

2016 9th RO-LCG Conference

GRID CLOUD

**AND HIGH-PERFORMANCE COMPUTING
IN SCIENCE**

Book of Abstracts

26-28 October 2016 Bucharest-Magurele, Romania



DEPARTMENT OF COMPUTATIONAL PHYSICS AND INFORMATION TECHNOLOGIES
HORIA HULUBEI NATIONAL INSTITUTE FOR RESEARCH AND DEVELOPMENT
IN PHYSICS AND NUCLEAR ENGINEERING

Grid, Cloud, and High-Performance Computing in Science

26-28 October 2016

Bucharest-Măgurele

BOOK OF ABSTRACTS

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Romanian Tier-2 Federation
RO-LCG



Horia Hulubei National Institute for
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National Authority for Scientific Research
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Romanian Association for Promotion of
Advanced Computational Methods in
Scientific Research



Grid, Cloud, and High-Performance Computing in Science

Bucharest-Măgurele, 2016

ISBN 978-973-0-22868-7

DTP: Mara Tanase, Adrian Socolov, Corina Dulea
Cover: Mara Tanase



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WELCOME MESSAGE

Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH) and the Organizing Committee have the pleasure to welcome you to the RO-LCG 2016 Conference, *"Grid, Cloud, and High-Performance Computing in Science"*.

The Conference is organized by the Department of Computational Physics and Information Technologies of IFIN-HH and the Romanian Tier2 Federation. RO-LCG 2016 is sponsored by the *National Authority for Scientific Research and Innovation*, the *Romanian Association for the Promotion of Advanced Computational Methods in Scientific Research*, *DELL Romania*, *Lenovo*, and *Logic Computer SRL*.

The Conference celebrates the 10th anniversary of the Romanian Tier2 Federation, which was founded in 2006 following the conclusion of the Memorandum of Understanding between CERN and the National Authority for Scientific Research. The event continues the tradition of annual meetings dedicated to 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, distributed computing, Big Data, Grid computing for the LHC experiments, cloud computing, algorithms and applications development.

We are confident that the RO-LCG 2016 Conference will stimulate a fruitful scientific dialogue between the participants and opportunities for initiating new collaborations.

We wish you all to enjoy the Conference and to have a memorable stay in Bucharest!

Dr. Mihnea Alexandru Dulea

Chairman of the Organizing Committee

Acad. Nicolae Victor Zamfir

Director General IFIN-HH

PROGRAM

26.10.2016		
08:45	Transportation from hotel	
09:15	REGISTRATION and Welcome coffee	
10:00	Welcome Address	Acad. Nicolae Victor ZAMFIR
10:05	Conference overview and logistics	Mihnea Dulea
SESSION: e-Infrastructures for Large-Scale Collaborations - Part I (10:10-12:40)		
10:10	One Decade of Computational Support for Advanced Research	Mihnea Dulea
10:30	EGI: advanced computing for research ... in Europe and beyond!	Yannick Legré
11:00	GÉANT Advanced Network Services Delivery for HPC in Science	Rudolf Vohnout
11:30	COFFEE BREAK (10')	
11:40	MICC – new targets for information technology and computing in JINR	Gheorghe Adam
12:10	Exploiting the Resources of a University HPC Center	Dana Petcu
12:40	Sponsor presentation: <i>Lenovo Solutions for Enterprises</i>	Aurel Netin
13:10	Sponsor presentation: <i>Dell EMC Modern Datacenter enabling the Future-Ready Enterprise</i>	Dan Bogdan
13:40	LUNCH BREAK (50')	
14:30	Industrial presentation: <i>Achieving the next phase of performance evolution on Supercomputing</i>	Boris Neiman
SESSION: e-Infrastructures for Large-Scale Collaborations - Part II (15:00-16:00)		
15:00	National Communication Infrastructure for Romanian Research Projects	Octavian Rusu
15:30	High Performance Computing Infrastructure of the Babes-Bolyai University	Virginia Niculescu
16:00	ROUND TABLE: Future advanced computing solutions for the research and academic community ELI-NP	
16:45	WELCOME COCKTAIL (45')	
17:30	Transportation to hotel	
27.10.2016		
09:00	Transportation from hotel	
09:30	Welcome coffee	
SESSION: Distributed Computing (10:00-11:30)		
10:00	DIRAC: from particle physics to other scientific domains	Andrei Tsaregorodtsev
10:30	Simulation of a Distributed Data Processing System for HEP Experiments	Andrey Nechaevskiy
11:00	Integration of HTC and HPC tools for solving complex problems in computational biology	Ionuț Vasile
11:30	COFFEE BREAK (10')	
SESSION: Algorithms and Applications Development - Part I (11:40-13:10)		
11:40	Classes of integrals in the automatic adaptive quadrature	Gheorghe Adam

