14th International Conference on

Advanced Scientific Computing

ICASC 2023

Cluj-Napoca, 2023

Organizing Committee INCDTIM

Claudiu-Ortensie Filip – president
Gabriel Alexandru Popeneciu
Felicia Diana Nicoară
Felix Fărcaș
Cristian Andrei Lupșe
Jefte Nagy
Izabella Szabó
Mihail Radu Cătălin Trușcă
Laurențiu-Victor Zârbo
Dulea Mihnea Alexandru – IFIN HH

Scientific Comittee

Adam Gheorghe	Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest, Romania
Balaž Antun	Institute of Physics Belgrade, Serbia
Argyrakis Panos	Aristotle University of Thessaloniki/GRNET, Greece
Buša Ján	Technical University of Košice, Slovakia
Dulea Mihnea Alexandru	Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Bucharest, Romania
Gasner Paul	Al. I. Cuza University of Iași, Romania
Zârbo Liviu-Petre	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Miclea Liviu-Cristian	Technical University Cluj-Napoca, Romania
Vázquez-Poletti José Luis	DSA Research Group, Madrid, Spain
Pușchiță Emanuel Dumitru	Technical University Cluj-Napoca, Romania
Trușcă Mihail Radu Cătălin	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania
Țăpuș Nicolae	Politehnica University of Bucharest, Romania
Filip Claudiu Ortensie	National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania

Welcome at ICASC 2023

The ICASC 2023 conference continues the series of the former 14 annual events of the Romanian LCG Federation (RO-LCG) on „Grid, Cloud and High-Performance Computing in Science" (2007-2022). Its title has been changed and the topics have been expanded to offer a more comprehensive coverage of the current evolution in scientific computing.

ICASC 2023 is devoted to recent developments on the application of advanced computing technologies and methods in physics research and related areas. The conference is addressed to specialists with various backgrounds of expertise, such as computer scientists and researchers in numerical methods, developers and users of software applications, quantum computing, providers and beneficiaries of data-intensive services, data center administrators.

Topics:

- Grid Cloud and HPC computing in research, economy and business
- Grid and applications, including eScience and eBusiness
- Quantum Computing
- Embedded and Pervasive Computing
- E-infrastructures for collaborative research
- National contributions to the computational support of large-scale collaborations
- Software and services for distributed computing infrastructures
- Numerical methods for physics
- Development and optimization of software applications in Grid / Cloud / HPC and Quantum environments
- Applications of machine learning methods in scientific research
- Monitoring, management and data organization tools
- Middleware, resource management, and runtime environments
- Processing and analysis of data in computational physics / chemistry / biology
- Distributed multimedia analysis and processing
- Multi-core and cluster computing

ABSTRACTS

The Pivotal Role of Input Validation for Robust and Reliable Bayesian Automatic Adaptive Quadrature

G Adam[1], S Adam[1]

[1]Department of Theoretical Physics Horea Hulubei National Institute for Physics & Nuclear Engineering, IFIN–HH Măgurele, Bucharest, Romania

E-mail: adamg@nipne.ro, adams@nipne.ro

Abstract: New developments are reported for the recursive algorithms of the Bayesian inference based automatic adaptive quadrature (BAAQ) of the one-dimensional Riemann integrals with the aim at securing robust and reliable automatic decisions at critical steps of the solution path. First, the integrand function conditioning at the ends of a subrange decision tree root is resolved within a Bayesian predictor–corrector algorithm, resulting in decisions characterized by uniqueness and reliability. Second, a new subrange strategy refinement enables the highest accuracy available output under cancellation by subtraction. All the reported advances to the reliable definition of the adaptive BAAQ path to the derivation of the automatic solution use appropriate input validation procedures. Index Terms—Bayesian automatic adaptive quadrature, Riemann integral, QUADPACK package, robustness, reliability, input validation, subrange decision tree, cancellation by subtraction.

