 21 November 2007

Last modified on : Wednesday 21 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 11

Harmonic Spectra in H2+ Molecule in the Presence of a Laser Field

We solve numerically the time-dependent Schroedinger equation for hydrogen molecular isotopes in the presence of strong laser pulses beyond the Born-Oppenhaimer approximation. The emitted spectra show the presence of satellite peaks around the usual odd harmonic lines. The spacing of such side-bands is given by the vibrational frequency of nuclear motion. Furthermore, an isotopic effect is evident in the spectra of the emitted radiation: the intensity of the spectral lines is strongly dependent on the nuclear mass. Moreover a wavelet analysis shows that the intensity of harmonic lines is modulated with the same period as the nuclear motion.

Primary authors : Mr. ORLANDO, Gianfranco (universita di palermo)

Co-authors : Mr. CASTIGLIA, Giuseppe (universita di palermo) ; Mr. CORSO, Pier Paolo (universita di palermo)

Presenter : Mr. ORLANDO, Gianfranco (universita di palermo)

Track classification :

Contribution type : --not specified--

Submitted by : Mr. ORLANDO, Gianfranco

Submitted on Wednesday 21 November 2007

Last modified on : Wednesday 21 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 12

High Performance Computing on the GRID infrastructure of COMETA

We present the High Performance Computing (HPC) projects jointly developed at the INAF - Osservatorio Astronomico di Palermo and at the Dip.S.F.A. - Universita` degli Studi di Palermo which benefit of the GRID infrastructure of COMETA. We have contributed to setup the infrastructure in order to run HPC applications on the GRID. We report on our experience regarding to porting HPC applications to the GRID and to the first HPC simulations performed. The most demanding simulations are about the interaction of a magnetized supernova shock wave with an interstellar gas cloud. We discuss the resources required for the simulations, the performance and the scalability of our code on the GRID. We present the first results.

Primary authors : Dr. ORLANDO, Salvatore (INAF - Osservatorio Astronomico di Palermo)

Co-authors : Prof. PERES, Giovanni (Dip.S.F.A. - Universita` degli Studi di Palermo) ; Prof. REALE, Fabio (Dip.S.F.A. - Universita` degli Studi di Palermo) ; Dr. BOCCHINO, Fabrizio (INAF - Osservatorio Astronomico di Palermo) ; Mrs. BONITO, Rosaria (Consorzio COMETA) ; Dr. MICELI, Marco (Consorzio COMETA) ; Dr. SACCO, Germano G. (Consorzio COMETA) ; Mr. PAGANO, Paolo (Dip.S.F.A. - Universita` degli Studi di Palermo) ; Dr. ARGIROFFI, Costanza (Dip.S.F.A. - Universita` degli Studi di Palermo) ; Dr. YELENINA, Tatiana (INAF - Osservatorio Astronomico di Palermo)

Presenter : Dr. ORLANDO, Salvatore (INAF - Osservatorio Astronomico di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. ORLANDO, Salvatore

Submitted on Wednesday 21 November 2007

Last modified on : Wednesday 21 November 2007

Comments :

Talk presentation

Status : SUBMITTED

Track judgments :

Abstract ID : 13

Structural determination as a tool for prediction of mutagenic activity of nitro-polycyclic aromatic hydrocarbons

Nitro-polycyclic aromatic hydrocarbons (nitro-PAHs), are widespread environmental pollutants mainly produced from combustion processes and reactions between PAH and NOx. These nitroaromatic species, which are also present in the food chain, are recalcitrant to degradation and may exhibit high mutagenic and carcinogenic potencies [1]. It is well recognized that mutagenic activity of nitro-PAHs is strictly connected to the nitro group position with respect to the plane of the aromatic system [2]. There are indications showing that metabolic pathways for mutagenic activation of nitro-PAHs involve reductive and/or oxidative reactions which are preceded by diffusion and binding to enzymes [1]. Mutagenic activities are governed by molecular characteristics, which can be predicted with reasonable accuracy by computational methods.
In this work we illustrate data of structure, electronic and vibrational properties of nitro-PAH series of isomers of great environmental interest. The principal aim is to explore the effects of the substituent position on these physico-chemical properties and elucidate possible relationships with mutagenic potencies available from the literature. To this purpose semiempirical, ab initio SCF-MO and density functional theory methods have been used. Calculations were performed through the Grid-based architecture within the PI2S2-COMETA project.
The results show that, near planar isomers are the most stable forms and exhibit electron affinity, electric properties and their derivatives higher than those of the corresponding less planar forms. Present findings mainly support nitroreduction mechanisms and substrate-enzyme binding affinity as crucial pathways for the different mutagenic behaviour of the studied nitro-PAH isomers.

References
[1] Rosenkranz and Mermelstein, Mutat. Res., 1983, 114, 217-267.
[2] Li, Y. S.; Fu. P. P.; Church, J. S. J. Mol. Struct., 2000, 550-551, 217-223.

Primary authors : Prof. LIBRANDO, Vito (Dipartimento di Scienze Chimiche)

Co-authors : Dr. ALPARONE, Andrea (Dipartimento di Scienze Chimiche) ; Dr. MINNITI, Zelica (Dipartimento di Scienze Chimiche)

Presenter : Dr. ALPARONE, Andrea (Dipartimento di Scienze Chimiche)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. ALPARONE, Andrea

Submitted on Wednesday 21 November 2007

Last modified on : Wednesday 21 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 14

A new paradigm to design, implement and deploy Grid oriented application: a biomedical use case

Nowadays, many biomedicine studies are dealing with large, distributed, and heterogeneous repositories as well as with computationally demanding analyses. Complex integration techniques are more often required to handle this complexity, even if for small sized applications, when they are intrinsically distributed: this particular scenario is frequently found in medical informatics applications, where the health care provider is not a single institution but a collection of actors that play different roles in the territory. The BM Portal is a Grid oriented platform thought to promote collaboration and cooperation among scientists and healthcare research groups, enabling the remote use of resources integrated in complex software platform services forming a virtual laboratory. It is designed to host several medical use cases and it is able to deploy several analysis algorithms. A set of independent applications could be published on the portal and either single algorithms or a combination of them might be invoked by the user through a workflow strategy that can be defined via a web interface. The scope of this work is both to present a Grid application with its own medical use case and empathize the benefit that a new Design Paradigm based on Grid could provide to research groups spread in different geographically distant sites. The implementation of the BM Portal system is based on gLite, the Grid middleware developed in the context of the EU co-funded EGEE Project and involves Computation of Algorithms, Data Management, and Security aspects. Data Management capabilities are made up by the adoption of the GSAF software layer and the Data Violation is avoided thanks to the interoperation with the Secure Storage Service.

summary :

The BM Portal Project is carried out by the University of Genoa, Department of Communication, Computer and System Sciences, BIOLAB laboratory with the cooperation of some Italian SMEs AITEK, NICE, IR, UNICO and the INFN (Department of Catania) as well as the Official Training and Support Team of EGEE. It provides methods and tools for accessing distributed data in a secure way without moving files on the net, for managing related metadata, for building and maintaining catalogues, for submitting jobs on the Grid together with all the needed parameters.

Primary authors : Dr. PORRO, Ivan (DIST Dipartimento di Informatica Sistemistica e Telematica, Università degli Studi di Genova) ; Dr. TORTEROLO, Livia (DIST Dipartimento di Informatica Sistemistica e Telematica, Università degli Studi di Genova)

Co-authors : Dr. BARBERA, Roberto (University of Catania and INFN) ; Dr. CORRADI, Luca (DIST Dipartimento di Informatica Sistemistica e Telematica, Università degli Studi di Genova) ; Dr. FATO, Marco (DIST Dipartimento di Informatica Sistemistica e Telematica, Università degli Studi di Genova) ; Dr. PARISI, Salvo (IR engineering s.r.l.) ; Dr. VENUTI, Nicola (NICE S.r.l.) ; Dr. SCARDACI, Diego (Istituto Nazionale di Fisica Nucleare, Sezione di Catania) ; Dr. SCUDERI, Giordano (Unico Informatica S.r.l) ; Dr. SCIFO, Salvatore (Consorzio Cometa) ; Dr. CALANDUCCI, Antonio (Istituto Nazionale di Fisica Nucleare, Sezione di Catania)

Presenter : Dr. SCIFO, Salvatore (Consorzio Cometa)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. SCIFO, Salvatore

Submitted on Thursday 22 November 2007

Last modified on : Thursday 22 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 15

A Parallel solver for Reaction-Diffusion systems in computational electrocardiology