PROGRAM

12:00	SpeechXRays. Multi-channel biometrics combining acoustic and machine vision analysis of speech, lips movement and face	Alexandru Nicolin
12:30	TraViS: GPU Accelerated Computing Tool for Monitoring and Analyzing Network Traffic	Mihai Carabaş
12:50	Numerical simulations for the propagation of laser beams	Victor Palea
13:10	LUNCH BREAK (50')	
14:00-15:00 – ARCAŞ Meeting		
SESSION: Algorithms and Applications Development - Part II (14:00-15:30)		
14:00	Sympathetic skin response analysis using exosomatic method, biomedical sensors and clustering technique	Maria Raluca Aileni
14:20	Big Data and Deep Learning Based Predictive Analytics of High Order Harmonics Generation Optimal Scenarios	Andreea Mihăilescu
14:40	Big data predictive analytics for bioheat transfer modeling	Maria Raluca Aileni
15:00	Geant4 simulation of cone shape attenuator for uniform spatial dose distribution for a proton beam generated by fs lasers	Sohichiroh Aogaki
15:30	COFFEE BREAK (15')	
SESSION: Status reports and activities of HTC/HPC installations - Part I (15:45-16:30)		
15:45	Overview of the national computing support for the LHC community	Mihnea Dulea
16:10	The evolution of the RO-16-UAIC grid site	Ciprian Pînzaru
SESSION: Cloud computing - Part I (16:30-17:00)		
16:30	HPC Cloud Application Orchestration through Self-Organization	Dana Petcu
17:00	Transportation to hotel	
19:30	CONFERENCE DINNER: "Caru' cu bere", http://www.carucubere.ro/en , http://www.carucubere.ro/ro	
28.10.2016		
09:00	Transportation from hotel	
09:30	Welcome coffee	
SESSION: Cloud computing - Part II (10:00-11:00)		
10:00	Implementation of a Decentralized Cloud Platform using 5G Networks	George Suciu
10:30	CLOUDIFIN, the first NGI-RO site participating to the EGI Federated Cloud	Ionuţ Vasile
SESSION: Status reports and activities of HTC/HPC installations - Part II (11:00-12:30)		
11:00	Status report of ISS Grid activities	Liviu Irimia
11:20	COFFEE BREAK (10')	
11:30	Support of Multiple LHC VOs in a Heterogeneous Grid Site	Mihai Ciubăncan
11:50	Current status and future upgrade at ITIM Grid site	Radu Truşcă
12:10	New Network Design for the Grid Infrastructure	Teodor Ivănoaica
12:30	CLOSING SESSION: Conference review	
13:00	LUNCH	
14:00	Transportation to Bucharest	



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WEDNESDAY OCTOBER 26, 2016
e-Infrastructures for Large-Scale Collaborations

One Decade of Computational Support for Advanced Research

Mihnea Dulea

*Department of Computational Physics and Information Technologies,
Horia Hulubei National Institute for Physics and Nuclear Engineering,
Bucharest-Măgurele, Romania*

The report reviews the significant achievements in the advanced computing infrastructure for research since the founding of the Romanian Tier2 Federation (RO-LCG), which is partner in the *Worldwide LHC Computing Grid (WLCG)* collaboration.

Motivated by the existence of a strong community of high energy physics scientists, the national IT support of large-scale research projects started with the development of Grid sites dedicated to the offline computing for the ALICE, ATLAS and LHCb experiments in CERN.

These have joined in 2006 in the RO-LCG Federation, which represents until today the main component of the national Grid infrastructure.

The development of the RO-LCG's infrastructure closely followed the evolution of WLCG's technical program, meeting the requirements of the experiments' research strategy in what regards their computing needs. It has undergone multiple evolution stages in terms of networking, data and job management, security, software and workflow optimizations.

The experience accumulated in the deployment, management and operation of the Grid and HPC technologies was beneficial for tackling the problem of computing support for another major project, *Extreme Light Infrastructure – Nuclear Physics (ELI-NP)*, expected to enter the operational phase in 2019. While the global computing requirements for storing and processing the data to be acquired are still to be defined, the researcher groups are already performing simulations and model experimental setups by using the HTC and HPC infrastructure of the GRIDIFIN resource centre.

The offering of support to the large scale projects such as WLCG and ELI-NP is but one of the targets of the *Romanian National Grid Infrastructure (NGI-RO)*. Smaller national research and academic communities dispersed in various fields, such as from biology, astronomy or engineering, often need uncorrelated IT assistance for shorter-time projects and/or for the occasional analysis of experimental data. It is generally acknowledged that the computational paradigm which fits best in these cases, that belong to what is known as the *long tail of science*, is the cloud computing.

The final part of the report reveals the strategy followed at IFIN-HH in order to provide cloud computing services for these communities and to join the *EGI's Federated Cloud*, in anticipation of the future *European Open Science Cloud*.



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e-Infrastructures for Large-Scale Collaborations

EGI: advanced computing for research ... in Europe and beyond!

Y. Legré, T. Ferrari, S. Andreozzi, G. Sipos, P. Solagna
on behalf of the EGI Federation

EGI Foundation – Science Park 140, Amsterdam 1098XG – the Netherlands

The EGI infrastructure is a publicly funded e-infrastructure put together to give scientists, access to more than 826,000 logical CPUs, 560 PB of storage capacity to drive research and innovation in Europe. Resources are provided by about 325 resource centres who are distributed across 56 countries in Europe, the Asia-Pacific region, Canada and Latin America. EGI also federates publicly funded cloud providers across Europe to contribute to the implementation of a European Open Science cloud to support data- and compute-intensive science.