Devising advanced computing solutions for scientific communities

D Ciobanu-Zabet[1], M Ciubancan[1], I Vasile[1], M Dulea[1]

[1]Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Măgurele, Romania

E-mail: mihnea.dulea@nipne.ro

Abstract: We present the advanced compute solutions that were implemented by DFCTI@IFIN-HH for supporting the national and international research communities. First, we overview the role that the Grid facility plays in providing resources for specific research topics. Then the recent developments of the Cloud IaaS services are detailed. The peculiarities of the two computing paradigms in satisfying different user groups' requirements are emphasized. Finally, we present a federated cloud solution that was recently designed and implemented for sharing resources with cloud centres located in different administrative domains.

A Python-based Approach for Monitoring and Troubleshooting Snort IDS in Distributed Firewall Environments

A D Tudosi[1]

[1]Ștefan cel Mare University of Suceava, 720229, Romania
Department of Computers, Electronics and Automation

E-mail: andrei.tudosi1@student.usv.ro

Abstract: This article provides a comprehensive analysis of a novel script-based framework for monitoring and troubleshooting Snort Intrusion Detection System in distributed firewall environments. The framework provides a comprehensive solution for continuous monitoring by utilizing Python scripting and key libraries, including subprocesses, requests, and time. The script contains crucial functions for evaluating network connectivity, database server availability, resource limitations, and Snort configuration. By performing these tests on a periodic basis, the framework effectively identifies potential issues that could compromise the optimal operation of Snort IDS. This research contribution is distinguished by its focus on distributed firewall environments and its script-based methodology. Real-world flexibility, scalability, and implementation simplicity are ensured by the framework's modular architecture and integration of widely used Python libraries. Through comprehensive evaluations and simulated experiments, the framework demonstrates its ability to identify network connectivity issues, promptly address database server problems, manage resource constraints, and validate Snort configuration. The script-based framework presented here makes a significant contribution to the field of network security by offering a dependable and effective solution for monitoring and troubleshooting Snort IDS in distributed firewall environments.

Enhancing biomarker detection using artificial neural networks

C A Pantis-Simut[1,2,3], M Cosinschi[1,2], N Filipoiu[1,2], A T Preda[1,2,3], G Necula[1], G A Nemnes[1,2,3]

[1] Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Măgurele, Romania
[2]University of Bucharest, Faculty of Physics, 077125 Măgurele-Ilfov, Romania
[3]Research Institute of the University of Bucharest (ICUB), Sos. Panduri 90, Bucharest Romania.

E-mail: mihaela.cosinschi@nipne.ro

Abstract: The development of machine learning techniques has taken off in the last years, and as a result, numerous research fields started to engage in exploiting them. They became popular in different science branches such as biology, physics and chemistry for their remarkable accuracy and response time when solving problems. Regarding the issue of correctly identifying biomarkers, that are associated with specific pathologies, is of great interest nowadays and may be improved by machine learning techniques. In this study, we bring a detailed description of 2D semiconductor heterostructures (i.e. zig-zag phosphorene nanoribbon upon hexagonal boron nitride), brought into contact with biomarkers of certain respiratory diseases (i.e. tuberculosis, SARS-CoV-2), which exhibit large tunabilities in the transport properties. The electronic properties of the system are investigated via DFT simulations, where enough instances are considered to form a complete dataset for the machine learning procedure. Since the conductance obtained from transmission function is sensitive to the molecule position and rotation, we employ artificial neural networks to predict the conductance for different biomarker configuration in the sensor vicinity. This involves the mapping between structural information and the transport properties.

Implementing the Open Science infrastructure at IFIN-HH

N Constantinescu[1], I Vasile[1], M Dulea[1]

[1] Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Magurele, Romania

E-mail: mihnea.dulea@nipne.ro

Abstract: In response to the growing needs of the research community, Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH) is on the way to developing services dedicated to data management and dissemination. Aiming at achieving integration compatibility of the National Library of Physics (NLP) with the European existing services for research data management, the concept of FAIR digital objects is currently implemented. If NLP is to meet the requirements of EOSC Interoperability Framework (EOSC-IF), the development of a strong and flexible infrastructure is required. As, according to the guidelines, the prevalent resources of the future scientific research will be the "*machine-readable artefacts that would support composable or executable workflow*s", we implement an appropriate software framework for managing data sets and many other forms of research outputs. This paper frames our efforts within the European and national policy boundaries and brings forward a solution to create a specialized digital repository. Software solutions and different architectures have been analysed arriving to a desired technical and technological arrangement suitable for future interoperability in the overall context of Open Science.