Recent advances in contemporary cardiac electrophysiology are progressively revealing the complex multiscale structure of the bioelectrical activity of the heart, from the microscopic activity of ion channels of the cellular membrane to the macroscopic properties of the anisotropic propagation of excitation and recovery fronts in the whole heart. In recent years, the experimental study of these complex phenomena has been accompanied by mathematical and physical modeling and numerical simulation. In particular, computation studies and numerical simulations have played an important role in electrocardiology. The most complete model of cardiac electrical activity is the Bidomain model. It consists of a system of two degenerate parabolic reaction-diffusion equations in 3D complex domain describing the intra and exsrtacellular potential in the cardiac muscle, coupled with a system of ordinary differential equations describing the ionic currents flowing through the cellular membrane resulting a large set of coupled ordinary differential equations. This model is computationally expensive because of the involvement of different space and time scales. The space discretization is based on the structured isoparametric Q_1 finite elements. In realistic three-dimensional models it is possible to have discrete problems with more than $\mathcal{O}(10^7)$ unknowns at every time step and simulations have to be run for several thousands of time steps. Large-scale simulations of the whole heartbeat using Bidomain model requires adaptive and parallel tools in order to reduce their high computational cost. While both tools can in principal be applied to both space and time, we have chosen to use adaptive methods in time and parallel solvers in space. Therefore we introduce a parallel solver for the Bidomain system and an adaptive time-stepping strategy that efficiently deals with the tree main phases (depolarization, plateau, repolarization) of a complete heartbeat. We use a se

Primary authors : Dr. BOSCARINO, Sebastino (Dipartimento di Matematica ed Informatica Catania)

Co-authors : Prof. PAVARINO, Luca (Dipartimento di Matematica Milano) ; Prof. RUSSO, Giovanni (Dipartimento di Matematica e Informatica Catania)

Presenter : Dr. BOSCARINO, Sebastino (Dipartimento di Matematica ed Informatica Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. BOSCARINO, Sebastino

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 16

Grid Secure Storage System

The security of the informations has always been one of the fundamental themes in the computing activity. With the advent of the Internet, in a Grid context of distributed computation, there is the possibility to access to a dynamic storage space, which is able to satisfy any requirement, also in fault-tollerance terms.
The data storage environement provided by a Grid architecture is a common environment, so that the possibility of having an exclusive access to the own data became an important requirement.
The present work has been oriented to the definition of an architecture, which permits to have the security of informations, security as the univocal possibility for user to access his own data.
To build this architecture, which permits the creation of a memorization space accessible only from the customer, we used cryptography technique with asymmetric key (RSA), and, to assure the efficiency and the usefulness of the system, the RSA has been associated to symmetrical cryptography (AES).
In our architecture, a layer is build over GFAL, providing a file service with crypto capability maintaining POSIX interface.
From user point of view gs3 library functions are similar to GFAL functions, all is traducted in a “gs3_*” call instead of “gfal_*” call.
Compared to POSIX interface the only difference consits on a initialize and finalize phases, necessary to setup the context for encryption (load key and open file system index).
Data security, as total user exclusive data access, is guaranted in memory, over the network and on storage because data are always encrypted. It is not possible to find unencrypted data except when the owner use them.
The encryption keys are stored into unswappable locations of central memory when they are used and always encrypted with user's public key on the distributed storage.
Time to file access are quite double than GFAL time access, this is due to build a file system structure on GFAL library and to data encryption.

Primary authors : CUNSOLO, Vincenzo Daniele (Universita' di Messina) ; Prof. SCARPA, Marco Lucio (Universita' di Messina)

Co-authors :

Presenter : CUNSOLO, Vincenzo Daniele (Universita' di Messina)

Track classification :

Contribution type : --not specified--

Submitted by : CUNSOLO, Vincenzo Daniele

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 17

GRID as a Bio-Informatic Tool in Plant Virology Investigations

The goal of TriGrid Project and PI2S2 is the creation of the first Sicilian regional computational Grid. In particular, it aims to build various software-hardware interfaces between the infrastructure and some scientific and industrial applications. In this context, we have integrated some among the most innovative computing applications in virology research inside these Grid infrastructure. Particularly, we have implemented in a complete workflow, various tools for pairwise or multiple sequence alignment and phylogeny tree construction (ClustalW-MPI), phylogenetic networks (SplitsTree), detection of recombination by phylogenetic methods (TOPALi) and prediction of DNA or RNA secondary consensus structures (KnetFold). This work will show how the ported applications decrease the execution time of the analysis programs, improve the accessibility to the data storage system and allow the use of metadata for data processing.

Primary authors : Dr. LOMBARDO, Alessandro (Consorzio Cometa, Dipartimento di Scienze e Tecnologie Fitosanitarie)

Co-authors : Dr. LANZALONE, Gaetano (INFN Sezione di Catania, Consorzio COMETA) ; Dr. MUOIO, Annamaria (INFN Sezione di Catania, Consorzio COMETA) ; Dr. IACONO-MANNO, Marcello (INFN Sezione di Catania, Consorzio COMETA)

Presenter : Dr. LOMBARDO, Alessandro (Consorzio Cometa, Dipartimento di Scienze e Tecnologie Fitosanitarie)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. LOMBARDO, Alessandro

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 18

GRID parallel simulations of a meshless method for Electromagnetic transients

The ever growing development of information and communication technology systems needs the use of ever more advanced computational tools able to predict, since the initial design stage, the compliance of the assigned EMC goals. Classical grid-based numerical methods can be successfully used in solving complex EM problems. However, the accuracy of numerical approximation depends on the connectivity laws among the grid nodes and on the geometry of the elementary cell. Moreover, when irregular geometry problems with diffuse non-homogeneity has to be treated, the grid construction could be a strong task; heavy computational resources have also to be used when locally adaptive schemes have to be introduced. A challenging way to overcome the previous difficulties could be the use of methods as those used in a hydrodynamic context.
The attractiveness and popularity of the method known as Smoothed Particle Hydrodynamics (SPH) are due to the evaluation of field functions and relative differential operators by means of an integral representation based on a suitable interpolating function. The integral representation is discretized by using a set of particles scattered in the problem domain.
A mesh-free particle method, based on SPH, adapted to solve Maxwell's equations in free space, is presented. The basic idea is to obtain numerical solutions for the partial differential equations describing the EM problem in time domain, by using a set of particles, considered as spatial interpolation points of the field variables. Irregular problems geometry and diffused non-homogeneous media can be modelled by an initial set of arbitrarily distributed particles. The program, written in C++ with MPI instructions, is executed on GRID environment.
The simulation shows a 6400 particle domain, representing a 2-D space of 0.8 x 0.8 m2. A Gaussian shaped pulse propagates freely into space. Absorbing conditions on boundaries are implemented by Berenger's PML (Perfectly Matched Layer).

Primary authors : Prof. ALA, Guido (Università degli Studi di Palermo) ; Prof. FRANCOMANO, Elisa (Università degli Studi di Palermo) ; Dr. SPAGNUOLO, Antonino (Università degli Studi di Palermo)

Co-authors :

Presenter : Dr. SPAGNUOLO, Antonino (Università degli Studi di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. SPAGNUOLO, Antonino

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 19

Finite Element electromagnetic analysis of Traveling Wave Tubes in GRID environment

The electromagnetic analysis of vacuum electronic devices, such as Traveling Wave Tubes (TWTs) leads to the management and the processing of huge quantity of data. In fact the need of accurate description of real 3-D geometries requires the generation of particularly refined meshes, above all in problem regarding either a full wave high frequency analysis or the tracement of particles trajectories.
Although the main goal of the simulation of a TWT is the electrons' tracement within the whole device, the electromagnetic analysis can be performed in a separate way for the three functional regions of the TWT: the electron gun, the interaction region, and the collector. From the numerical analysis viewpoint two different approaches can be followed: the former is a steady-state approach suitable for the electron gun and the collector regions; the latter is a full-wave approach required for the modeling of the interaction regions. Several solutions have been studied in order to solve this kind of problems, but only the possibility to adopt grid computing can lead to realistic simulations of real devices with reasonable computing time.
Consequently the know-how, earned during the development of specialized finite element codes for TWT, allows us to set up some algorithms able to solve this kind of problems in the GRID environment, in the framework of the PI2S2 project. In particular in the simulation of electron gun and collector, which requires the tracement of a high number of particles, the possibility of splitting the beam in a set of small beams and of launching these very time consuming tracement jobs on a computer grid allows us to drastically reduce the simulation time. The same approach can be also applied to the electromagnetic characterization of the helix slow wave structure which requires the eigenmode computation of the structure for different values (one for job) of phase shift of the RF electromagnetic field within a period of the slow wave structure.

Primary authors : Dr. POLLICINO, Giuseppe (Università di Catania)

Co-authors : Prof. COCO, Salvatore (Università di Catania) ; Dr. LAUDANI, Antonino (Università di Catania)

Presenter : Dr. POLLICINO, Giuseppe (Università di Catania) ; Prof. COCO, Salvatore (Università di Catania) ; Dr. LAUDANI, Antonino (Università di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. POLLICINO, Giuseppe

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 20

QoS management in Grid environments.

Providing and guaranteeing quality of service (QoS) of resources shared in a Grid environment are crucial challenges to obtain a flexible and dynamic services management. This represents the basic requirement to orient Grids towards concept of trading services, wherein providers and consumers of services and their relationship are clearly defined.

This paper focuses on modelling QoS in a gLite platform and designing suitable protocols to manage different kinds of constraints on supplying QoS guarantees.

