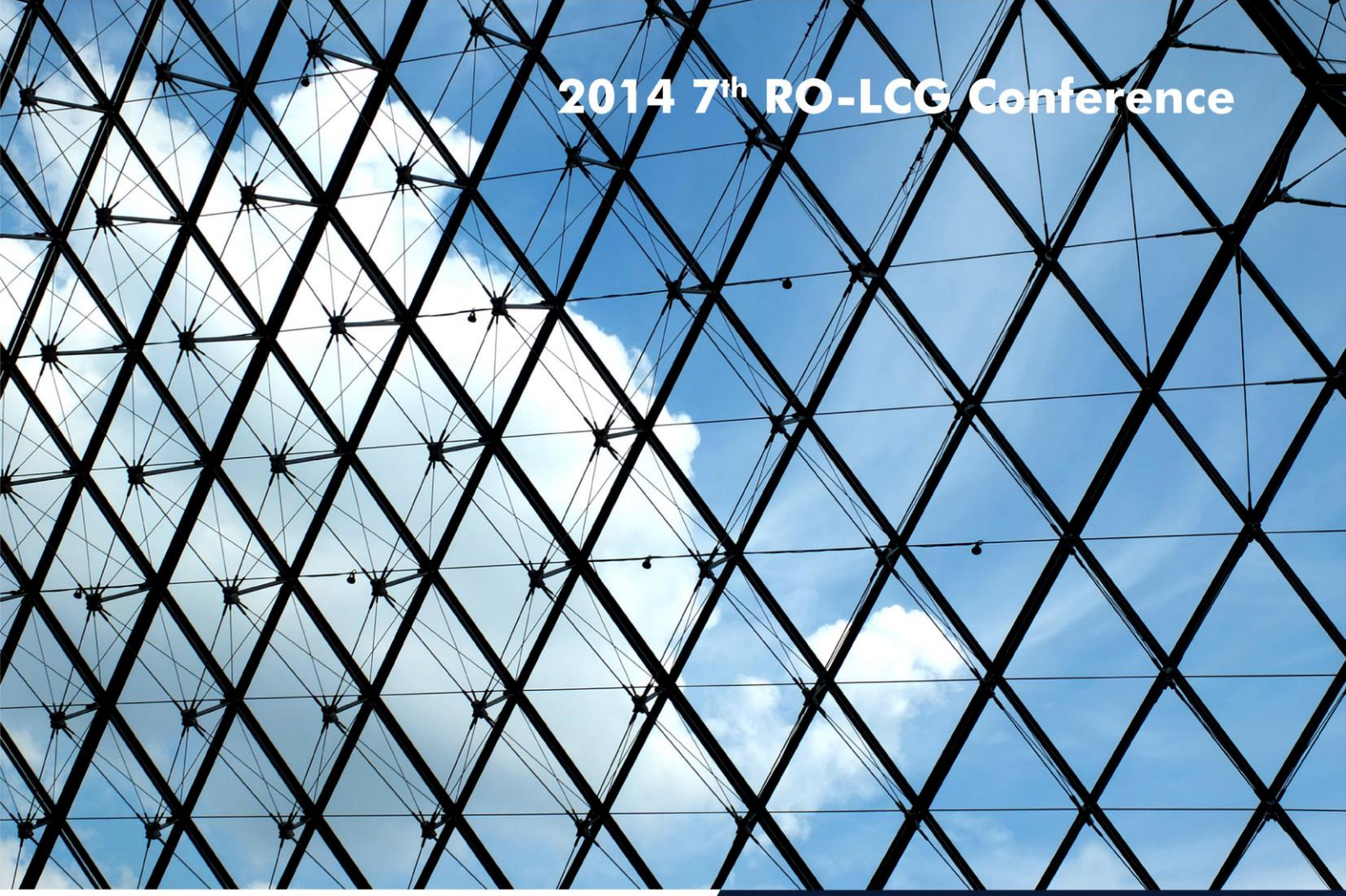

2014 7th RO-LCG Conference

GRID CLOUD

AND HIGH-PERFORMANCE COMPUTING IN PHYSICS RESEARCH

Book of Abstracts

3-5 November 2014 Bucharest-Magurele, Romania

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HORIA HULUBEI NATIONAL INSTITUTE FOR RESEARCH AND DEVELOPMENT
IN PHYSICS AND NUCLEAR ENGINEERING

Grid, Cloud, and High-Performance Computing in Physics Research

3-5 November 2014

Bucharest-Magurele

BOOK OF ABSTRACTS

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Grid, Cloud, and High-Performance Computing in Physics Research

Bucharest-Magurele, 2014

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WELCOME MESSAGE

Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH) and the Organizing Committee cordially welcome you to the RO-LCG 2014 Conference, "*Grid, Cloud, and High-Performance Computing in Physics Research*".

