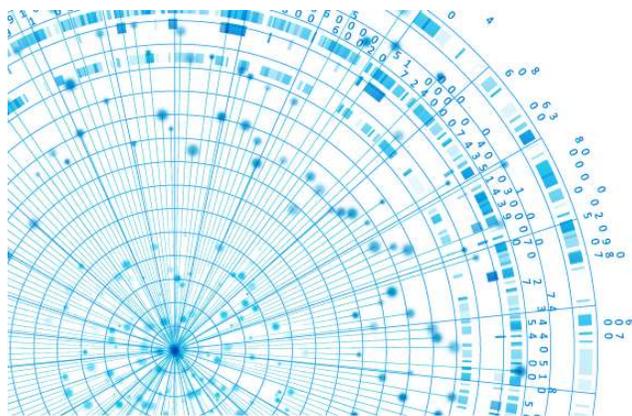


PROGRAM BOOK & ABSTRACTS



15th USERS CONFERENCE

16 - 17 September 2021



RED ESPAÑOLA DE
SUPERCOMPUTACIÓN



Online Conference

September 2021

@RES_HPC #JURES21

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Welcome

Dear RES user,

For the second year, we are forced to meet again online instead of our annual face-to-face meetings. Although we are witnessing some clear signs of recovery due to vaccination campaigns, we have decided that this 15th edition will be held online again. We are going virtual but, since 14th edition was planned to be held in Cáceres, we will bring some of the cultural and artistic beauties of such wonderful city to each of you. So be ready to enjoy this new edition of JURES!

During this last year, RES has faced many important challenges:

- We had the first call for data management projects, with a high level of participation and with high quality proposals received. It is without any doubt the era of data, and a supercomputer center that generates vast amounts of data from your research activities needs to provide data services. The next call will open by the end of this year 2021.
- RES network has increased with the incorporation of new members. Institutions such as the public entity Navarra de Servicios y Tecnologías (NASERTIC), the Port d'Informació Científica (PIC) and the Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT) have joined the network that currently totals 14 institutions providing access to supercomputing power to the research community.
- Eight RES members have engaged in the creation of the HPC Spanish Competence Centre (<https://eurocc-spain.res.es>) under the framework of the EuroHPC JU funding program. This Competence Centre will deal with the mapping and the development of HPC competences for SMEs and public administrations. This will be complementary with the forthcoming regional Digital Innovation Hubs (DIH). We are witnessing the opening of HPC to businesses and industry to enhance their overall competitiveness.
- A new RES Strategic Plan has been elaborated for the period 2021-2024, in parallel with the update of the Spanish ICTS (Infraestructuras Científicas y Técnicas Singulares) map and the related investment plans. Hopefully, the new EU Next Generation funding scheme will bring additional funds to the computing infrastructures, aiming at providing wider access to all project applications.

Despite the difficulties encountered, RES has again performed successfully thanks to the strong commitment of the nodes and to the cooperation and understanding of RES users community.

We deeply thank our kind sponsors Huawei, Fujitsu, HP Enterprise, HPCNow! and AMD that will make it possible to feel closer by sharing a breakfast at home.

We hope to meet all of you in person for the 16th Users Conference in September 2022. Join us for this exciting new experience that brings HPC science directly to you!

Sergi Girona, RES coordinator

Cáceres, the city of three cultures (virtual visit)¹

The traditional ochre-and-alabaster streets of Cáceres look like a scene from an old sepia photograph come to life. Located in Extremadura, Spain's least touristy region, Cáceres' old town, a unique mix of Roman, Islamic, Gothic and Renaissance architecture surrounded by large stone walls, is a UNESCO World Heritage Site.

Streets, squares, palaces, churches and walls, in a magnificent state of preservation, will take you back to a glorious past, in which you will relish the marvellous artistic manifestations that the three cultures - Christian, Islamic and Jewish - left in our city. This diversity will allow you to enter the Monumental City through a Roman door, come across the beautiful Old Jewish Quarter at the exit of an Almohad tower or behold a Renaissance palace next to a Mudejar façade. The cultural coalescence has bequeathed us an excellent Monumental Patrimony at the same time that it has forged the hospitable personality of the people of Cáceres.

There is not a better time to visit this amazing city than the afternoon. Let me show you Cáceres, World Heritage, UNESCO and Third Best Preserved Monumental City in Europe, which becomes magical when sun sets. Join me for a superb walking tour to the Old Town and feel yourself a star of history.

We will begin at the Main Square and immerse in an amazing labyrinth of charming narrow streets and breath-taking squares. Palaces here, towers above, shields everywhere. . . Cáceres is an incredible compilation from medieval and Renaissance times. Come with me and discover all the secrets that only a few locals really know!

See the program to attend the virtual visit.