The QoS management requires exploiting various middleware functionalities:

- (i) a first set of features are related to the management and negotiation of QoS parameters in a Grid; these functionalities have to be provided at collective layer;
- (ii) a second set is related to the low level tools to guarantee advance reservation, to drive the allocation and the scheduling of resources. This is obtained by working directly on Job Management System maintained on a Computing Element.

The highlighted features are strictly related: managing QoS at collective layer requires low level mechanisms and policies to monitor and guarantee the assignment of a resource to a job (or user) for a specific time slot. The QoS management protocols are built on the low level components to support choices related to negotiation and providing of guaranteed services.

This paper is divided into two parts. The first part deals with issues directly related to QoS management: defining the SLA related to a negotiation, clearifying the roles of participants to a negotiation, facing the issues related to the composition of services, and defining the mechanisms of monitoring QoS levels. The second part of the paper copes with the issues related to advance reservation and allocation: introducing scheduling policies in accordance with the requested QoS, performing the advance reservation of a resource, and introducing policies and mechanisms to improve the overall resource utilization.

Primary authors : Dr. ZITO, Daniele (DIIT) ; Dr. MORANA, Giovanni (DIIT) ; Prof. DI STEFANO, Antonella (DIIT)

Co-authors :

Presenter : Dr. ZITO, Daniele (DIIT)

Track classification :

Contribution type : --not specified--

Submitted by : Mr. ZITO, Daniele

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 21

GRID Technology to Treatment Planning Validation by Monte Carlo application

The international guidelines to implement a treatment planning system (TPS) in the clinical practice reports the necessity to validate it and to understand the limit of its application. The Monte Carlo is a useful method to valuate the TPS calculation, now clearly recognized by medical physics community. In our work we simulate the Elekta Gamma Knife unit, a radio-surgical device used to treat brain disorders, and a complete real clinical case. The simulation of machine complex geometry and the many radiation configurations used in the clinical application needs a long computational time run. In order to calculate the dose space distribution in a reasonable time, we exploited the GRID technology, using the production testbed available within the COMETA consortium. The implementation of this technology inside a GEANT4 Monte Carlo application don't need to change any line code but only the installation of the GEANT4 libraries on worked node. In comparison to the cluster use the implementation of the GRID technology need to change the methodology to split the work. The nodes that provide CPU cycles in a GRID system have more likely to vary greatly. A node might be a high-end supercomputer, or a low-end personal computer. In addition, these nodes are geographically widely distributed and not centrally manageable. A node may go down or became inaccessible without notice while it is working on its task. Therefore, a slow node might became the bottleneck of the whole computation if the assembly of the final result must wait for the partial result generated on this slow node. For this reason we used the N-out-of-M strategy, in this way more subtasks, than are needed, are actually scheduled, therefore, none of these subtasks will became a "key" subtask and we can tolerate at most M-N delayed or halted subtask. Our work shows that the GRID technology can represent in general a solution to a long calculation time of Monte Carlo simulations.

Primary authors : Dr. RUSSO, Giorgio (Consorzio COMETA)

Co-authors : Prof. BARBERA, Roberto (Department of Physics, University of Catania, Catania, Italy) ; Dr. CUTTONE, Giacomo (Laboratori Nazionali del Sud, Istituto Nazionale di Fisica Nucleare, Catania, Italy) ; Dr. GIORGIO, Emidio (Istituto Nazionale di Fisica Nucleare, Catania's Department, Catania, Italy) ; Dr. ROMANO, Francesco (Department of Physics, University of Catania, Catania, Italy) ; Dr. FORONI, Roberto (Gamma Knife Center, Borgo Trento Hospital, Verona, Italy) ; Dr. SABINI, Maria Gabriella (Department of Imaging, Cannizzaro Hospital, Catania, Italy)

Presenter : Dr. RUSSO, Giorgio (Consorzio COMETA)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. RUSSO, Giorgio

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 22

Parallelizing the Multi Layer Model to analyze microarray data

Nucleosomes are the fundamental repeating units of eukaryotic chromatin. Nucleosomes position can be regulated in vivo by multi-subunit chromatin remodeling complexes, influencing gene expression in eukaryotic cells. Alterations in chromatin structure, and hence in nucleosome organization, can result in a variety of diseases, including cancer, highlighting the need to achieve a better understanding of the molecular processes modulating chromatin dynamics [1].
To measure nucleosome positions on a genomic scale, a DNA microarray method, based on the Hidden-Markov Model (HMM), has been recently used to identify nucleosomal and linker DNA sequences on the basis of susceptibility of linker DNA [2]. However, this approach does not take into account the signal shape.
Here, a new method called Multi-Layer Model (MLM) [3] is presented and its parallelization on high performance computer system is outlined. We have shown [3] that it provides a better structural view of the input data when compared to the HMM on tiled microarray data of the Saccharomyces cerevisiae. Up to now optimized serial implementations of both HMM and MLM are not feasible to analyse very large sets of microarrays (e.g for 100 microarray of 4x10^5 spots requires about 3 days of computation on a 3GHz INTEL XEON). The parallelization of MLM is ongoing on 32 AMD OPTERON dual core processors (~1800 MHz clock). The signal derived from the microarray data is partitioned into 64 overlapping regions. Taking in account of the overhead due to the information exchange in the shared regions the estimated total computation time for a data set of 4x10^7 microarray spots is 120minutes (speedup of about 35).

[1] Jacobson S., Pillus L. (1999), Curr. Opin. Genet. Dev. (9), 175-184.
[2] Yuan G-C., et al. (2005), Science (309), 626-630.
[3] Corona D. et al. (2007), LNAI, KES (3), 862-869.

Primary authors : Prof. DI GESU', Vito (Univesrita' degli Studi di Palermo)

Co-authors : Dr. CORONA, Davide (Istituto Telethon Dulbecco, c/o Università di Palermo, Italy) ; Dr. LO BOSCO, Giosuè (Dipartimento di Matematica e Applicazioni, Università di Palermo, Italy) ; Dr. PINELLO, Luca (Dipartimento di Matematica e Applicazioni, Università di Palermo, Italy) ; Prof. YUAN, Guo-cheng (Department of Biostatistics , Harvard School of Public Health, USA)

Presenter : Prof. DI GESU', Vito (Univesrita' degli Studi di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. DI GESU', Vito

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 23

MHD modeling of Coronal Mass Ejections on GRID/COMETA high performance computing systems

The Coronal Mass Ejections are plasma clouds expelled from the Sun into the interplanetary medium. We study the propagation of shock waves in the solar corona generated during Coronal Mass Ejections by means of a numerical multi-dimensional MHD model. The model describes the MHD evolution of a compressible plasma in an ambient magnetic field including tensor thermal conduction, radiative losses as main physical effects.
We use the MHD version of the FLASH parallel hydrodynamic code with adaptive mesh refinement, originally developed at the University of Chicago (USA). The code is highly modular and made efficiently parallel with the Message Passing Interface library.
We analyze the diagnostic signatures of shock fronts generated by supersonic CME fragments detectable with the UltraViolet Coronagraphic Spectrometer on board the SoHO mission. To this aim we perform 3D MHD simulations of the shock propagation for the time it takes to cross the UVCS slit positioned at a distance of a few solar radii from the solar surface. In the presence of highly effective thermal conduction the simulation takes ~200000 time steps to cover ~1000 s of evolution. Considering a 3-D domain of 256x256x512 grid cells this kind of simulations requires thousands of hours of computer time and therefore high performance computing (HPC) systems. Sample simulations were run on the COMETA HPC system in Palermo using the FLASH code ported for execution on the GRID. We show simulation results and some implications for UVCS observations.

Primary authors : PAGANO, Paolo (University of Palermo/INAF Osservatorio Astronomico di Palermo)

Co-authors : Prof. REALE, Fabio (University of Palermo/INAF Osservatorio Astronomico di Palermo) ; Prof. RAYMOND, John C. (Harvard-Smithsonian Center for Astrophysics) ; Dr. ORLANDO, Salvatore (INAF Osservatorio Astronomico di Palermo) ; Prof. PERES, Giovanni (University of Palermo/INAF Osservatorio Astronomico di Palermo)

Presenter : PAGANO, Paolo (University of Palermo/INAF Osservatorio Astronomico di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : PAGANO, Paolo

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 24

Supernova remnants and grid computing at INAF-OAPa

We present the grid computing activities at the INAF-Osservatorio Astronomico Vaiana di Palermo to study supernova remnants. Our approach includes both high performance computing and data analysis. We present preliminary hydrodynamic simulations performed on the HPC system of the COMETA grid (Palermo) and simulating the evolution of the stellar fragments ("shrapnels") ejected in a supernova explosion. To this end we use the FLASH code, an advanced hydrodynamic code made parallel with MPI directives and ported on the grid. In particular, we address the Vela SNR, the nearest middle-aged SNR, where we recently detected X-ray emitting shrapnels. We also report on the analysis of X-ray spectra observed in the supernova remnant IC 443 with the XMM-Newton X-ray telescope. We use a "farming" approach, particularly suited for the grid, to rapidly analyze a huge amount of data.