The Conference is organized by the Department of Computational Physics and Information Technology of IFIN-HH and the RO-LCG Federation. RO-LCG 2014 is held under the aegis of IEEE – Romania Section, and sponsored by the Ministry of National Education, the Academy of Romanian Scientists, ARCAS Association, DELL Romania, FUJITSU Romanian Branch, and Q-East Software.

The Conference continues the 8-year tradition of annual meetings established since the foundation of the RO-LCG Federation, as a forum for the discussion of recent developments in the application of advanced computing technologies in scientific research. This year, the topics of the Conference cover areas such as e-infrastructures for large-scale collaborations, software tools development, LHC Computing Grid, high-performance computing in scientific research, algorithms and applications development.

We hope the Conference will stimulate fruitful communication between the participants and opportunities for initiating new collaborations.

We whish you to enjoy the Conference and to have a nice stay in Bucharest!

Dr. Mihnea Alexandru Dulea

Chairman of the Organizing Committee

Prof. Nicolae Victor Zamfir

Director General IFIN-HH

PROGRAM

03.11.2014		
8:45	Transportation from IBIS Hotel	
9:00	REGISTRATION	
10:00	Welcome Address	Prof. Nicolae Victor ZAMFIR
10:05	Conference overview and logistics	Dr. Mihnea DULEA
Session: e-Infrastructures for Large-Scale Collaborations (10:10-13:30)		
10:10	Contributions to the advanced computing for scientific research in Romania	Dr. Mihnea DULEA
10:30	Development of distributed computing technologies and BigData in LIT-JINR	Prof. Vladimir KORENKOV
11:00	Overview of Grid and High Performance Computing activities in Serbia	Vladimir SLAVNIC
11:30	COFFEE BREAK	
11:50	High Performance Computing Applications in Bulgaria	Dr. Emanouil ATANASSOV
12:20	National Infrastructures for computational sciences and their development in Greece	Dr. Ioannis LIABOTIS
12:50	Computing as a Service - Roundtrip of the HPC Services at Wigner RCP	Máté F. NAGY-EGRI
13:10	Grid and Cloud Computing in INCDTIM	Dr. Felix FARCAS
13:30	LUNCH BREAK	
14:30	Industrial presentation	
Session: Software tools (15:00-16:40)		
15:00	Long Term Digital Preservation Using Cloud Services	Dr. Daniel POP
15:30	Building Scientific Workflows on the Grid: A Comparison between OpenMole and Taverna	MSc. Bojana KOTESKA
16:00	Graphical User Interface Application for EMI UI	Dr. Ionel STAN
16:20	Temperature and Active Power Monitoring in INCDTIM Data Center	Radu Catalin TRUSCA
16:40	WELCOME COCKTAIL	
17:45	Transportation to IBIS Hotel	
04.11.2014		
8:45	Transportation from IBIS Hotel	
Session: LHC Computing Grid (09:30-13:10)		
9:30	WLCG: The challenges of LHC Run2 and 3	Dr. Markus SCHULZ
10:00	ATLAS Distributed Computing Readiness for the LHC Run-2	Dr. Eric LANÇON
10:30	ATLAS Tier-2s in the LHC Run-2	Prof. Andrej FILIPČIČ

11:00	Participation of DFCTI in the WLCG collaboration	Dr. Mihai CIUBĂNCAN
11:30	COFFEE BREAK	
11:50	Network performance improvement based on perfSONAR survey	Șerban CONSTANTINESCU
12:10	ISS resources deployment for GRID infrastructures	Dr. Adrian SEVCENCO
12:30	LHCb Romania GRID and Local Computing	Teodor IVĂNOAICA
12:50	Monitoring and Status Report of the RO-16-UAIC site	Dr. Ciprian PÎNZARU
13:10	Discussions	
13:30	LUNCH BREAK	
14:45	Industrial presentation: *Advancing Scientific Discoveries with Dell IT Solutions*	Marius PURICE
Session: High-Performance Computing in Scientific Research (15:20-17:20)		
15:20	Mathematical modeling of physical problems and HPC on the heterogeneous cluster HybriLit	Prof. Gheorghe ADAM
15:50	Measuring HPC Speedup for Evolutionary Algorithms with Dynamic Chromosome Length	Prof. Boro JAKIMOVSKI
16:20	Strong field physics applications and HPC computing	Daniel BERÉNYI
16:50	Recent developments of the IFIN_BC high performance computing platform	Ionuț VASILE
17:10	Modeling the drug-protein interaction on DFCTI's HPC platform	Dr. George NECULA
17:30	Transportation to IBIS Hotel	
19:30	CONFERENCE DINNER: "Caru' cu bere", http://www.carucubere.ro	
05.11.2014		
8:45	Transportation from IBIS Hotel	
Session: Algorithms and Applications Development (09:30-11:30)		
9:30	Fast Bayesian automatic adaptive quadrature	Prof. Gheorghe ADAM
10:00	Symbolic and numerical computing for Bose-Einstein condensates	Dr. Alexandru NICOLIN
10:30	Transport approaches to pygmy resonances for ELI-NP	Prof. Virgil BĂRAN
11:00	Framework for feature extraction on satellite images	Prof. Emil SLUȘANSCHI
11:30	COFFEE BREAK	
11:50	Round Table: Computational support for the ELI-NP experiments	
13:00	LUNCH	
14:30	2014 Annual General Assembly of the ARCAS association	