EGI is supporting 'grids' of high-performance computing (HPC) and high-throughput computing (HTC) resources and is also ideally placed to integrate new Distributed Computing Infrastructures (DCIs) such as clouds, supercomputing networks and desktop grids.

The EGI cloud infrastructure is based on open standards allowing a seamless user experience over the cloud sites belonging to the federation through standardised interfaces. Advanced services are available to manage computing services and datasets in a distributed environment hiding the complexity of the geographical distribution to the developers of scientific applications and services. Users automatically find their software available in all the federation nodes supporting their research and mechanisms to create the computing services close the data to process are also envisaged. The EGI Federated Cloud allows to publish, use and reuse datasets, according to their access policy, stored into the federated resources, promote the spreading of open research data and offer interfaces towards well-known public services for data discovery like OpenAIRE.

EGI is committed to contribute to the Open Science Commons, including the knowledge commons aiming at making knowledge, competences and support services openly available to the whole European Research Area. This is concretely realized through a network of community-driven centres of excellence. EGI aims at providing – together with other key players – a European federation of Centres of Excellence providing services relevant to all the digital assets needed to support European e-Science. For more information about the Open Science Commons vision see: <http://go.egi.eu/osc>.

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GÉANT Advanced Network Services Delivery for HPC in Science

Rudolf Vohnout^{1,2}, Vincenzo Capone²

¹*CESNET*

²*GÉANT*

GÉANT is the Pan-European Research and Education Network operator, providing reliable modern networking services to a wide range of application: from pure Photonic Transmission, to Circuits, Virtual Private Networks, Wireless, Testbeds, IP, Performance monitoring, Trust & Identity, underpinning High Performance Computing/GRID/Cloud. GÉANT currently has more than 50 million users around Europe, and more than 10 thousand connected institutions in 40 countries, including leading research infrastructures as associate members (e.g. CERN, EBI). The service provision to such, high demanding partners is a notable challenge, to which GÉANT has to suitably answer.

GÉANT also carries out research activities in the field of networking technologies, usually jointly with those European National Research and Educational Network operators that support research activities, along with the usual operational activities. Thanks to this ongoing collaboration, GÉANT could achieve 100% monthly IP availability, with over 2,000 Terabytes/day of data transferred across the whole GÉANT network.

As a long-term partner of PRACE and EGI (and related research infrastructure projects using their resources), GÉANT has a significant experience in delivering state-of-the-art end-to-end network services and related support. In close cooperation with users, a top-down approach could be implemented. Performance and resources monitoring is one of the key services, together with user identification (AAI services) and traffic monitoring.. As for the security aspects, GÉANT can provide L2+L3 multi-domain VPN services, or virtual private circuits over the MPLS backbone, as well as optical private circuits (lambdas) with reserved bandwidth.



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e-Infrastructures for Large-Scale Collaborations

National Communication Infrastructure for Romanian Research Projects

Octavian Rusu

Agency ARNIEC/RoEduNet, Iasi NOC, Carol I, 11, Iasi, Romania

Romanian National Research and Education Network has been established two decades ago and evolved from 9600 bps star topology to 100 Gbps mesh topology based on own dark fiber network. The network development was very slow before and immediately after Romania joined GEANT, a big step forward was the installation of the DWDM equipment nationwide at the end of 2008¹, providing multiple 10G links for the regional NOCs and 1G for almost every POP over 4200 km of dark fiber.

First 100G lambda in the Romanian NREN has been installed as a testbed in the late 2011² and further research was conducted to show that, over Ciena's coherent technology, alien lambdas could be installed, managed and operated³. Later on, all regional NOCs were connected to the national NOC using this technology, bringing the 100G national backbone to the research and education community.

Network evolution, current and future topologies as well as actions to be taken to improve the support for big research communities and in Romania will be presented.

¹ <http://www.fiberopticsonline.com/doc/romania-roedunet-educational-network-0001>

² <http://www.capacitymedia.com/Article/2868043/Ciena-to-deploy-100G-in-Romania.html>

³ [dx.doi.org/10.1109/RoEduNet-RENAM.2014.6955326](https://doi.org/10.1109/RoEduNet-RENAM.2014.6955326)

WEDNESDAY OCTOBER 26, 2016

e-Infrastructures for Large-Scale Collaborations

Exploiting the Resources of a University HPC Center

Dana Petcu

Computer Science Department, West University of Timisoara, Romania

The hardware and human resources of a usual university HPC center are mainly serving the needs of the university research activities. However, such activities cannot be done in isolation from the activities of other centers or the research collaborators. Giving priority European collaboration activities has the potential to enhance the research activities scope and to strengthen of result visibility.

Best practices of the HPC center of West University of Timisoara are intended to be shared in the presentation. The main topics are related to: engage SMEs to use HPC (related to the H2020 action SESAME-NET), engage multi-national scientific communities to use HPC (related to H2020 action VI-SEEM), migration of HPC to HPC2 (HPC Cloud services, related to the H2020 action CloudLightning) and cluster services for Big Data (related to H2020 action DICE) or for deploying portable Cloud-enabled applications (related to PNII action AMICAS).