Primary authors : Dr. MICELI, Marco (Consorzio COMETA - INAF OAPa)

Co-authors : Dr. BOCCHINO, Fabrizio (INAF-OAPa, Consorzio COMETA) ; Dr. ORLANDO, Salvatore (INAF-OAPa, Consorzio COMETA) ; Dr. TROJA, Eleonora (Universita' di Palermo, INAF-IASF Pa) ; Prof. REALE, Fabio (Universita' di Palermo, INAF-OAPa, Consorzio COMETA)

Presenter : Dr. MICELI, Marco (Consorzio COMETA - INAF OAPa)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. MICELI, Marco

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :
Oral presentation

Status : SUBMITTED

Track judgments :

Abstract ID : 25

Air shower simulation with CORSIKA for the GAW experiment

The cosmos and its evolution are studied using all radiation, in particular electromagnetic waves. The observable spectrum extends from radio waves to ultra-high energy gamma ray. One of the intents of the ground based gamma-ray astronomy is to obtain a sky survey in the TeV region. GAW, acronym of Gamma Air Watch, is an experiment whose main goal is explore the feasibility of large field of view Imaging Atmospheric Cherenkov Telescopes in this range of energy. It is an array of three relatively small Cherenkov telescopes that use a refractive optics system as light collector with a large field of view capability and use of single photoelectron counting as detector working mode.
To explore the capability of the telescope, its efficiency it is required a big amount of simulated air showers originated in different configurations; such a huge set of data has been simulated with CORSIKA taking advantage of the GRID services. The high statistics of simulated data will allow to properly test the methods of direction and energy reconstruction and to properly discriminate gamma ray from the cosmic-ray dominant background.

Primary authors : TORRESI, Domenico (Consorzio Cometa e IASF-Palermo/INAF)

Co-authors :

Presenter : TORRESI, Domenico (Consorzio Cometa e IASF-Palermo/INAF)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. TORRESI, Domenico

Submitted on Friday 23 November 2007

Last modified on : Thursday 29 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 26

X-ray emission from protostellar jets

In order to investigate the physical mechanisms governing the X-ray emission observed in Herbig-Haro (HH) objects, we developed a hydrodynamic numerical model (including thermal conduction and radiative losses) of a continuous supersonic protostellar jet propagating through an uniform medium. Such a model explains the detected X-ray sources as the emission from the shock formed by the interaction between the jet and the ambient medium. Albeit this moving shock model answers many of the previous questions, the physical scenario suggested by the observations seems more complex than expected. Here we briefly discuss new configurations of the jet/ambient system which may describe satisfactorily the observations. In particular, as a follow up of our work, we have started to explore new models, describing the interaction between a continuous supersonic jet and inhomogeneities of the ambient medium, and the auto-interaction between "blobs" ejected from the proto-star at different epochs, i. e. the scenario of a pulsed jet. This project takes advantage of the PI2S2 GRID infrastracture.

Primary authors : BONITO, Rosaria (Universita' di Palermo -- OAPa -- COMETA - INAF)

Co-authors : Dr. ORLANDO, Salvatore (INAF -- OAPa -- COMETA) ; Dr. FAVATA, Fabio (ESA) ; Prof. PERES, Giovanni (INAF -- OAPa --COMETA)

Presenter : BONITO, Rosaria (Universita' di Palermo -- OAPa -- COMETA - INAF)

Track classification :

Contribution type : --not specified--

Submitted by : BONITO, Rosaria

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :
Poster

Status : SUBMITTED

Track judgments :

Abstract ID : 27

Hydrogene molecule in intense laser fields

We study the single and double ionization yields and the dissociation dynamics of a one-dimensional two-electron molecule exposed to a laser pulse of intensity IL in the range 10^{14} - 10^{16} W/cm^2 and photon energy ħω_L = 3,18 eV for different pulse durations (from 2 to 16 optical cycles). The calculations are carried out in the case both of fixed and movable nuclei. At low IL the ionization curves have a power law shape IL^n that is interrupted by a knee at higher intensity. Such a knee structure is due to non-sequential ionization effects introduced by the electron-electron interaction. We investigate such a non-sequentiality as function of the pulse duration and compare the results with those obtained for He atom. The laser intensity strongly affects the nuclear dynamics of the molecule allowing for either vibrational motion or Coulomb explosion.
A temporal comparison between nuclear motion and electron ionization shows a strong correlation between nuclear dynamics and ionization yields and is co-responsible of the break of the power law. A detailed investigation of the emitted spectra associated to vibrational motion shows the presence of satellite peaks around odd harmonics, regularly spaced by the vibrational frequency. Such satellite peaks can be used as a tool for spectroscopic investigations.

Primary authors : Dr. CASTIGLIA, Giuseppe (Cometa) ; Dr. CORSO, Pier Paolo (Università deli studi di Palermo) ; Prof. DANIELE, Rosalba (Università deli studi di Palermo) ; Prof. FIORDILINO, Emilio (Università deli studi di Palermo) ; Prof. MORALES, Francesca (Università deli studi di Palermo) ; Dr. ORLANDO, Gianfranco (Università deli studi di Palermo) ; Prof. PERSICO, Franco (Università deli studi di Palermo)

Co-authors :

Presenter : Dr. CASTIGLIA, Giuseppe (Cometa)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. CASTIGLIA, Giuseppe

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 28

Access to EGEE computational grid using smart card and X.509 certificate

The User Interface (UI) of the gLite middleware allows the user to access the grid infrastructure using X.509 certificates. These certificates are stored in the file system of the machine, the User Interface is installed on. There are two ways for accessing the UI: the first consists in locally installing the UI on the owner's machine, while the second assumes that the UI is accessed remotely through a ssh tunnel.
The X.509 certificate stored in the UI contains a public key and a private key associated with the user. Both keys are encoded using the PEM certificate format. The private key must be accessed only from the user it is associated to. For the time being, this certificate may be subjected to possible fraudulent use by people logged to the UI (e.g. the system administrator).
The user certificate is used for generating a new temporary certificate (proxy certificate) that grants access to grid resources. This certificate is signed using the user's private key, stored in the X.509 certificate.
In this work we present our innovative solution for storing and using the private key in a secure way, when the UI in installed in the user's machine.
We have performed a new access method for interacting with the PEM X.509 certificate stored on a smart card. All the cryptographic operations on the user's certificate are performed in a secure way through the smart card itself. The signature of the proxy certificate is now produced by the smart card using the certificate it stores.
We have modified the source code of the voms-proxy module that generates the proxy certificate. With this hack, the module signs the proxy certificate using the smart card. In order to have a certificated signed, the voms module computes the hash of the proxy certificate. This sequence of data is sent to and processed by the smart card, according to the software procedures we have developed. Finally, the smart card encodes this data utilizing the private key it stores.

summary :

With the proposed solution, it is impossible to have multiple copies of a private key. In addition, each operation that needs to access the user's private key (i.e. the signature) is made on the smart card itself. This mechanism introduces an extra level of security in the EGEE accounting architecture, since it makes virtually impossible to retrieve the user's private key.
In order to pursue such goal, we have developed a dynamic library that includes a set of functions which allow to interact with the cryptographic device.

Primary authors : Dr. TRIOLO, Gianluca (Facoltà di Ingegneria Università di Messina)

Co-authors : Dr. TUSA, Francesco (Facoltà di Ingegneria Università di Messina) ; Prof. VILLARI, Massimo (Facoltà di Ingegneria Università di Messina) ; Prof. PULIAFITO, Antonio (Facoltà di Ingegneria Università di Messina)

Presenter : Dr. TRIOLO, Gianluca (Facoltà di Ingegneria Università di Messina)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. TRIOLO, Gianluca

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 29

3D finite element models of ground deformation and stress field in a viscoelastic medium

A 3D finite element model was carried out for evaluating the time dependent ground deformation and the stress change caused by a pressure source embedded in a viscoelastic medium. In volcanic areas, the presence of inhomogeneous materials and high temperatures produce a lower effective viscosity of the Earth’s crust that calls for considering the thermal regime of crustal volume surrounding the magmatic sources. A coupled thermo-mechanical numerical model allows for evaluating the temperature dependency of the viscoelastic solution. Both temperature distributions and ground deformation are firstly evaluated by solving an axi-symmetric problem to estimate the effects of thermo-viscoelastic response of the medium. Numerical results show that viscoelastic relaxation is responsible for significant time-dependent changes in long-term deformation and quasi-static stress field around the magmatic sources. These effects can be used for the interpretation of the spatio-temporal evolution of the seismicity associated with magmatic pressurization. In order to review the expected ground deformation on Mt Etna during the 1993-1997 inflation phase, we set up a fully 3D finite element model in which the real topography and seismic tomography were taken into account.