CONTENTS

CONTENTS

Contributions to the advanced computing for scientific research in Romania

Mihnea Dulea

Department of Computational Physics and Information Technology,
Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Magurele, Romania

A brief overview of the current realizations of three advanced computing paradigms (Grid, High-Performance, and Cloud) in the national e-infrastructure for science is presented. The computational resources provided by the main public institutions of research and education are reviewed, together with the user communities they serve. As a general feature, although teams of high professional competence are engaged in various international collaborations and scientific projects supported by the Grid and HPC infrastructures, the global coordination and sustainable funding of the resource providers is lacking. Arguments are reiterated for the integration of the available resources in a national Cloud for scientific research and education, that will offer platform as a service and software as a service under the coordination of a legal, non-profit association.

The second part of the presentation focuses on the role currently played by IFIN-HH within the national e-infrastructure for scientific research. The projects sustained by its Grid computing and HPC facilities are shortly reviewed. Also, prospects of future involvements in the computational support for large scale collaborations, such as the ELI ESFRI project, are discussed.

Development of distributed computing technologies and BigData in LIT-JINR

Gh. Adam[1,2], V. Korenkov[1], D. Podgainy[1], T. Strizh[1]

[1]*Laboratory of Information Technologies, JINR, Dubna, Russia*
[2]*IFIN-HH, Bucharest, Romania*

The report presents the main activities done in the Laboratory of Information Technologies (LIT) of the Joint Institute for Nuclear Research (JINR), with emphasis on the development of distributed computing.

The discussion starts with an outline of the contribution of the LIT staff to the development of computational models for experiments at the Large Hadron Collider (LHC) at CERN.

A brief overview is given of the projects devoted to the development of distributed computing which were carried out by LIT staff in Russia, CERN, the USA, China, and JINR Member States. Special emphasis is devoted to two projects which are of particular importance to the JINR: the creation in Dubna of a Tier1 level center for the CMS experiment at the LHC and the development of computational models for the mega-project NICA.

Finally, the work done on the integration of HPC, grid, cloud, and BigData technologies for large international projects is analyzed.

Overview of Grid and High Performance Computing activities in Serbia

Vladimir Slavnic

Scientific Computing Laboratory
Institute of Physics Belgrade, Serbia

In this talk the current status of Grid and High Performance (HPC) activities in Serbia will be presented. These efforts are coordinated by Academic and Educational Grid Initiative of Serbia (AEGIS) that seeks to unify HPC in Serbia integrating it into robust national, regional and pan-European infrastructures. AEGIS members are researchers and academic institutions in Serbia that use, provide and/or develop Grid and HPC resources.

Serbia's engagement in recently finished and ongoing Grid and HPC initiatives and projects such as EGI-InSPIRE, SCI-BUS, agINFRA, SemaGrow and series of PRACE projects will be described, as well as supported scientific communities.

Grid sites and HPC infrastructure deployed in Serbia will be presented with the focus on recently upgraded HPC PARADOX Cluster located at Scientific Computing Laboratory (SCL) of the Institute of Physics Belgrade.

Overview of some tools and portals that were developed for supported scientific communities will be given, such as tools developed for agriculture community in agINFRA project or AEGIS CMPC science gateway developed at SCL within the framework of the SCI-BUS project that was created to provide seamless access to the applications developed for Serbian condensed matter physics community.

High Performance Computing Applications in Bulgaria

Emanouil Atanassov

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria

The Bulgarian research community has a long history of using advanced HPC systems for parallel applications in various domains of science. Novel mathematical methods have been developed and applied to problems from physics, chemistry, biomedicine, etc.

The acquiring of the Blue Gene/P system has been a stimulus for further development of such applications or for studies in new areas of science. Recently resources based on GPGPU computing devices and Xeon Phi co-processors were integrated in the Bulgarian HPC e-infrastructure and motivated development of new algorithms and software targeting such architectures.

The recent advances in several applications from the domains of statistical physics, semiconductor modelling, financial mathematics, will be presented. The methods and tools used will be compared and the numerical performance will be studied from several points of view.