WEDNESDAY OCTOBER 26, 2016

Sponsor presentation

Dell EMC Modern Datacenter enabling the Future-Ready Enterprise

Dan Bogdan

Infrastructure Solutions Lead SEE, Dell EMC Central & Eastern Europe

Michael Dell, chairman and CEO of Dell Technologies, said, "We are at the dawn of the next industrial revolution. Our world is becoming more intelligent and more connected by the minute, and ultimately will become intertwined with a vast Internet of Things, paving the way for our customers to do incredible things. This is why we created Dell Technologies. We have the products, services, talent and global scale to be a catalyst for change and guide customers, large and small, on their digital journey."

Dell Technologies blends Dell's go-to-market strength with small business and mid-market customers and EMC's strength with large enterprises and stands as a market leader in many of the most important and high-growth areas of the \$2 trillion information technology market, including positions as a "Leader" in 20 Gartner Magic Quadrants and a portfolio of more than 20,000 patents and applications. Dell Technologies <<http://www.delltechnologies.com/>> is a unique family of businesses that provides the essential infrastructure for organizations to build their digital future, transform IT and protect their most important asset, information. The company services customers of all sizes across 180 countries – ranging from 98% of the Fortune 500 to individual consumers – with the industry's most comprehensive and innovative portfolio from the edge to the core to the cloud.

"Together, we have an incredibly powerful set of capabilities. Our goal is to be your most trusted, most innovative partner...We believe we've created the next great technology company...and we've created it just for you" said Michael Dell with the occasion of EMC acquisition. Let the digital transformation journey begin with Dell Technologies, the No. 1 provider for: solutions in converged infrastructures, storage, virtualised data center infrastructures, server virtualisation software, Cloud IT or the world's most secure business-class laptops.

WEDNESDAY OCTOBER 26, 2016
e-Infrastructures for Large-Scale Collaborations

MICC – new targets for information technology and computing in JINR

Gh. Adam^{1,2}, V.V Korenkov¹, T.A. Strizh¹

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²*Horia Hulubei National Institute for Physics and Nuclear Technologies (IFIN-HH), Bucharest-Măgurele, Romania*

In the modern scientific research, computing has become an integral part of theory, experiment, and technology development. The Multifunctional Information and Computing Complex (MICC), under development in the Laboratory of Information Technologies (LIT) of the Joint Institute for Nuclear Research (JINR) in Dubna is planned to be implemented at the state-of-the-art information technology parameters enabling integral fulfillment of the needs of the JINR scientific projects in accordance with the new Seven-Year Plan of Development for 2017-2023.

The noticeable diversity of the scientific goals defined for the JINR research, together with the accumulated LIT expertise, pointed to the necessity, for the time being, of eight distinct undertakings needed to reach the proposed MICC targets: multi-functionality, high performance, task adapted storage, high reliability and availability, security, scalability, user customized software environment, inner and outer high speed connections.

The implementation of the computing infrastructure itself comprises five distinct activities:

- (i) Design and creation of a dedicated infrastructure (characterized by robust long term data storage, reliable and efficient data processing and analysis) for the support of the NICA-based projects – BM@N, MPD, SPD.
- (ii) Development of the CMS Tier-1 centre (covering the needs foreseen within the CMS collaboration and the RDMS CMS collaboration frameworks).
- (iii) Addition of new features to the existing configuration of the Grid JINR Tier-2 site, upgrade of the outdated compute elements (CE) and data storage elements (SE). The Tier-2 site provides support to the virtual organizations (VOs) enabling the participation of JINR groups to the large scale experiments at the LHC (ALICE, ATLAS, CMS, LHCb), FAIR (CBM, PANDA), as well as to other VOs within large scale international collaborations. Traditionally, the tasks of the non-grid JINR users asking for sequential computing resources are supported within this activity as well.



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- (iv) Design and implementation of a cloud structure aimed at expanding the range of services provided to local and remote users /user groups/ and at creating an integrated cloud environment of the JINR Member States.
- (v) Significant enlargement of the modular heterogeneous computing cluster HibriLIT, the basic resource for the solution of high performance computing (HPC) in JINR.

There are, in addition, three underlying activities which are indelibly connected with the safe and efficient MICC operation:

- (vi) A multicomponent engineering infrastructure supplying basic resources (electricity, climate control).
- (vii) The high throughput JINR telecommunication channels and the high speed local area network (LAN), which will need substantial extension and improvement to cope with the inside and outside huge throughputs of data transfer volumes.
- (viii) Exhausting monitoring/control of the functioning of all the MICC elements.

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e-Infrastructures for Large-Scale Collaborations

High Performance Computing Infrastructure of the Babeş-Bolyai University

Virginia Niculescu, Darius Bufnea and Adrian Stercă

Babeş-Bolyai University, Cluj-Napoca

The High Performance Computing Center of the Babeş-Bolyai University was established in 2015, founded by a European Union infrastructure project. The HPC infrastructure is constituted from two parts: **the HPC Cluster** and **the HPC Cloud System**.