Primary authors : Dr. SCANDURA, Danila (INGV-sezione Catania)

Co-authors : Dr. CURRENTI, Gilda (INGV-sezione Catania) ; Dr. DEL NEGRO, Ciro (INGV-sezione Catania)

Presenter : Dr. SCANDURA, Danila (INGV-sezione Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. SCANDURA, Danila

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 30

NEMO Monte Carlo application

The opening of the high energy neutrino astronomy, that will provide new information about the most violent phenomena occurring in the Universe, requires detectors with volume of 1 km^3 or more. NEMO is an advanced R project for the constructor of a neutrino telescope in the deep Mediterranean Sea. Preliminary design for an underwater km^3 detector was performed on the basis of Monte Carlo simulations aimed at the optimization of the detector performance.
With the purpose to study the performances of a detector is necessary to simulate the detector response to astrophysical neutrino fluxes. Since the predicted neutrino fluxes are weak it is necessary to take into account the expected background noise. The main sources of noise are atmospheric muons and atmospheric neutrinos, produced by the interaction of the cosmic rays with the atmosphere.
The simulation code simulates the physic interaction of the cosmic rays with the atmosphere and the muon propagation in the atmosphere up to the sea surface and in water up to the detector. The simulation needs a wide statistic and big processing time, therefore GRID is the ideal tool to simulate this huge amount of events. The porting of simulation codes has been performed and first submission attempts have been carried out.

Primary authors : Dr. CALCAGNO, Rosalba (INFN-LNS)

Co-authors :

Presenter : Dr. CALCAGNO, Rosalba (INFN-LNS)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. CALCAGNO, Rosalba

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 31

3D MHD modelling of accretion processes in young stars with the PLUTO code

As shown by observations, many young stars (age < 5 Myr) harbour a circumstellar disk and accrete material from it through the star-disk magnetosphere. Despite the large amount of observational data in the infrared, optical and X-ray bands, different issues regarding star-disk interactions are yet open. Many of these issues need detailed physical models of the star-disk system for a better insight. To this end, we are developing a model describing the interaction between the accreting material and the star atmosphere, using the 3D MHD code PLUTO developed at the University of Torino . We plan to perform a set of demanding 3D simulations on the PI2S2 GRID infrastructure. Here, we describe the model, the results of some tests on the most recent PLUTO version , which we ported on the GRID, and the first runs of the PLUTO code performed on the PI2S2 GRID.

Primary authors : Dr. SACCO, Giuseppe Germano Sacco (Consorzio Cometa)

Co-authors : Dr. MIGNONE, Andrea (Dipartimento di Fisica - Universita' di Torino) ; Dr. MATSAKOS, Titos (Dipartimento di Fisica - Universita' di Torino) ; Dr. ARGIROFFI, Costanza (Dipartimento di Fisica - Universita' di Palermo) ; Dr. YELENINA, Tatiana (Osservatorio Astronomico di Palermo-INAF) ; Dr. ORLANDO, Salvatore (Osservatorio Astronomico di Palermo-INAF) ; Dr. PAGANO, Paolo (Dipartimento di Fisica - Universita' di Palermo) ; Prof. PERES, Giovanni (Dipartimento di Fisica - Universita' di Palermo) ; Prof. REALE, Fabio (Dipartimento di Fisica - Universita' di Palermo)

Presenter : Dr. SACCO, Giuseppe Germano Sacco (Consorzio Cometa)

Track classification :

Contribution type : --not specified--

Submitted by : SACCO, Giuseppe Germano Sacco

Submitted on Friday 23 November 2007

Last modified on : Friday 23 November 2007

Comments :

requested contribution type: Poster

Status : SUBMITTED

Track judgments :

Abstract ID : 32

The phenomenon of separation in 2D flows and a comparison with Boundary Layer theory

Turbulence is a phenomenon of great relevance in aerodynamics and fluid dynamics. The apparently chaotic/random behaviour of turbulent flows makes their study a challenging problem. The Navier-Stokes equations represent the basic mathematical model for a viscous flow. Typically turbulent flows are characterized by high Reynolds number. The presence of a solid boundary makes the problem even more difficult because, in this case, the onset of turbulence is due to unsteady separation of the flow from the body. The separation requires an accurate study of the behaviour of the flow in a thin region near the body, where a huge amount of vorticity is generated. The Boundary Layer theory predicts that close to the boundary, in the limit of infinite Reynolds number, the NS equations can be replaced by the simpler Prandtl's equations. Unsteady separation in Prandtl's equations is related to the blow up of the streamwise gradient of the velocity. The study of the flows at high Reynolds numbers requires an efficient numerical scheme and high computer precision (double double precision or quadruple precision). We use a spectral-finite differences scheme and, to resolve the NS equations close to the boundary, we adapt the computational grid to concentrate the grid points close to the wall. For Reynolds number of order 10^4-10^5 in 2D we find it necessary to use a resolution from 2048x2048 to 8192x8192 grid points. In this talk I'll show the separation phenomenon for a 2D flow past a cylinder and for a vortex array interacting with a rectilinear boundary. The high resolution we have used prevents the occurrence of numerical instability observed in literature close to separation time. NS solutions and Prandtl's solution show good agreement until the interaction between the viscous boundary layer and the outer flow begins. Some parameter such as the streamwise pressure gradient are analyzed to the determine when this interaction became relevant in the motion of the fluid.

Primary authors : Dr. GARGANO, Francesco (Dipartimento di Matematica ed Applicazioni)

Co-authors : Prof. SAMMARTINO, Marco (Dipartimento di Matematica ed Applicazioni) ; Dr. SCIACCA, Vincenzo (Dipartimento di Matematica ed Applicazioni)

Presenter : Dr. GARGANO, Francesco (Dipartimento di Matematica ed Applicazioni)

Track classification :

Contribution type : --not specified--

Submitted by : GARGANO, Francesco

Submitted on Saturday 24 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 33

TAA-Variation: In-silico experiments using the Sicilian Grid

Introduction to biological problem
Many viruses, bacteria and parasites have developed ways of evading immune system. Every year we are hit by new strains of influenza virus, which have mutated so they are no longer destroyed by the antibodies and T-cells that we developed to a previous infection.
This process is called Antigenic Variation.
Tumors also shed their tumor antigens or change their structure spontaneously to avoid immune system elimination.
Is it possible to predict the action of a vaccine against an antigenic variation?

Experiments Overview
SimTriplex uses 12 bit array to represent the Tumor Associated Antigen.
We considered the case of "1 and 2 bits" TAA variation, then we have 12 TAA-1bit and 67 TAA-2bits variated for mouse.
We simulated 4 Triplex-Therapy for each mouse and we run the simulations on a population of 100 mice.
The amount of submitted jobs is 4800 (TAA-1bit) plus 26800 (TAA-2bit), for a total of 31600 jobs.
We used an automatic procedure to submit pool of jobs (1340 for TAA-2bits and 240 for TAA-1bit) and to retrieve related output accessing from DIIT and INFN user interface. We submitted 7579 jobs to DIIT,8427 to DMI, 26997 to UNIPA, 18668 to INAF for a total of 61671 submissions, comprensive of pre-experiments test.
We retrieve output for 2,5G and we had 30511 successfull jobs on 31600,with a success rate of 96,553%
The experiments have been taken 10 days,in a single PC it would be required 658 days.
We used a MySQL Db to store datas and to analyze it.

First results
In silico results show that small antigenic variations of TAA are well covered by Triplex vaccine, in particular we obtained the following survival results on Triplex-Chronic vaccination: 81.75% for TAA-1bit and 81.5% for TAA-2bits. Results have to be validated by in vivo experiments.

summary :
In the current abstract we present a study of "TAA-Variation by In-silico experiments" using the using the Sicilian PI2S2-Grid.
Our in silico results show that small antigenic variations of TAA are well covered by Triplex vaccine, in particular we obtained the following survival results on Triplex-Chronic vaccination: 81.75% for TAA-1bit and 81.5% for TAA-2bits. These results, obtain with an heavy use of the Grid, have to be validated by in vivo experiments.