An overview of other results of the big national project for establishing a Center of Excellence in Supercomputing Applications (SuperCA++) will be given as well as the perspectives for expansion of the infrastructure and applications in the near-term.

National Infrastructures for computational sciences and their development in Greece

Ioannis Liabotis

Greek Research & Technology Network,
Athens, Greece

The Greek Research and Technology Network (GRNET S.A. www.grnet.gr) is a state-owned company, operating under the auspices of the Greek Ministry of Education - General Secretariat for Research and Technology.

Its mission is to provide high-quality Infrastructure and services to the academic, research and educational community of Greece, and to disseminate ICT to the general public.

GRNET is the National Research and Education Network (NREN) provider. GRNET also plays a key role at national level in the field of distributed and large-scale research infrastructures including Grid, Cloud and HPC.

The talk focuses on the development of those infrastructures over the years, the lessons learned and their impact within the Greek and as well as the European research communities.

Computing as a Service - Roundtrip of the HPC Services at Wigner RCP

Máté Ferenc Nagy-Egri

Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary

High Performance Computing has been a buzzword in physics ever since computers have been employed for scientific use. Parallel and distributed computing has become the de-facto means of efficiently increasing computational power for the past two decades. Massively parallel computing (aka GPGPU) can be considered mainstream today, while focus is continuously shifting towards heterogenous programming.

The readily available computing expertise at Wigner has made way to a strong collaboration with CERN, which culminated in the CERN@Wigner project. The brand new Wigner Datacenter not only harbors state of the art IT infrastructure with mission critical availability, it also serves as the basis of the Wigner Computing Cloud. Researching the newest techniques in massively parallel calculations, Wigner's GPU-Lab lends both hardware resources and programming expertise to those wishing to accelerate their scientific simulations and analysis.

Grid and Cloud Computing in INCDTIM

Felix Fărcaș

National Institute of Research and Development of Isotopic and Molecular Technology, IT - Department - Cluj-Napoca, Romania

Grid Computing is a relatively new, but at the same time mature technology, whose principles were first devised by I. Foster and C. Kesselman in 1998. Since then, it had an important role in key sectors like scientific research, education, various business areas, industry, and many others.

Significant improvements in the delivery of the grid computing services, especially for businesses, have led few years ago to Cloud Computing. Both domains share the same idea of "connecting" together processors and storages of distributed computers in order to make efficient use of all available resources to solve large problems much quicker.

This paper will discuss recent problems encountered at the RO-14-ITIM Grid site and the new direction developed in the last year in private cloud computing at the National Institute for Research and Development of Isotopic and Molecular Technology (ITIM) from Cluj Napoca.

Long Term Digital Preservation Using Cloud Services

Daniel Pop, Dana Petcu, Marian Neagul

Department of Computer Science
West University of Timisoara
Timisoara, Romania

Cloud computing is adopted nowadays by various activity sectors. Libraries implementing Cloud-based solutions for their digital preservation environment can also benefit from the advantages offered by combining private Cloud deployments with public Clouds usage.

This paper particularly addresses the deployment of digital preservation solutions over Multi-Cloud environments. After discussing different Cloud deployment strategies, we are presenting the overall architecture of a digital preservation environment and how its components can be assigned to different Clouds.

Building Scientific Workflows on the Grid: A Comparison between OpenMole and Taverna

Bojana Koteska, Boro Jakimovski, and Anastas Mishev

Ss. Cyril and Methodious University,
Faculty of Information Sciences and Computer Engineering,
Rugjer Boshkovikj 16, 1000 Skopje, Macedonia

Scientific workflows are used in a number of different scientific domains. The interest for using workflows grows because of the progress of Grid computational techniques and the increased resources availability. Moreover, there are a number of scientific workflow systems that allow building workflows needed for different scientific applications and scientific experiments.

In this paper, we analyze the characteristics of two open source scientific workflow systems: OpenMole and Taverna. Both systems are designed to provide environments for parallel execution of processes, to support graphical workflow design, to offer scalability and remote execution of workflows (grids, clusters, clouds). The former is relatively new, but both are open to users if they want to contribute to their development. Although these two systems have a number of common features, they differ in the way of workflow composition, execution and implementation logic.

In order to show and verify the similarities and differences between these two scientific workflow systems, we designed a workflow and we implemented it in both systems.

Graphical User Interface Application for EMI UI

Ionel Stan, Adrian Sevcenco, Sorin Zgură, Liviu Irimia

Institute of Space Science, ISS
Magurele, Romania

In this paper we describe a graphical user interface application build in Qt framework specially for EMI User Interface.