The **HPC Cluster** is built on the IBM NextScale computing architecture, it consists of 68 computing nodes each having two 10-core Intel Xeon v3 CPUs, 128 GB RAM memory and 1 TB HDD storage, two management nodes, two NSD nodes and a backup tape library machine for data archiving. The data network of the HPC cluster is Infiniband FDR with 1:1 subscription rate operating at 56Gb/s. The external storage system is IBM GPFS 4.x with a total raw disk space of 72TB. The theoretical Rpeak performance achieved by our system is 62Tflops and the practical Rmax performance is 40Tflops. Some of the compute nodes have also two Nvidia K40x GPU and Intel Phi coprocessors. The Management of the HPC Cluster is done using IBM Platform HPC 4.2 and xCat.

The **Cloud system** is built on IBM Flex System architecture and has ten Flex System virtualization servers with two Intel Xeon v2 CPUs, 128 GB RAM memory and 2x 240Gb SSD storage disks and one management node. The Cloud operating software is OpenStack. The management and monitor software is IBM Flex System Software Stack. The virtualization software is Vmware vSphere Enterprise 5.1.

Within the same EU-funded project, a Research Center of Modeling, Optimization and Simulation has been created in order to strengthen the development of high performance interdisciplinary research. The team is formed of computer scientists and mathematicians that have strong collaborations with different groups from other research fields.

We consider that the High Performance Computing Center of the Babeş-Bolyai University and the affiliated team could offer a high potential infrastructure for different multidisciplinary research projects.



THURSDAY OCTOBER 27, 2016

Distributed Computing

DIRAC: from particle physics to other scientific domains

A. Tsaregorodtsev

CPPM, Aix Marseille Université, CNRS/IN2P3, Marseille, France

DIRAC is a framework for building distributed computing infrastructures for scientific communities needing access to a large volume of computing and storage resources. First developed for the LHCb experiment at LHC, CERN, it was adopted as a basis for production systems of some other experiments in High Energy Physics and other domains. In this contribution we will make a brief review of the DIRAC project status and describe different applications of the DIRAC framework in large scientific experiments. We will present also activities of DIRAC services provided by several grid infrastructure projects for various scientific user communities.

THURSDAY OCTOBER 27, 2016**Distributed Computing**

Simulation of a Distributed Data Processing System for HEP Experiments

Andrey Nechaevskiy, Darya Pryahina

Joint Institute for Nuclear Research, Dubna, Russia

The distributed complex computing systems for data storage and processing are in common use worldwide. The development of a HEP (High Energy Physics) computing system aiming at processing, analyzing and storing experimental data is a complex and difficult task due to the need of a sophisticated design under evolving user requirements. The superconducting accelerator complex NICA at the Joint Institute for Nuclear Research (JINR) is now in an advanced stage of implementation. NICA underlies the BM@N, MPD and SPD experiments, each of which is characterized by specific requirements.

Starting from the existing grid simulation program GridSim (www.gridbus.org/gridsim), an advanced HEP computing system simulation program called SyMSim is developed at LIT-JINR with the aim to provide necessary computing background for NICA complex. The wider grasp of the simulation system allows improving the efficiency of the grid/cloud structures development accommodating the work quality indicators of specific real systems. The simulation program SyMSim has allowed to develop the infrastructure for the CMS JINR Tier1 site. Based on the SyMSim simulation program a proper architectures can be tailored for the specific experiment computing infrastructure. SyMSim facilitates making decisions regarding a required equipment.

The paper describes results obtained within the above mentioned framework.



THURSDAY OCTOBER 27, 2016

Distributed Computing

Integration of HTC and HPC tools for solving complex problems in computational biology

Dragoş Ciobanu-Zabet¹, Dragoş Hont², George Necula¹, Ionuţ Vasile¹,
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Molecular modeling makes extensive use of high-throughput computing for operations such as database interrogations, massive data retrieval and conversion, high-throughput VLS, protein structure and function prediction, genomics, and high-performance computing for molecular dynamics, chemical structure calculations, etc.

The molecular modeling of complex cellular subsystems requires both sequential and parallel computing steps in order to obtain physically significant results, such as the description of drug-protein interaction in bacterial membranes. The researcher is often overwhelmed by the multitude of different software tools and data transfers one must use to get these results.

Here we report the implementation status of a new integrated system for molecular modeling we recently designed for the study of the substructures of the Gram negative bacteria, that considerably eases the user's burden.

The system consists of an extensible and scalable pool of HTC and HPC resources which are accessible to the user through a graphical frontend (portal).

The data handling and processing through various retrieval, conversion and modeling tools is managed by means of automatic, programmable and reusable workflows.

THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Classes of integrals in the automatic adaptive quadrature

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The high performance computing in physics research frequently asks for fast and reliable computation of Riemann integrals as part of the models involving evaluation of physical observables. The progress toward the implementation of Bayesian automatic adaptive quadrature (BAAQ) algorithms (see, e.g., the overview [1] and the reports [2-4]) has resulted in significant departure from the standard automatic adaptive quadrature (SAAQ) approach [5, 6].

The present report provides a discussion of the basic criteria which enable both the inheritance of the best features of the SAAQ approach and the consistent definition of distinct classes of integrals. There are two basic features which must be counted in the implementation of generally valid, efficient, and consistent BAAQ algorithms.