Primary authors : Dr. MASTRIANI, Emilio (University of Catania) ; Dr. PAPPALARDO, Francesco (University of Catania)

Co-authors : Dr. PENNISI, Marzio (University of Catania) ; Dr. CATANUTO, Roberto (University of Catania) ; Prof. MOTTA, Santo (University of Catania)

Presenter : Dr. MASTRIANI, Emilio (University of Catania) ; Dr. PAPPALARDO, Francesco (University of Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. MASTRIANI, Emilio

Submitted on Saturday 24 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 34

ImmunoGrid-PI2S2 Integration Architecture

We present here an overview of the system architecture designed to implement a solution for the integration of the Grid Web Server (IWS) and the PI2S2 infrastructure. ImmunoGrid (IG)is a simulation framework to model the Human Immune System utilising Grid technologies.
It also integrates other developed modules such as SimTriplex, C-ImmSim and other prediction models which simulate antigen processing and presentation. The main goal is to equip the ImmunoGrid web server with the capabilities to launch jobs also on the PI2S2-Grid, simplifying the submission process for the user. One of the main conventions followed during the development of ImmunoGrid was to allow access to a wide variety of resource through the same mechanism or interface. The IG project has developed a solution which is made up of a single web-based interface which is coupled with a job broker. This job broker/launcher accesses PI2S2, UNICORE or AHE via command line tools and web services via standard SOAP protocols. The main benefit of this setup is the ability to launch jobs on different Grid platforms, local resources and web services all through a single interface. The access to Grid services is made by a Virtual User Interface (VUI) The virtual machine is run by VM-Ware application installed on the Web server. The authentication step from IWS to the VUI is made by SSH without password using public key authentication with an agent. The credentials to use the Grid services is obtained by pk12 Gilda Certs. The integration between IWS and PI2S2-Grid is made by a pool of scripts that are able to:initialize the voms-proxy for the user, create the needed environment to submit job,submit the job,wait for the "Done" status of the job showing the current state of the job,and retrieve the output of submitted job.we are able to launch single or batch jobs onto the PI2S2 grid via gLite,Local clusters,computers and globus enabled resources via AHE.With additional development, we'll be able to sumbit MPI jobs

summary :

We present here an overview of the system architecture designed to implement a solution for the integration of the ImmunoGrid Web Server (IWS) and the PI2S2 infrastructure. One of the main conventions followed during the development of ImmunoGrid was to allow access to a wide variety of resource through the same mechanism or interface. The ImmunoGrid project has developed a solution which is made up of a single web-based interface which is
coupled with a job broker. This job broker/launcher accesses PI2S2, UNICORE or AHE via command line tools and web services via standard SOAP protocols. The main benefit of this setup is the ability to launch jobs on different Grid platforms, local resources and web services all through a single interface. In our opinion, a Grid solution is only as good as the interface provided to the users. For this reason we have concentrated on providing an easy to use, familiar web based interface which can be used to access every single resource on the Grid,
regardless of the middleware used to access it. This is achieved by the separation of the web interface from the job broker and the Grid implementations. Currently we are able to launch single or batch jobs onto the PI2S2 grid via gLite, Local clusters, computers and globus enabled resources via AHE and other resources via simple web services. With additional
development, we will also be able to submit MPI jobs to these resources.

Primary authors : Dr. MASTRIANI, Emilio (University of Catania) ; Dr. HALLING-BROWN, Mark (School of Crystallography - Birkbeck College)

Co-authors : Prof. SHEPHERD, Adrian (School of Crystallography - Birkbeck College) ; Prof. MOTTA, Santo (University of Catania)

Presenter : Dr. MASTRIANI, Emilio (University of Catania) ; Prof. SHEPHERD, Adrian (School of Crystallography - Birkbeck College)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. MASTRIANI, Emilio

Submitted on Saturday 24 November 2007

Last modified on : Saturday 24 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 35

Structure-dynamics-function of proteins: Molecular Dynamics simulations of Myoglobin in water and complex solvents

Standard Molecular Dynamics simulations allow studying medium size protein/water systems (Natoms < 50000) on the nanosecond time scale. Atomistic simulations on longer scales, or in complex solvent (G. Cottone, J. Phys. Chem. B 2007, 111, 3563) in which the the ergodic properties of the system are sizably reduced, require the use of massive calculation to obtain a reliable estimate of structure/dynamics properties.
It appears useful to describe the simulated system as related to a few important degrees of freedom (or collective variables, CVs) and a much larger set of degrees of freedom acting as a thermal bath. The Free Energy (FE) landscape underlying the CVs has a large number of valleys and saddle points, separated by higher barriers than the available thermal energy. Recently, numerical techniques have been developed and exploited to explore the FE even at low temperatures via an artificial sampling of the dynamics of the CVs, suitable coupled to the dynamics of the rest of the system (L. Maragliano et al., Chem. Phys. Lett., 2006, 426, 168).
The technique is exploited to study the carbon-monoxide (CO) diffusion inside Myoglobin (Mb), in water solutions; it is well known that the protein matrix control the ligand funnel to/from the solvent, in a time scale of hundreds of nanoseconds or longer (F. Schotte et a, Science, 2003,300,1944).
Preliminary results from this study are here presented. The system is formed by a Mb molecule, the CO ligand and explicit water. Several short simulations (hundred of picoseconds) are independently performed, corresponding to different dynamical parameters of the CVs; this allows the ligand exploring different regions inside the protein matrix, and eventually escaping to the solvent. At the end, the procedure will allow to represent the FE space of CO diffusion inside Mb as a three dimensional map, from which a complete picture of barriers, binding sites and pathways to/from the external solvent would be available.

Primary authors : Dr. COTTONE, Grazia (DSFA, Universita' di Palermo)

Co-authors : Prof. CORDONE, Lorenzo (DSFA, Università di Palermo) ; Dr. MARAGLIANO, Luca (Courant Institute of Mathematical Sciences) ; Prof. VANDEN-EIJNDEN, Eric (Courant Institute of Mathematical Sciences) ; Prof. CICCOTTI, Giovanni (Dipartimeto di Fisica, UNiversità di Roma La Sapienza)

Presenter : Dr. COTTONE, Grazia (DSFA, Universita' di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. COTTONE, Grazia

Submitted on Saturday 24 November 2007

Last modified on : Saturday 24 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 36

Grid Time Dependent Monte Carlo Simulations of Nano Catalytic Systems

An algorithmic time dependent Monte Carlo (tdMC) model, developed to study bi- and three-phase reactions, involving the production of light petrol- and fine-chemical derivatives on nano-structured catalysts, is reported with preliminary simulation results on the reaction test, namely the but-2-ene isomerization on Pd/H-ZSM-5 supported zeolites, used to develop the here ANSI C 89 code.

The code is based on a quantum-stochastic approach, in which the dynamical tdMC simulations use, preliminarily gained, quantum-chemistry (qc) information. The latter gives local insight on the system while the former reconstructs – starting from the microscopic details – bulk properties that can be compared with similar laboratory results.

The approach, which should be able to reproduce the inmost physical and chemical characteristics of heterogeneous system, accounts for events as absorption, diffusion and desorption, occurring on surfaces also embedded in 3-D frameworks. These are generated by subroutines, which, using experimental or calculated structural data, construct a matrix, representing the catalytic material, which can be used in the code.

The results on the but-2-ene isomerization, obtained by using DFT structural and kinetic data calculated at B3LYP/6-31G**+LANL2DZ level through the Gaussian 03 program package, are in well agreement with our model-experimental results obtained in the frame of the NANOCAT project, showing the heuristic properties of the approach.

Besides the simulations of real or fictitious systems, the qc-tdMC code can be used to:
- manage the effects of temperature gradients and hindrance interactions,
- validate the local qc information,
- find exotic parameters, characterizing heterogeneous interface processes.

For these applications, which we are now attempting, recursive ODEs solutions and fit procedures, easily implemented by parallel programmation in the qc-tdMC code, are required while GRID technology strongly enhance their run performances.

Primary authors : Prof. DUCA, Dario (Dipartimento di Chimica Inorganica e Analitica "S. Cannizzaro")

Co-authors : Dr. BALDISSIN, Gael (Dipartimento di Chimica Inorganica e Analitica "S. Cannizzaro")

Presenter : Dr. BALDISSIN, Gael (Dipartimento di Chimica Inorganica e Analitica "S. Cannizzaro")

Track classification :

Contribution type : --not specified--

Submitted by : Prof. DUCA, Dario

Submitted on Saturday 24 November 2007

Last modified on : Saturday 24 November 2007

Comments :

Scientific Results Obtained Using Grid Technology

Status : SUBMITTED

Track judgments :

Abstract ID : 37

Industrial Fluid Dynamics in a GRID environment: case studies

Opening a GRID infrastructure to industrial users is an essential aspect of current GRID research and development towards the long term sustainability of the infrastructure.

Within the PI2S2 project, the SCIRE consortium role is to bring in the industrial consultancy experience and real industrial test cases to the GRID infrastructure.
We are going to present some computational fluid dynamics test cases mainly (but not exclusively) from the automotive industry.
Specifically we will present a detailed analysis of some aeroacoustics test cases for the evaluation of the noise signature and shape optimization of some automotive components.
The main objective of our work at this stage is to set up a reproducible methodology that can be transferred to industrial end-users whoa re experts in their domain, but not familiar with GRID technology, and to evaluate the impact on the design cycle, devising different business cases for various user scenarios, both in terms of time to results and in terms of accuracy.