With this application Grid users can find in a very simple manner information about Grid resources, authenticate and authorized to use Grid resources, launches jobs, get the status and results of the submitted jobs and transfer files in Grid.

Temperature and Active Power Monitoring in INCDTIM Data Center

M.R.C. Truşcă, Ş. Albert, M. L. Soran, F. Fărcaş

Datacenter Department
National Institute of Research and Development of Isotopic and Molecular Technology
Cluj-Napoca, Romania

The massive proliferation of data centers in recent years together with the exponential increase in computing capacity required cost effective solutions for power management, which rely upon the accurate monitoring and accounting of the parameters of interest.

Within the computing center at the National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM) data are continuously processed and stored for various research projects and experiments. The temperature in the computer room, which should be kept constant by four air conditioning systems, requires continuous monitoring.

In this paper a software application (Data Logger for UPT210) is presented that was developed for the monitoring/accounting of temperature and power consumption inside a data center with multiple air cooling systems. The implementation of the monitoring system in the INCDTIM's data center is discussed.

WLCG: The challenges of LHC Run2 and 3

Markus Schulz

IT DEPARTMENT /SDC, CERN

The presentation is focussed of the changing requirements and how WLCG can cope with them. It will also give an overview of the efforts to integrate new computing paradigms. Special emphasis will be given on the likely development of the multi Tier architecture of WLCG.

ATLAS Distributed Computing Readiness for the LHC Run-2

Eric Lançon

CEA-Irfu,
Gif/Yvette 91191, France

ATLAS software and computing is in a period of intensive evolution. The current long shutdown presents an opportunity to assimilate lessons from the very successful Run 1 and to prepare for the substantially increased computing requirements for Run 2 (from spring 2015).

Run 2 will bring a near doubling of the energy and the data rate, high event pile-up levels, and higher event complexity from detector upgrades, meaning the number and complexity of events to be analyzed will increase dramatically. At the same time operational loads must be reduced through greater automation, a wider array of opportunistic resources must be supported, costly storage must be used with greater efficiency, a sophisticated new analysis model must be integrated, and concurrency features of new processors must be exploited.

This presentation will survey the distributed computing aspects of the Run 2 upgrade program.

ATLAS Tier-2s in the LHC Run-2

Andrej Filipčič

Jozef Stefan Institute
University of Ljubljana, Slovenia

The ATLAS computing model changed drastically after the first period of LHC operation in order to prepare for the challenging requirements of data processing and Monte-Carlo production during the upcoming LHC Run-2.

The Monarc model of strict Tier-0, 1, 2 and 3 hierarchy of data distribution and processing was relaxed for faster computing task turnaround and more efficient data placement and storage. In order to achieve the maximum flexibility, the Tier-1 and Tier-2 disk storage will be used with much less strict boundaries, the stable and fast Tier-2s will effectively play the same role as Tier-1 disk storage. A good network connectivity between all the WLCG sites is a must for an efficient data storage and distribution.

The new ATLAS production system Prodsys-2 and the new data-management system Rucio will be commissioned by the end of this year, and the new task distribution and data placement paradigms will be tested and tuned for the upcoming dynamic distributed computing challenges of Run-2.

Participation of DFCTI in the LHC Computing Grid

Mihai Ciubăncan, Teodor Ivănoaica, Mihnea Dulea

Department of Computational Physics and Information Technology,
Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Magurele, Romania

This presentation addresses the recent achievements of the Department of Computational Physics and Information Technology (DFCTI) of IFIN-HH within the Worldwide LHC Computing Grid Collaboration (WLCG).

The IT group from DFCTI started its participation to LCG in 2004, and coordinates the Romanian Tier-2 Federation from its establishment, in 2006. Since then, the group has significantly contributed to the offline computing support for ALICE, ATLAS and LHCb, which was sustained through the advanced computing and networking infrastructure of the department.

After an overview of the global results obtained by RO-LCG during the recent period, the presentation focuses on the last year's accomplishments of DFCTI in preparation of the Run 2 at LHC. The surveyed topics include the implementation of multicore support for ATLAS VO, the attachment to FAX (Federated ATLAS storage systems using XRootD), and the qualification as a Tier2 site with Data for the LHCb experiment, of the main Grid site, RO-07-NIPNE. Measures for data transfer optimization and for improving the Grid activity monitoring are also discussed.

Network performance improvement based on perfSONAR survey

Șerban Constantinescu

Department of Elementary Particle
Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Magurele, Romania

A survey on network throughput to and from the perfSONAR service of the RO-02-NIPNE grid site is presented.

The local perfSONAR has a 10 Gbps ethernet card, so it can easily saturate a destination site having 1 Gbps ethernet card. This survey tries to find the best configuration on the local service to improve the throughput performance both for source-destination connection and destination-source connection, based on MTU (Maximum Transfer Unit) value, the TCP-IP buffer size and the Congestion Control Algorithm.