The first feature follows from the *extension of the integration domain*. Within the multiscale approach [4], it was shown that each length scale necessarily associates a *characteristic quadrature rule*. While the characteristic quadrature rules associated to the *microscopic*, *mesoscopic*, and *macroscopic* integration domain lengths proposed in [4] are valid, we have subsequently found that their use for macroscopic lengths carries distinct features in the cases of *macroscopic finite* and *macroscopic with asymptotic tail* integration domain lengths.

The second feature follows from the *range of variation of the integrand function*. Its investigation enables consistent identification of *easy exceptional cases*, of *easy Riemann integrals* asking nothing but SAAQ approach, and *difficult Riemann integrals*. It is for the last case only that Bayesian inferences are to be used.



THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

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THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

**SpeechXRays. Multi-channel biometrics combining
acoustic and machine vision analysis of speech, lips
movement and face**

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The SpeechXRays project will develop and test in real-life environments a user recognition platform based on voice acoustics analysis and audio-visual identity verification. SpeechXRays will outperform state-of-the-art solutions in areas such as: security (high accuracy solution), privacy (biometric data stored in the device or in a private cloud under the responsibility of the data subject), usability (text-independent speaker identification, i.e., no pass phrase), low sensitivity to surrounding noise and cost-efficiency (through the use of standard embedded microphone and cameras in mobile devices).

The project will combine and pilot two proven techniques, namely acoustic driven voice recognition (using acoustic rather than statistical only models) and multi-channel biometrics incorporating dynamic face recognition (machine vision analysis of speech, lip movement and face).

The vision of the SpeechXRays project is to provide a solution combining the convenience and cost-effectiveness of voice biometrics, achieving better accuracies by combining it with video, and bringing superior anti-spoofing capabilities. The project lasts 36 months and is coordinated by Oberthur Technologies, world leader in digital security solutions for the mobility space.



THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

**TraViS: GPU Accelerated Computing Tool for Monitoring
and Analyzing Network Traffic**

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This paper provides an innovative solution for real-time application traffic monitoring using Graphics processing unit. TraViS is built upon commodity hardware and offers an optimized kernel module for fast data processing and classification.

Keywords: GPU; GPU Direct RDMA; application detection; real-time statistics

THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Sympathetic skin response analysis using exosomatic method, biomedical sensors and clustering technique

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This paper presents an application for the processing of the data regarding galvanic skin response for monitoring the bioelectrical conductivity measured from the surface of the skin and reflecting change of the bioelectric properties. The bioelectric conductivity at the skin level is in function of the degree of stress or relaxation of human body, and in direct relation with skin humidity caused by disorders or emotions.

For data capture and record was used a smart sensors system based on low power ATmega328 from Atmel, based on a RISC microcontroller chip, sensors, a Bluetooth device and flexible electrodes. In the experimental part the continuous-time signal was sampled to discrete time intervals and subsequently converted to digital values. For choosing suitable time interval we used clustering technique applied for received data logger.

Keywords: sensors, biomedical, clustering algorithms, data mining, galvanic skin response, monitoring, bioelectric, humidity, conductivity



THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Numerical simulations for the propagation of laser beams

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Motivated by some computational problems associated with the propagation of laser beams, we investigate here by numerical means the dynamics of the beam profile within the framework of one- and two-dimensional Schrödinger equations for various beam profiles. We use finite difference methods whose errors we determine for the simplified case of a Gaussian beam profile to determine beam properties such as the width of the laser beam, the direction of the beam, and the self-focusing. We control the accuracy of our numerical simulations through the size of the time and space grids and check our results for consistency through a one-to-one comparison between the output of different methods on different platforms.

Our numerical results will help experimental groups to better control the laser beam properties through customized modulation functions.

THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Big Data and Deep Learning Based Predictive Analytics of High Order Harmonics Generation Optimal Scenarios

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The interaction of ultrashort and intense laser pulses with solid targets and dense plasmas is a rapidly developing area of physics, this being mostly due to the significant advancements in laser technology we have witnessed over the past decades. There is thus, a growing interest in characterizing as accurately as possible the numerous phenomena related to the absorption and reflection of laser light occurring during the interaction. In particular, high order harmonics generation (HHG) is one of the challenging applications in this field. The goals are numerous: achieving higher conversion efficiency for higher harmonics orders, increasing harmonics power and brilliance, reducing their durations towards the attosecond range. Conventionally, HHG theoretical investigations rely heavily on Particle-In-Cell (PIC) simulations. Albeit the extensive improvements this method has seen over the last years, there are some compelling issues related to certain non-physical behaviours that these codes tend to exhibit, not mentioning the considerable computational resources they require.

This paper discusses a novel approach to theoretical investigations of HHG by combining PIC simulations with deep learning and big data with the ultimate goal of constructing a predictive system. Hence, over 4TB of interaction data have been processed using Deep Neural Networks implemented on a private cloud platform built using Hadoop. The optimal configurations of the networks have been determined by deploying a grid search algorithm in conjunction with dropout and constructive learning techniques. Alternatively, some ensemble learning implementations have also been tested. Such predictive systems have the potential of being a reliable tool for estimating optimal interaction scenarios for HHG, scenarios leading towards higher order harmonics or harmonics with particular features such as a particular wavelength range, a particular harmonic pulse duration or intensity.



THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Big data predictive analytics for bioheat transfer modeling

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In this paper are presented some aspects regarding signal processing and big data analytics for bioheat transfer modeling using biomedical sensors. Big data received from sensors and stored in private cloud can be used for predictive analyses with Hadoop technology. For behavior modeling of the certain diseases, the vital signs analyze must be made taking into account the thermoregulation mechanism (internal control system for maintain internal body temperatures in range values for physiological set point for all type of environmental condition) and environmental parameters (pressure, temperature, humidity).

The bioheat transfer is influenced by metabolic processes, blood transport through tissue and blood flow rate. In the experimental part data were received from sensors in contact with skin (noninvasive method). Big data regarding the temperature must be correlated with cardiovascular monitoring, in order to provide a real insight into the causes and effects arising from certain diseases.

Keywords: sensors, cloud, predictive, big data, analytics, bioheat, biomedical, cardio, temperature, signal processing, physiological.

THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Geant4 simulation of cone shape attenuator for uniform spatial dose distribution for a proton beam generated by fs lasers

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E5 experimental area of Extreme Light Infrastructure – Nuclear Physics (ELI-NP) in Măgurele, Romania, will host two high power laser beamlines (1 PW, 25 fs). The interaction of the high power laser and a solid target can generate a broad energy range proton beam (kinetic energy < 100 MeV, number of protons per pulse $< 10^{12}$) and also electrons, gamma-ray, and ion beams. These multi-energetic and multi-component beams will be used to model the outer space radiation environment and study the effect of complex radiation on materials and biological samples [1].

The simulation of interaction between materials and such a multi-energetic beam is very difficult, when using an analytical approach. Thus, we used Geant4 simulation which is a Monte-Carlo approach to solve this problem. The main goal of the simulation is to obtain a beam attenuator for a uniform dose on a wide area (96 well plate, 127.7×85.48 mm²). In the center of the plate, the beam produces a hot spot due to its angular characteristics. The attenuator makes the beam uniformly dense leading to a uniform dose irradiation of the plate. We report here the algorithm of estimating the attenuator shape and dimensions as obtained using a Grid.

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THURSDAY OCTOBER 27, 2016

Algorithms and Applications Development

Improving of the GRID computing system efficiency

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A current problem with a great impact both on the environment and on computers users, is the efficient operation of computing systems. For this purpose should be considered a number of parameters such as: the use of some equipments with low energy consumption as well as server systems that use new low voltage CPUs, storage systems and auxiliaries with high energy efficiency. For maintaining of the environmental parameters within the limits of optimal functioning (e.g. temperature in the range 20 – 23 °C), use of air conditioning systems effective. The present study follows to obtain an improved activity in Data Center and this starts with monitoring of the number of jobs, the power consumption and the temperature variation in time. A correlation of these data was performed in order to reduce the power consumption using the existent equipments.

The next step in the improving of Data Center activity is to establish the influence of the use of the new technologies on energy consumption. We will rely on the use of new technologies in computing systems and on the use of the latest generation air conditioning systems, because they have the greatest impact on energy consumption in a Data Center.

THURSDAY OCTOBER 27, 2016

Status reports and activities of HTC/HPC installations

Overview of the national LCG sites

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This introduction to the reports of the individual Grid sites briefly presents the global contribution of the RO-LCG Federation to the computing support of the LHC experiments.

Technical commonalities and the peculiarities of the centres are emphasized and discussed.

The overall grid activity, as sum of individual sites contribution, and its sharing per virtual communities during the last 12 months is presented.

Also, the recommendations of the International Computing Committee which recently reviewed the RO-LCG infrastructure are discussed and conclusions regarding the future strategy are outlined.



THURSDAY OCTOBER 27, 2016

Status reports and activities of HTC/HPC installations

The evolution of the RO-16-UAIC grid site

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Since commissioned in 2011, the grid site of the A. I. Cuza University of Iași contributed with more than 10% to the total CPU hours accounted at the national level. The site is integrated within the ATLAS French Cloud, providing high-availability support for Monte Carlo simulations.

This communication presents the infrastructure of the site and the results obtained in the last year within the ATLAS and ATLASM8 virtual organisations.

Special emphasis is put on solutions implemented for ensuring the integrity and efficiency of data transfer, and on the use of network statistics monitoring tools in order to improve the security and availability of the site.

THURSDAY OCTOBER 27, 2016

Cloud computing

HPC Cloud Application Orchestration through Self-Organization

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With the widespread adoption of cloud computing and the emergence of new business models, novel approaches on how various services are delivered are identified. Such changes can be identified in how various high performance computing (HPC) resources are obtained and provisioned in cloud environments. In this paper present components identified to play a crucial role in the process of resource acquisition for HPC applications.

We present the architecture of a system aimed in supporting the modeling, deployment and orchestration of HPC Cloud Applications. We introduce the extensions envisioned for existing standards like TOSCA and CAMP, and also we propose interfaces for bridging TOSCA and CAMP middleware with underlying backends supporting the proposed interfaces.