Primary authors : Dr. FILIPPONE, Salvatore (Università ROma Tor Vergata)

Co-authors : Mr. TESTA, Mario (NUMIDIA s.r.l.) ; Prof. BELLA, Gino (Università ROma Tor Vergata)

Presenter : Dr. FILIPPONE, Salvatore (Università ROma Tor Vergata)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. FILIPPONE, Salvatore

Submitted on Saturday 24 November 2007

Last modified on : Wednesday 28 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 38

High Performance Computing for Design Space Exploration: A Case Study

In this paper we present a case study of Design Space Exploration (DSE) of a complex highly parameterized VLIW based System-on-a-Chip (SoC) platform.
In this case study we test the use of High Performance Computing (HPC) as a viable solution to tackle with DSE related problems. Experiments on a set of multimedia applications are given, demonstrating that it is possible to achieve up to one order of magnitude reduction in exploration time.

summary :

The increasing complexity of modern electronic systems, together with increasing time-to-market pressure, has led the embedded system industry to adopt pre-designed System-on-a-Chip (SoC) architectures known as SoC platforms. From one hand a SoC platform has to be general enough to be used in different application scenarios, so as to offset the design, verification and manufacturing costs involved. On the other hand, it has to be specific in order to meet the typical design constraints like silicon area, performance, and power dissipation. A SoC platform is typically made up of a number of parameterized
intellectual property (IP) cores communicating via an interconnection system which is also parametric. Each parameter has an associated range of discrete values within which it can vary. When a value is set for each parameter the system is said to have been configured. As the number of possible configurations that can be mapped on a parametric system is equal to the product of the cardinalities of the ranges of variation for each parameter, the size of the space of configurations grows exponentially as the number of parameters increases. The capacity to find a good trade-off between the requirements, respecting the design constraints, is the challenge now facing Design Space Exploration (DSE) methods. However each visited system configuration must be evaluated by means of a system-level simulation which typical is a computational intensive
task.
In this paper we present a case study of design space exploration of a complex highly parameterized VLIW based SOC platform. The 18 free parameters which characterize the platform span a design space of over 10^9 system configurations. Even considering an evaluation time of a few seconds for each configuration, exhaustive exploration would take hundreds of years on single machine. We test the use of High Performance Computing (HPC) as a viable
solution to tackle with DSE related problems. For the best of our knowledge, all the DSE techniques proposed in literature relies on the use of a computation infrastructure which is typical mono-processor in nature. We believe that the availability of distributed or grid computational infrastructures should be exploited and analyzed in the context of DSE to cope with the ever growing increase in complexity of current and next generation SOC platforms.

Primary authors : Dr. DI NUOVO, Alessandro (DIIT - Università degli Studi di Catania)

Co-authors : Dr. PATTI, Davide (DIIT - Università degli Studi di Catania) ; Dr. DE FRANCISCI MORALESI, Gianmarco (DIIT - Università degli Studi di Catania) ; Dr. PALESI, Maurizio (DIIT - Università degli Studi di Catania) ; Prof. CATANIA, Vincenzo (DIIT - Università degli Studi di

Catania)

Presenter : Dr. DI NUOVO, Alessandro (DIIT - Università degli Studi di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. DI NUOVO, Alessandro

Submitted on Saturday 24 November 2007

Last modified on : Saturday 24 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 39

Airfoils Characterization by means of CFD Simulations in GRID Environment

The present paper deals with the implementation of a Computational Fluid Dynamic (CFD) based application for airfoil characterization by means of supercomputing GRID system. Such results are really useful to advance possible profiles solutions for the blades of high-efficiency micro-wind turbines.
In order to build up a database of the lift and drag coefficients versus air speed of different profiles, CFD running have been carried out using GRID trivially-parallel method.
Thus, the implemented database represents a useful reference for the machine designer, allowing him to chose the proper solution to shape the rotor blades of wind turbines.
In more details, each job run calculate specific airfoil performance varying air speed, as well as air speed inclination with reference to the profile cord.
The job uses the trivially parallel method to evaluate the complete airfoil performance and MPI run for each specific airfoil performance point.
Thus, the implemented method allows to run the complete airfoil performance curve using less global time than using a serial approach.

Primary authors : Dr. BRUSCA, Sebastian (DIIM - University of Catania)

Co-authors : Dr. GIUFFRIDA, Antonio (DIIM-University of Catania) ; Prof. LANZAFAME, Rosario (DIIM-University of Catania)

Presenter : Prof. LANZAFAME, Rosario (DIIM-University of Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. BRUSCA, Sebastian

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 40

Use of GRID technologies with ALICE experiment

ALICE (A Large Ion Collider Experiment) is one of the four experiments installed at the LHC (Large Hadron Collider) facility at CERN, and will start to take data in 2008. This experiment is specifically designed to study the Quark-Gluon Plasma in heavy ion collisions. As for other LHC experiments, ALICE requires huge resources in terms of CPU and storage capacity. For this reason its computing model relies strongly on GRID infrastructure, by means of which the data will be stored and analysed. To fullfill its specific requirements, the ALICE collaboration has developed its own middleware, AliEn, that provides an full environment for data management and job submission and monitoring.
We first give an overview of ALICE experiment and its computing model; we then introduce its dedicated middleware AliEn and finally present the use of ALICE GRID resources from a user (physicist) point of view.

Primary authors : Dr. VERNET, Renaud (Consorzio COMETA)

Co-authors :

Presenter : Dr. VERNET, Renaud (Consorzio COMETA)

Track classification :

Contribution type : --not specified--

Submitted by : Dr. VERNET, Renaud

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 41

Three-dimensional meshes segmentation and partitioning

Segmentation and partitioning of three-dimensional meshes are common tasks in many fields of research. In particular, we are interested in surface segmentation by using geometrical and differentiable properties. The general graph partitioning problem is NP, thus these problems are computational expensive as the quality and size of models increase. Generally, partitioning and dynamic load balancing of processors are performed by considering information not directly available on open distributed systems as GRID and HPC (e.g. the processors assignment policy, the memory availability, the communications costs). This contribution presents a three-dimensional segmentation method and a general parallel framework for local mesh analysis.

The serial implementation considers the edges as the intersection of smooth surfaces and assigns to each arc of the mesh a weight proportional to the local bending of the surface:

- Each arc is labeled with a bend degree to calculate the slope of the local curvature of the surface of the object.

- The resulting candidate edges are connected into patches, that satisfy geometric and perceptive properties.

- Post processing as patch dilation and thinning improves the appearance of the final result.

The main features of the parallel framework are:

- The partition is obtained through a Inertial Moment Bisection technique.

- A hierarchical approach is used and the communication pattern of processors is modeled as a binary tree.

The following percentages refer to the average time spent on a high resolution mesh with respect to the serial implementation:

Serial: 100%
2 CPUs: 19%
4 CPUs: 16%
8 CPUs: 13%
16 CPUs: 11%

Primary authors : CIPOLLA, Marco (Dipartimento di Matematica e Applicazioni. Universita' di Palermo)

Co-authors : DI GESU', Vito (Dipartimento di Matematica e Applicazioni. Universita' di Palermo) ;
VALENTI, Cesare (Dipartimento di Matematica e Applicazioni. Universita' di Palermo)

Presenter : CIPOLLA, Marco (Dipartimento di Matematica e Applicazioni. Universita' di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : VALENTI, Cesare

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 42

Non-parametric parallel Harris-affine detector

Feature detector algorithms are fundamental for many advanced image processing methodologies like 3D reconstruction, object detection and mosaicing. A new non-parametric Harris-affine detector is introduced here. This is an image processing algorithm for extracting a particular kind of image features, known as Harris corners. The new proposed implementation automatically tries to select best features with respect to local-to-global image properties in a scale-space domain: different image knowledge can be acquired at different observation scales simulated by Gaussian convolution. The proposed algorithm consists of the following steps computed for each scale: image enhancement and feature mask computation by using z-scored local windows, simple Harris-corner extraction and selection, and refinement of the final result by an iterative procedure computed on every feature.
The algorithm uses statistical filters with a variety of kernel size, which cause a bottleneck on a serial implementation. Time required to process different data on different scales, but also in the same one, is highly variable; thus an unusual MPI implementation has been developed to avoid unbalanced computational workload distribution among different processors. Multithreaded server-client MPI routines have been created to dynamically distribute workload to working threads on every processor. This distribution strategy has been based on statistics obtained from communication with other client threads that run on different processors. Only the server and client threads are allowed to communicate between different processors; eventually, they can modify the working threads status.
The following percentages refer to the average time with respect to serial the implementation:
Serial: 100%
2CPU: 53%
4CPU: 39%
8CPU: 22%
16CPU: 15%
24CPU: 9%

Primary authors : BELLAVIA, Fabio (Dipartimento di Matematica ed Applicazioni, Universita' di Palermo)

Co-authors : VALENTI, Cesare (Dipartimento di Matematica ed Applicazioni, Universita' di Palermo) ; TEGOLO, Domenico (Dipartimento di Matematica ed Applicazioni, Universita' di Palermo)

Presenter : BELLAVIA, Fabio (Dipartimento di Matematica ed Applicazioni, Universita' di Palermo)

Track classification :

Contribution type : --not specified--

Submitted by : BELLAVIA, Fabio

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 43

A strategy for balancing resources handling replica files

When accessing data files on a Grid environment, users are free to choose one among the available replica. Since, it is unknown how the dynamic of requests coming from users will vary at runtime, the Grid environment could experience overload in some hosts.

We propose a strategy to dynamically suggest users which host provides the shortest response time when having to access data files. This strategy takes into account that delays on the communication of data about usage of replicas could be common because of the large distance among parts of the network. Hence, the proposed strategy is adaptive, moreover, an a priori analysis of delays that might occur allows a degree of confidence to be calculated for the suggestions.