The YeAH-TCP (Yet Another Highspeed TCP) Congestion Control Algorithm was chosen after a study of the characteristics of this algorithm.

It resulted a configuration improving the connection throughput for both 1 Gbps and 10 Gbps destination sites.

ISS resources deployment for GRID infrastructures

Adrian Sevcenco and Ionel Stan

Institute of Space Science, ISS
Magurele, Romania

An overview of both hardware and software installations for GRID infrastructure within the Institute for Space Science is provided.

The topics include the hardware installation architecture for GRID and near and long term plans for hardware upgrade and expansion, the software, optimization and monitoring employed and some details about the GRID deployments, EMI and AliEN middlewares and their components.

LHCb Romania GRID and Local Computing

Teodor Ivănoaica

Department of Computational Physics and Information Technology,
Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Magurele, Romania

The LHCb Romanian team takes part in WLCG with the grid site RO-11-NIPNE and also runs tests and simulations on a smaller local cluster.

This communication presents the recent evolution of the two computing facilities since the change of the computing model of the LHCb collaboration, which now allows user analysis to be performed on *Tier-2 sites with Data*.

This year the site's hardware has been replaced and upgraded, such that the processing capacity was doubled. As a consequence of the connectivity improvement to the Tier-1, a constant load of the site of over 80% was maintained during the last months.

Monitoring and Status Report of the RO-16-UAIC site

Ciprian Pînzaru

Digital Communications Department
Alexandru Ioan Cuza University
Iasi, Romania

Grid and, more recently, cloud technologies are used on a large scale for distributed computing in scientific domains like physics, chemistry, biology, meteorology, earth sciences, in engineering, industry, and even in army.

Because many applications can benefit on the use of these technologies, the number of interconnected grid sites and computer clusters is continuously growing, which implies increased security measures against cyber-attacks.

This paper surveys the infrastructure and the results recently obtained at the RO-16-UAIC site, which supports grid production for the ATLAS virtual organization. It also presents the network monitoring system of RoEduNet and methods of traffic analysis that provide statistics and valuable information for discovering cyber-attacks. One example of DdoS bandwidth exhaustion attack is discussed.

Mathematical modeling of physical problems and high-performance computing on the heterogeneous cluster HybriLit

Gh. Adam[1,2], D. Belyakov[1], V. Korenkov[1], D. Podgainy[1], O. Streltsova[1], M. Vala[1,3], P. Zrelov[1]

[1]Laboratory of Information Technologies, JINR, Dubna, Russia
[2]IFIN-HH, Bucharest, Romania
[3]Institute of Experimental Physics of the Slovak Academy of Sciences, Kosice, Slovakia

The overwhelming part of the research done in the Joint Institute for Nuclear Research (JINR) Dubna and in Institutes, from both JINR Member States and other countries, cooperating with JINR Laboratories, results in mathematical problems the solutions of which ask for intensive computing.

The scientists in the Laboratory of Information technologies (LIT) of JINR provide a twofold contribution to the solution of such problems. On the one side, they develop a devoted computer and information infrastructure within the JINR Central Information and Computing Complex (CICC) implemented at LIT. On the other side, they contribute to the mathematical modeling of specific problems, unveiling their well- or ill-posedness, the right approach to the derivation of sound numerical or computer algebra algorithms, and the implementation of these algorithms into efficient computer programs, adapted to the existing hardware and software environment.

The purpose of this lecture is twofold. First, we illustrate the mathematical modeling process for a few selected topics solved in LIT-JINR. Second, we describe the progress achieved so far in the development of the newest component of the JINR CICC, the heterogeneous cluster HybriLit (hardware configuration, primary software environment), and illustrate its use to the solution of a number of case study and actual research problems.

Measuring HPC Speedup for Evolutionary Algorithms with Dynamic Chromosome Length

Jane Jovanovski[1], Boro Jakimovski[1], Dragan Jakimovski[2]

[1]Faculty of Computer Science and Engineering
[2]Faculty of Natural Sciences and Mathematics
Ss. Cyril and Methodius, Skopje

Evolutionary Algorithms (EAs) are a very powerful optimization technique which can be easily parallelized on High Performance Computing (HPC) systems. However, measuring the speedup for such parallel implementations presents a big problem. Some EAs experience variable execution time for fitness function evaluations, due to dynamic length of the chromosomes.

Having random genetic material in every optimization run, the total execution time needed for optimization of the same problem is variable in each run. In our previous work we have developed a novel two step EA approach that produces an analytical solution of a system of ordinary differential equations using Genetic Programming and Genetic Algorithms.