FRIDAY OCTOBER 28, 2016

Cloud computing

Convergence of Decentralized Cloud Platforms and 5G Networks

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From a user's point of view, Cloud Computing can be described in simple terms as accessing and storing information over the Internet from any computer in any remote location instead of accessing it on the own computer's storage. With the exponentially increased capabilities of 5th generation (5G) mobile networks, MCC (mobile cloud computing) will become even more powerful and will develop to such an extent that it is anticipated to have a significant impact on social life.

In this paper we present the implementation of a Cloud Platform making use of 5th generation mobile network capabilities, hardware equipment like Universal Software Radio Peripheral (USRP) and GNU Radio. The purpose is to create a decentralized cloud computing platform that can be used for "disaster recovery" or enterprise data backup making use of smartphone devices and tablets. Finally, a series of tests and simulations assess the platform's interoperability security and performance.

Keywords: MCC; 5G; USRP; GNU Radio; Cloud



FRIDAY OCTOBER 28, 2016

Cloud computing

CLOUDIFIN, the first NGI-RO site participating to the EGI Federated Cloud

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We report the recent implementation of a new cloud computing site, CLOUDIFIN, at the Operations Centre of the National Grid Infrastructure (NGI-RO).

The purpose of the site is twofold: first, to provide infrastructure-as-a-service (IaaS) - virtual machines - to the national research and education community; second, to support within the EGI Federated Cloud the European ESFRI projects in which Romania is involved, such as ELI, DANUBIUS, etc.

The site runs OpenStack Mitaka version on the CENTOS7 platform and the EGI extensions are installed.

At present the site accepts two virtual organisations (VOs) for operational purposes (ops and dteam), and one VO that provides resources for applications prototyping and validation (fedcloud.egi.eu).

The site is currently in tests for FedCloud registration.



FRIDAY OCTOBER 28, 2016

Status reports and activities of HTC/HPC installations

Status report of ISS Grid activities

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Institute of Space Science

In this presentation we will describe the existing datacenter topology and the hardware as well as the architecture and components of main Grid middlewares as well as a status report of ISS performance numbers as seen by the Grid monitoring tools.

FRIDAY OCTOBER 28, 2016

Status reports and activities of HTC/HPC installations

Support of Multiple LHC VOs in a Heterogeneous Grid Site

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Unlike the other RO-LCG Grid sites, RO-07-NIPNE was designed to offer support to all the three LHC experiments which are investigated in Romania (Alice, ATLAS and LHCb).

In this paper the current software and hardware status of the site and its recent upgrades are presented.

In the first part of the article the hardware infrastructure is described, with all its 3 components: computing, storage and network.

In the second part we discuss the software solutions deployed in the last period in order to improve the ATLAS job processing efficiency. These include the implementation of two multi-core queues, each one deployed using a different technology (ARC-CE based on SLURM and CREAM-CE based on Torque+Maui), and the allocation of more resources for the multi-core jobs than for the single-core jobs.



FRIDAY OCTOBER 28, 2016

Status reports and activities of HTC/HPC installations

Current status and future upgrade at ITIM Grid site

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It is important to find ways to make the most of the resources you already have. In sectors like research, life science and many others significant improvements have been realized through grid computing. This domain allows us to link together the processors, storage and/or memory of distributed computers to make efficient use of all available computer resources to solve large problems quicker.

This paper will discuss a major upgrade of the site RO-14-ITIM situated at the National Institute for Research and Development of Isotopic and Molecular Technology (ITIM) from Cluj Napoca, a key computing center in the Nord-West part of Romania.

FRIDAY OCTOBER 28, 2016

Status reports and activities of HTC/HPC installations

New Network Design for the Grid Infrastructure

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Started almost 14 years ago as a need defined by the High Energy Physics communities, used to analyse and process the data sets generated at the Large Hadron Collider, and presented as generating "colossal amounts of data"⁴, the WLCG network infrastructure handles a tremendous load triggered by experiments. "Approximately 600 million times per second, particles collide within the Large Hadron Collider (LHC). Each collision generates particles that often decay in complex ways into even more particles. Electronic circuits record the passage of each particle through a detector as a series of electronic signals, and send the data to the CERN Data Centre (DC) for digital reconstruction."⁵

All this is generating for the Tier2 Grid sites, be it locally or distributed all over the world, plenty of issues regarding their connectivity to the Tier1's, to other sites, or just issues regarding the connection of the worker nodes to the computing elements in the same Data Centre.

In our case the migration to IPV6, as it is already tested for general services within IFIN's network even if still not yet usable/deployed for *all* the Grid services, will manage to cover the IP addressing needs that cannot be covered by IPv4 addresses for the increasing requirements of the Grid computing sites, and will lower the latencies for the data transfers.

As a first step for upgrading the network infrastructure the splitting of the broadcast domains is required, implementing separate subnets for each Grid site, followed by the implementation of High Availability Layer 3 protocols for the three big Grid Computing sites which are hosted in IFIN. This will improve the performance of the entire network infrastructure in terms of latency, delay, availability and reliability.

⁴ <https://home.cern/about/computing>

⁵ <https://home.cern/about/computing>

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