Primary authors : TRAMONTANA, Emiliano (Dipartimento di Matematica e Informatica, Universita' di Catania)

Co-authors : PAPPALARDO, Giuseppe (Dipartimento di Matematica e Informatica, Universita' di Catania) ; GIUNTA, Rosario (Dipartimento di Matematica e Informatica, Universita' di Catania) ; MESSINA, Fabrizio (Dipartimento di Matematica e Informatica, Universita' di Catania) ; TOSCANO, Luigi (Dipartimento di Matematica e Informatica, Universita' di Catania)

Presenter : TRAMONTANA, Emiliano (Dipartimento di Matematica e Informatica, Universita' di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : TRAMONTANA, Emiliano

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 44

Using the Pi2S2 Grid to simulate peer-to-peer large-scale Grid environments

In a very large scale distributed environment, a "peer-to-peer" model gives many advantages over a conventional hierarchical one, in terms of reliability, efficiency and scalability. In such environments, new resource finding algorithms have to be used, which exploit the decentralised architecture by means of a classical P2P "request-forwarding" policy. We propose an algorithm based on a suitable navigation strategy that forwards a request from node to node, until one is found which offers the desired amount of resources. Strategies envisaged are based on "spatial computing" concepts, whereby the overlay network, with its nodes labelled by the amount of available resources, is viewed as a three-dimensional surface. On it, valleys represent areas more endowed with resources. The proposed navigation strategies result in following a path leading to the global resource maximum or close to it.

The proposed approach is experimentally evaluated by means of a Java-based software simulator, which has been run on the powerful PI2S2 project's Grid, for the sake of cutting execution times and allowing several test suites to be run at once. The simulator accepts an initial configuration file whence all job-related files are automatically produced, i.e. the JDL file, the JAR Java bytecode and additional parameter files. These are all that is needed to run extensive simulation experiments.

Several combinations of the sensitive parameters (navigation strategies, number of nodes, their workload, the origin (node) of the resource request, etc.) have been tested. Several test cases have been produced, converted into independent jobs and submitted to the grid. The results gathered, which will be reported in the paper, show the effectiveness of the algorithm, and also help assessing its sensitivity to the chosen initial parameters. The computational power made available by the Pi2S2 Grid has turned out to be crucial to securing these valuable experimental results.

Primary authors : Prof. PAPPALARDO, Giuseppe (Dipartimento di Matematica e Informatica, Università di Catania) ; SANTORO, Corrado (Dipartimento di Matematica e Informatica, Università di Catania) ; DI STEFANO, Antonella (Dipartimento di Ingegneria Informatica e delle Telecomunicazioni, Università di Catania) ; MESSINA, Fabrizio (Dipartimento di Matematica e Informatica, Università di Catania) ; TOSCANO, Luigi (Dipartimento di Matematica e Informatica, Università di Catania)

Co-authors :

Presenter : Prof. PAPPALARDO, Giuseppe (Dipartimento di Matematica e Informatica, Università di Catania)

Track classification :

Contribution type : --not specified--

Submitted by : Prof. PAPPALARDO, Giuseppe

Submitted on Sunday 25 November 2007

Last modified on : Sunday 25 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 47

S-Sicilia – a Grid-based infrastructure for business applications

It is commonly recognised that nowadays a large part of business processes are carried out through the Internet, and thereby many companies need to enable their businesses to use this mean in a secure, reliable and performing way. Different technologies have been used so far for such a purpose, although two have emerged as the most appropriate to offer more advanced services with reduced costs: Web services along with the SOA paradigm and the Grid. The combination of those two paradigms will leverage the emerging concept of service oriented market. Business relationships will be regulated by business contracts which will contain the level of the services in terms of quality, reliability, time constraints, responsibility, penalties and methods of payment. The aim of the S-Sicilia project, a 2-year collaboration between Oracle and the COMETA consortium, is to setup a business infrastructure Grid-based able to make the aforementioned scenario real. The infrastructure consists of first the SLA engine which aims to provide the mechanisms to handle business contracts (SLAs) on which B2B and B2C relationships are based. This module acts from one side as the interface with customers, providing access to the whole infrastructure. On the other side, it interfaces with the lower Grid infrastructure, which deal with the low level resources. Second the QoS engine, that works at the Grid layer, providing the QoS functionalities that the Grid infrastructure does not provide natively. Decisions are taken by considering computation (CPU and RAM), storage and network resources. It also provides a prediction service to the SLA engine, that gives an estimate on the particular service upon it's been enquired. Third the Virtualization, which allows running applications with particular requirements, offering isolation and security mechanisms complementary to operating system, customization and encapsulation of entire application environments, and support for legacy applications.

Primary authors : RAGUSA, Carmelo (Univ. of Messina) ; PULIAFITO, Antonio (Univ. of Messina)

Co-authors :

Presenter : RAGUSA, Carmelo (Univ. of Messina)

Track classification :

Contribution type : --not specified--

Submitted by : BARBERA, Roberto

Submitted on Monday 26 November 2007

Last modified on : Monday 26 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 48

Computational challenges in high-energy astrophysics

The study of many astrophysical phenomena involves highly nonlinear physical processes and therefore has become possible only after the advent of reliable fast computational tools. Today supercomputers and grid networks have become the basic instruments not only to analyze data and scan archives and databases, but also primarily to elaborate and test physical models involving complex phenomena. In this review I shall concentrate on some aspects of the field of high-energy astrophysics that require large scale computations due to the complexity of the physical processes involved. They aim to understand fast dynamical phenomena, like stellar collapse, accretion onto black holes, launching of relativistic jets; while many evolutionary phases of astrophysical objects are characterized by a relatively slow pace and can be studied through quasi-stationary equilibrium models, high-energy phenomena involve a strong link between dynamics and microphysics and require a non-equilibrium treatment. Several research groups in Italy have developed an internationally recognized expertise in these studies, especially after the availability of national and local supercomputer centers and their linkage with international grids.

Primary authors : FERRARI, Attilio (Univ. di Torino e Univ. di Chicago)

Co-authors :

Presenter : FERRARI, Attilio (Univ. di Torino e Univ. di Chicago)

Track classification :

Contribution type : --not specified--

Submitted by : BARBERA, Roberto

Submitted on Thursday 29 November 2007

Last modified on : Thursday 29 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 49

The Organic Grid: designing self-organizing computations based on the principle of emergence

We propose to use self-organization as a model for the programming of very large collections of heterogeneous computing resources. In a representative application, this model is the base for the design of a truly general purpose version of desktop grids, able to run high performance computing (HPC) applications that are too large for current supercomputers. Self-organizing computation based on emergent design is a type of computation in which the desired global organization of the system emerges from local and long range interactions among component parts. This concept is very general and has been applied in the past to fields such as artificial neural networks, adaptive systems, connectionist learning, organization of social insects, and biological networks.

In our approach, a large scale computation is divided into self-contained independent units, each provided with its own autonomous behavior; only local information, or a modest amount of
non-local information, is used by each unit to take the decisions needed to carry out the computation. Allowing global coordination to emerge from a distributed collection of components addresses the shortcomings associated with centralized coordination, such as i) scalability (a central coordinator can become the performance bottleneck), ii) robustness (if the coordinator fails, the whole systems halts), and iii) control overhead (the overhead incurred in gathering and updating the information about the system).

In this project we are investigating the theoretical foundations of self-organization applied to HPC. The challenges of developing a theoretical framework for the self-organizing approach can be summarized by the two following fundamental questions: given a description of the local behavior, is it possible to make predictions about the emerging global organization of computation? Is it possible to provide design guidelines for the local behavior needed to achieve the emergence of a desired global behavior?

Primary authors : LAURIA, Mario (TIGEM)

Co-authors :

Presenter : LAURIA, Mario (TIGEM)

Track classification :

Contribution type : --not specified--

Submitted by : BARBERA, Roberto

Submitted on Thursday 29 November 2007

Last modified on : Thursday 29 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 50

The Grid paradigm in Italy

In this presentation the status of grid activities going on in Italy will be presented.

Primary authors : ANDRONICO, Giuseppe (INFN) ; MAZZUCATO, Mirco (INFN)

Co-authors :

Presenter :

Track classification :

Contribution type : --not specified--

Submitted by : BARBERA, Roberto

Submitted on Thursday 29 November 2007

Last modified on : Thursday 29 November 2007

Comments :

Status : SUBMITTED

Track judgments :

Abstract ID : 51

The COMETA Project

In this presentation the status of the PI2S2 Project and the activities of the Consorzio COMETA will be presented.

Primary authors : BARBERA, Roberto (Univ. di Catania e INFN)

Co-authors :

Presenter : BARBERA, Roberto (Univ. di Catania e INFN)

Track classification :

Contribution type : --not specified--

Submitted by : BARBERA, Roberto

Submitted on Thursday 29 November 2007

Last modified on : Thursday 29 November 2007

Comments :

Status : SUBMITTED

Track judgments :