OpenStack in higher education and academic research: A case study on benchmarking Big Data processing tools

M I Cluci[1], C Pînzaru[1], M Fotache[1], O Rusu[1,2] , P Gasner[1,2]

[1]Alexandru Ioan Cuza University, Iași, Romania

[2]ARNIEC/RoEduNet Agency

E-mail: marius.cluci@uaic.ro

Abstract. Despite many generous grants and discounts provided by major suppliers of cloud resources for academia and/or research teams, the cost incurred by the deployment and operationalization of cloud storage and processing is far from trivial. Hybrid cloud open-source solutions such as OpenStack can prove extremely important for institutions lacking generous financial resources. This is the case with the RaaS-IS platform installed at Alexandru Ioan Cuza University of Iasi which hosts a large variety of research projects on Big Data, Machine Learning, Text Mining, Molecular Biology, etc. developed by research teams from various institutions. This paper introduces a technical solution built on OpenStack, designed to assess the performance of data processing—specifically SQL queries—across a broad spectrum of Big Data tools, such as Apache Hadoop and Spark. The aim of the solution is to evaluate SQL query performance as data volume scales from hundreds of gigabytes to terabytes. The evaluation considers various query parameters, including the number of joins specified in the FROM clause, predicate filters in the WHERE clause, attributes in GROUP BY, conditions in the HAVING clause and many more.

InfiniBand clusters on demand in a distributed container environment

D Ciobanu-Zabet[1], I Vasile[1], M Dulea[1]

[1] Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no.30, P.O.BOX MG-6, Magurele, Romania

E-mail: zdragos@nipne.ro

Abstract: Motivated by the need for providing a versatile parallel computing environment in IaaS Clouds, a new HPC-as-a-service solution was developed for implementing virtual clusters on demand on OpenStack, endowed with MPI capabilities and low latency interconnects. Virtual clusters were deployed by using the InfiniBand (IB) Single Root I/O Virtualization (SR-IOV) interfaces and creating Virtual Functions on the compute nodes. Ubuntu-based flavor VMs were configured using Mellanox OFED (OpenFabrics Enterprise Distribution) with OpenMPI, and their performance was compared with that of udocker containers endowed with OFED and OpenMPI. The HPC users were provided with automatic means of generating MPI clusters, that offer familiar compute environments and resource management systems. To this goal, a tool has been developed in Python that uses libvirt module to attach the Virtual Functions of the IB network device to any new virtual machine. Scaling benchmarks conducted on the CLOUDIFIN OpenStack site showed no significant differences when running the same application on VM and udocker HPC clusters.

Molecular Modelling of Photochemical Properties in Molecules and Supramolecular Assemblies

A A Farcaș[1] and A Bende[1]
[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, 400293 Cluj-Napoca, Romania

E-mail: attila.bende@itim-cj.ro

Abstract: Molecular modelling techniques for computing the most common photochemical properties of molecules and supramolecular sets based on first-principles quantum mechanics methods are reviewed. Accordingly, the framework of the comparision of the electronic absorption and emission spectra obtained using density functional methods and experimental techniques is discussed. Cases for molecular structures with strong radiationless relaxation or spin transition via intersystem crossing are presented in detail. The role of different environmental conditions, like pH, nature of the solvent, solute concentration on the fluorescence emission spectra as well as the quantum yield of the electronic excitation relaxation is also discussed. Various quantum chemical softwares that can be used to model a wide range of photochemical properties will also be presented.