In this paper we propose a modificiation of this EA algorithm for finding a solution of one ordinary differential equation. The modified EA approach uses dynamic length of chromosomes, and therefore measuring the speedup of the algorithm in the HPC environment can be quite difficult.

The goal of our research is to introduce a new adjusted measurement of the speedup for parallel EAs with dynamic chromosome length on HPC platforms.

Strong field physics applications and HPC computing

Daniel Berenyi

Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest, Hungary

Pair production in strong fields is of fundamental interest in quantum field theories. In electrodynamics it marks the onset of the non-linear QED regime, where the extreme field strengths start to separate electron-positron pairs from the vacuum. This regime seems to be accessible in the near future with extreme laser facilities. In QCD an analogue process happens in heavy-ion collisions when the colliding nuclei are separating and gluonic strings form between the quarks inside them and produce quark-anti quark pairs.

We present the Dirac-Heisenberg-Wigner formalism as a theoretical model of these processes and focus on the computational cost of the interesting special cases in QED. As the resulting differential-equation systems are computationally demanding to solve we discuss the current possibilities of solving these equations on large scale utilizing Graphical Processing Units (GPUs). We briefly review how high-level programming techniques and staged compiling can shorten the development time of such GPU codes.

Recent developments of the IFIN_BC high performance computing platform

Ionuț Vasile, Dragoș Ciobanu-Zabet, Mihnea Dulea

Department of Computational Physics and Information Technology, Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest-Magurele, Romania

The recent changes in the software environment of the IFIN_BC high performance computing platform are reported. The evergrowing parallel processing needs for the time evolution of complex biomolecular systems must be sustained by an optimal hardware and software arhitecture. Thus, constant optimization of the core software is needed, as well as reoptimization and readjustment of the simulation packages used on our multiuser cluster.

This lecture aims at providing an insight of the software and hardware changes which occurred recently on IFIN_BC. We present the implementation of two different job management systems (Torque PBS and SLURM) which coexist on the same management server. Also, we discuss the deployment of the latest OFED Infiniband drivers and MPI implementations provided. Finally, we provide some experience notes regarding the CentOS release 7 and its usefulness in HPC systems.

Modeling the drug-protein interaction on DFCTI's HPC platform

G. Necula, D. Ciobanu-Zabet

Department of Computational Physics and Information Technology, Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest-Magurele, Romania

We report results of numerical modeling of ligand-protein interactions in multiple drug resistance (MDR) bacteria, which is an ever-increasing worldwide public heath problem caused by improper use of antibiotics. There are generally two mechanisms that enable MDR in bacteria: accumulation of resistance plasmids and overexpression of efflux pumps. Thus overexpressed efflux pumps have become targets for therapeutic drugs.

Several studies of MDR efflux mechanisms in S. aureus indicated that NorA is predominant protein efflux pump. NorA induces resistance to fluoroquinolones, cationic dyes, cationic inhibitors and tetraphenylphosphonium. Since the NorA structure was not resolved we have constructed a homology model using crystallographic structures of related molecules as templates. The NorA model was inserted in a POPE bilayer and the whole complex was solvated with TIP3 water molecules. Molecular dynamics of the system was simulated with NAMD program using CHARMM force field for a total time of 100 ns. A frame extracted after complete equilibration of the model was used for docking and virtual ligand screening with the aim of revealing the binding mode of known NorA inhibitors and discovering novel NorA inhibitors. The parallel performance of NAMD program scales very well on DFCTI's HPC platform with significant speedup gains even with hundreds of processors.

Virtual ligand screening was performed with AutoDock Vina parallelized using MPI thus reducing overall calculation time.

A large proportion of compounds used in virtual ligand screenings are available in online databases only as 1D (SMILES) or 2D representations that need to be converted to appropriate 3D structures To optimize ligand 3D structures we used GAUSSIAN 09 with Density Functional Theory (DFT) QM methods. The advantages of DFT methods is processing efficiency while the results obtained are comparable to the ones obtained with ab initio methods. Parallel performance of GAUSSIAN 09 DFT optimizations scales well up to 48 processors after which we noticed a steep decline of speedup.

Symbolic and numerical computing for Bose-Einstein condensates

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The experimental achievement of atomic Bose-Einstein condensates has been a long scientific endeavor that spanned over the seven decades which separate the theoretical prediction of Satyendranath Bose and Albert Einstein (1924-1925) from the first results obtained in the groups of E. A. Cornell, W. Ketterle, and C. E. Wieman in 1995. The scientific effervescence that followed the experimental results covers a wide range of research topics which go from nonlinear quantum optics to high-performance scientific computing and solid state physics to complex systems.

Scientific numerical computing has been a particularly active area of research, as the standard theoretical formalism used to describe the 0 K dynamics of a condensate, the so-called Gross-Pitaevskii equation, provides limited analytical insight and usually relies on specialized numerical treatment.

In the first part of the presentation we survey the state of the art on the symbolic and numerical computing methods used to investigate the dynamics of Bose-Einstein condensates, with special emphasis on effective equations of reduced dimensionality.

In the second part of the presentation we show how to derive effectively one- and two-dimensional equations for cigar- and pancake-shaped condensates, respectively, that have cubic nonlinearities.

Fast Bayesian automatic adaptive quadrature

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The aim of the Bayesian automatic adaptive quadrature (Baaq) is to provide reliable solutions of (proper or improper) Riemann integrals for integrand functions which are continuous almost everywhere inside the integration domain, irrespective of the local distribution of the finite number of zero measure or singular abscissas at which the integrand shows non-smooth behaviour. The proposed approach to the reliability enforcement [1, 2] brings the abscissas of irregular behaviour at the subrange ends defining the adaptively created partition of the input integration domain. This procedure is heavily based on the check of a hierarchically ordered set of well-conditioning criteria, prior to the activation of the local quadrature rules approximating the solution of the problem. While this approach was found to work, it is disproportionately time consuming for integrals involving well-conditioning integrands (asking perhaps for a moderate subdivision process).

In this paper we propose a significant improvement of the Baaq, based on three pillars:

(i) selection of the suitable local quadrature rule for the problem at hand in terms of the value got for the floating point degree of precision (slightly redefined with respect to [3]), pointing to one of the four possible domain length ranges (vanishing, microscopic, mesoscopic, or macroscopic);

(ii) for macroscopic domain lengths (which cover the overwhelming fraction of the practical problems), abandonment of the standard QUADPACK local quadrature rules [4] in favour of an implementation based on the principle of redundancy (yielding a local numerical estimate of the integral and its associated error from a pair of quadrature sums spanned by statistically independent distributions of the fractionary reduced quadrature knots);

(iii) inclusion of any resolved piecewise linear range of variation of the integrand into the class of exceptional cases asking for immediate definition of its actual extension to machine accuracy.

Then rapid solution is got for an 'easy' integral, while both the a posteriori [5] and a priori [1, 2] analysis of the integrand profile proceed fast and consistently.

(Continued)

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Transport approaches to pygmy resonances for ELI-NP

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The electric dipole response of nuclei, including the exotic systems, was intensively explored during the last decade through a variety of experimental methods and probes which include Nuclear Resonance Fluorescence using bremsstrahlung photons, excitation with photons resulting from Compton backscattering, alpha or proton scattering, and Coulomb excitations. From the data emerge the evidence that for many systems an additional dipole strength is present below the Giant Dipole Resonance (GDR) response which manifests as a resonant-like structure. It was concluded that it exhausts few percentages out of the total Energy-Weighted Sum Rule (EWSR) associated to the dipolar response and it is larger with the increase of the number of neutrons in excess. The position of the peak changes from around 7.35 MeV for 208Pb to 9.8 MeV in the case of 68Ni. However it is not yet clear if some systematic correlations can be established between the position of the energy peak, the sum-rule attributed to this low-lying mode, the possible substructure and the mass or isospin content of the nuclei, the neutron skin or the properties of the symmetry energy below saturation. Moreover, the nature of the response, collective or rather single-particle excitations is still under intense debate. Indeed some theoretical models provide evidences for a collective mode while other approaches suggest a rather non-collective structure involving some neutron excitations from the skin. Answering to such questions clearly requires high accuracy, systematic experimental studies over an extended domain of nuclear masses and/or isospin covering an energy range from well below the energy particle threshold until GDR response.

It is very likely that at the future ELI-NP facility in Bucharest various open questions can be addressed. In this context systematic theoretical investigations of the same questions can provide interesting hints. The goal of this presentation is to present such systematic results obtained within a microscopic transport model based on the Vlasov equation. This equation is obtained as the semi-classical limit of Time-Dependent Hartree-Fock equations. In the linear regime the Vlasov equation will correspond to Random Phase Approximation and therefore is well suited to explore the collective features of nuclear systems.

Framework for feature extraction on satellite images

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This paper presents a software for region classification in large satellite images from the map of Romania using textural measures, namely Haralick features and tonal information.

Two classification techniques are proposed: one of them uses the Mahalanobis distance to get the most appropriate class and the other uses a machine learning algorithm, Support Vector Machines (SVMs).

SVM is a powerful technique recently applied to remote sensing data classification problems, which seems to be efficient in many cases. Our experimental results using the SVM method indicate an average accuracy of 89% which is very promising. This software could be useful to build an automatic tool for tracking the environmental changes and keeping the maps updated according to a recent set of satellite images.

AUTHOR INDEX

AUTHOR INDEX

AUTHOR INDEX

AUTHOR INDEX

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