Automated Detection and Management of Deprecated Helm Releases in Kubernetes

I C Donca[1], L C Miclea[1] and O P Stan[1]

[1]Technical University of Cluj-Napoca, Automation Department, Cluj-Napoca, Romania

E-mail: ionut.donca@aut.utcluj.ro

Abstract. This article introduces a Golang application that revolutionizes Helm release management in Kubernetes clusters. Helm, a popular package manager for Kubernetes, simplifies the deployment of applications. However, managing and identifying deprecated Helm releases can be challenging. The Golang application leverages the Kubernetes Go client library and the Helm Go client library to fetch Helm releases from the cluster. Using intelligent algorithms, the application automatically identifies deprecated releases based on their status codes. The article provides a detailed guide on building and running the application, ensuring administrators can efficiently monitor and address deprecated Helm releases. It highlights the significance of proactive actions to maintain the stability and security of the Kubernetes environment. With automated identification of deprecated releases, Kubernetes administrators can optimize their infrastructure, reduce risks, and enhance operational efficiency. The application empowers administrators to stay ahead of potential pitfalls, making Helm release management seamless and hassle-free.

Computing and beyond at INCDTIM

F Fărcaș[1], C Lupșe[1], J Nagy[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: felix.farcas@itim-cj.ro

Abstract: Grid Computing, Cloud Computing, High Performance Computing are three different domain with the same idea, the processing and storing of data. Grid is standardized, Cloud is one step toward standardization and HPC is an ongoing project around the world with a lot of in-house possibility. At National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM) we are processing data for the last 15 years at Grid site RO-14-ITIM and at the HPC system of 7 TFlop for the last 8 years, but would like to add a cloud computing system at our Institute. This paper describes what we have at the Institute and what projects we have to fulfill our long last dream of having a public/private cloud at our location.

Phonon signatures in Majorana mode detection for quantum computing

L Máthé[1], D Sticleț[1] and L P Zârbo[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: levente.mathe@itim-cj.ro

Abstract: The Majorana zero modes could serve as an ideal platform for topological quantum computation where the topological qubits store quantum information nonlocally and thus they provide robust protection against decoherence. We consider a setup consisting of a quantum dot connected to the ends of a topological superconducting nanowire which enables the detection of the Majorana bound states. The dot-nanowire junction forms a loop structure and is threaded by a tunable magnetic flux, which allows one to control the electron transport in the system. In particular, we study the phonon-assisted transport properties in the device when the quantum dot interacts with a single long-wave optical phonon mode. The presence of phonon mode significantly affects the expected Majorana signature. Most importantly, we found that when the two Majorana bound states are unhybridized, the zero-temperature linear conductance has a 2π periodicity as a function of magnetic flux phase, independent of the electron-phonon interaction, the quantum dot energy, or the finite values of dot-Majorana couplings. For a finite overlap between the Majorana bound states, the linear conductance periodicity generally changes to 4π either due to a finite electron-phonon coupling strength, or a dot energy level that is tuned away from the Fermi level.

UAS-based Antenna Radiation Pattern Measurements: A Practical Approach

A Oprea[1,2], G Kovács[1,2], R Nelega[1,2], E Surducan[1], V Surducan[1], F Turcu[3], E Pușchiță[1,2]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania
[2]Faculty of Electronics, Telecommunications and Information Technology, Technical University of Cluj-Napoca, 400027 Cluj-Napoca, Romania
[3]Faculty of Physics, Babeș-Bolyai University, 400084 Cluj-Napoca

E-mail: Emanuel.Puschita@com.utcluj.ro

Abstract: The scope of this work is to indicate, test, and validate a practical approach that provides the radiation pattern of an directive antenna using UAS through in-field RF measurements. The proposed RF measurement method is useful for in-field measurements in remote areas. The UAS performs flights on different altitude ranges around the antenna to be characterized. During the measurements, the antenna is positioned horizontally as well as vertically. At the end of the measurement procedure, the data collected with the help of a spectral analyzer is processed using a custom-built application, which provides the antenna radiation pattern in both the H-plane and E-plane.

Fluxonium qubits for quantum computing

L M Pioraș-Țimbolmaș[1,2], L P Zârbo[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania
[2]Faculty of Physics, Babeș-Bolyai University, 1 Kogălniceanu, 400084 Cluj-Napoca, Romania

E-mail: larisa.timbolmas@itim-cj.ro

Abstract: Quantum bits, or qubits, are the fundamental units of quantum processing. Because of the versatility in tailoring their Hamiltonian, superconducting circuits are one of the most successful approaches for creating qubits. Material refining and circuit parameter adjustment are two methods for improving a superconducting qubit. We analyze and characterize devices based on fluxonium qubit architecture, investigating our system's interaction with the environment when coupled to a readout resonator.

Tackling management complexity in an evolving Grid computing infrastructure

M Ciubancan[1], I Vasile[1], M Dulea[1]

[1]Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), Str. Reactorului no. 30, P.O.BOX MG-6, Măgurele, Romania

E-mail: ciubancan@nipne.ro

Abstract: This communication is an overview of the recent years' development that the DFCTI's Grid infrastructure for particle physics has undergone in order to ramp up its contribution to the computational support for the Run 3 research activities at the Large Hadron Collider. The structural changes that the Romanian Tier 2 Federation underwent during this period, which aimed at the global simplification of management, led to the increase in the role of the Grid site managed by DFCTI. This one took charge of tasks previously carried out by other sites, currently ensuring the entire national Grid support for the LHCb experiment and for the ATLAS analysis. Besides, measures were implemented for reducing the complexity of the site. The adopted technical solutions, the resource upgrades and the achievements obtained are presented in detail.

Development of Grid Computing in the last years at INCDTIM

F Fărcaș[1], J Nagy[1], C Lupșe[1], M R C Trușcă[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: felix.farcas@itim-cj.ro

Abstract: Grid Computing Site RO-14-TIM, situated at the National Institute for Research and Development in Informatics (INCDTIM) in Cluj-Napoca, Romania, has witnessed significant growth and development over the past five years. This abstract provides a concise overview of the evolution and advancements made at this site, which serves as a crucial hub for grid computing in the region. Since its inception, Site RO-14-ITIM has been a pivotal player in the field of grid computing. It has contributed to research in ATLAS experiment through CondeGrid projects. The past five years have seen notable developments in infrastructure, research collaborations, and the deployment of advanced technologies. Grid Computing Site RO-14-ITIM at INCDTIM, Cluj-Napoca, has demonstrated substantial growth and development in the last five years. Through infrastructure expansion, strategic collaborations, technological innovation, and a broadening of application domains, the site has strengthened its position as a vital resource for researchers, scientists, and academics. The ongoing commitment to excellence in grid computing and scientific research continues to make Site RO-14-ITIM a valuable asset in the field of advanced computing and data analysis.

Experimental Control Of Thermal Processes To Increase The Availability And Reliability In Datacenters

J Nagy[1], M R C Trușcă[1]

[1]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donat, 400293 Cluj-Napoca, Romania

E-mail: jefte.nagy@itim-cj.ro

Abstract: Optimizing thermal processes within data centers to decrease energy consumption and reduce environmental impact has always been a significant challenge. Exploring solutions to enhance current cooling systems and decrease energy inefficiency can be approached in various ways.

This study aimed to refine the thermal processes in INCDTIM's data center by introducing a smart cooling system that delivers targeted cooling as and when required. Temperature sensor readings are stored in the Cloud for statistical analysis and pattern identification. Using these patterns, temperature regulation can be further honed. Experimental methods were employed, incorporating both passive (pipes, plenum optimizations) and active strategies (active grilles for efficient air regulation, and remote automation using PLC integrated with Cloud applications). Our methodology began with a 3D model of the data center, which was followed by simulations of current thermal conditions using the Ansys CFD (Computational Fluid Dynamics) software module. These simulations pinpointed problem areas and identified cold pockets, facilitating the creation of an enhanced cooling system. Subsequent to this, we compared the improved thermal conditions with the initial state to validate that the physical implementation mirrored our theoretical model.

Automation needs to be built in order to control the thermal processes. Connecting the PLC to a Cloud-based platform is the aim to optimize and control the thermal processes via the Cloud