¹ <https://time.com/collection/worlds-greatest-places-2021/6079226/caceres-spain/><https://turismo.caceres.es/en>

<https://turismo.caceres.es/en/>

Program

Thursday, September 16th

- 14:30** *Registration*
- 15:00** *Welcome address*
José I Doncel, Ministerio de Ciencia e Innovación
Sergi Girona, RES, Barcelona Supercomputing Center, BSC-CNS
José Luis González, CénitS-COMPUTAEX
- 15:15** *RES Presentation & updates*
Sergi Girona, RES, Barcelona Supercomputing Center, BSC-CNS
- 15:30** Keynote scientific lecture: *The European Genome-phenome Archive. Why and how we keep human genomic data safe and visible at the same time*
Teresa d'Altri, EGA, Center for Genomic Regulation, CRG
- 16:15** 2020 RES Award: *The quest for room-temperature superconductivity guided by first-principles calculations*
Ion Errea, Donostia International Physics Center, UPV/EHU
- 16:45** *RES Users Committee (CURES): presentation and activity report*
Miguel A. Aloy, CURES Chair, University of Valencia, UV
- 17:00** Sponsor talk: *Leading the new era of HPC*
Simón Viñals Larruga, Business Development Manager Spain & Portugal, AMD
- 17:15** BREAK
- 17:30** *Structural analysis by cryo EM of SARS Cov-2 spike*
Laura del Cano, JM^a Carazo, Centro Nacional de Biotecnología (CNB-CSIC)
- 17:50** *QM/MM computational studies of the main protease of SARS-CoV-2: towards the design of new inhibitors*
Vicent Moliner, Universitat Jaume I, UJI
- 18:10** *Impact of the COVID-19 lockdowns upon air pollution at the European level*
Oriol Jorba, Barcelona Supercomputing Center, BSC-CNS
- 18:30** *Early perturbation of the Ab42 conformational landscape by novel curcumin azobioisosteres*
Tiziana Ginex, Centro de Investigaciones Biológicas, CIB-CSIC
- 18:40** *Revealing the key factors of direct activation mechanism of AMPK based on isoform-dependent complex*
Carolina Estarellas, Universidad de Barcelona, UB
- 18:50** *Three-dimensional models of magnetorotational core-collapse supernovae*
Martin C Obergaulinger, University of Valencia, UV
- 19:05** SOCIAL ACTIVITY: Guided visit to Cáceres old Medieval quarter

Friday, September 17th

- 8:45** Program updates - Welcome 2nd day, RES
- 9:00** Sponsor talk: *DNN workload on large-scale parallel environment*
Kohta Nakashima, Senior Director of Fujitsu ICT Labs
- 9:15** Keynote technology lecture: *Quantum computation from zero*
José I Latorre, University of Barcelona, UB
- 10:00** *The noisy intermediate-scale quantum computing era*
Alba Cervera, University of Toronto
- 10:20** *Investigating the practical complexity of quantum computations*
Juan José García-Ripoll, Consejo Superior de Investigaciones Científicas, CSIC
- 10:40** *HPC simulations of hybrid quantum algorithms*
Artur Garcia, Barcelona Supercomputing Center, BSC-CNS
- 11:00** Sponsor talk: *The Road to Exascale*
Adriano Galano, Head of HPC and Artificial Intelligence for Southern Europe, Hewlett Packard Enterprise, HPE
- 11:15** BREAK / CATERING AT HOME
- 11:30** Sponsor talk: *When portability and reproducibility also meets performance*
Jordi Blasco, CTO, HPCNow!
- 11:50** *Numerical modeling of double-polarity subduction*
Mireia Peral, Geociències Barcelona, Geo3Bcn-CSIC
- 12:10** *Database generation for 2.5D borehole resistivity measurements using refined isogeometric analysis*
Ali Hashemian, Basque Center for Applied Mathematics, BCAM
- 12:30** *Study of how the eccentricity factor of elliptical nozzle affects the primary atomization using Direct Numerical Simulation*
Lucas A. González-Montero, Universitat Politècnica de València, UPV
- 12:50** *Simulations of defects and nucleobases adsorption in 2D materials by DFT-based calculations*
Blanca Biel, University of Granada, UG
- 13:10** Magnetism, topology and optics of novel 2D materials
Alejandro Molina-Sánchez, Institute of Materials Science, University of Valencia, UV
- 13:30** BREAK

- 15:00** *Homogeneous nucleation of NaCl in supersaturated solutions*
Cintia Pulido, Universidad Complutense de Madrid, UCM
- 15:20** *The role of light on the contemporary composition of the genetic material: are other alternative building blocks viable?*
Inés Corral, Universidad Autónoma de Madrid, UAM
- 15:40** *In silico study of Li6PS5Cl Argyrodite electrolyte degradation at contact with bare and coated metallic Li anode*
Andrey Golov, CIC energiGUNE
- 16:00** *Predicting the structure and oxidation state of complex materials under reaction conditions*
Jon Quinlivan, Albert Bruix, Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, UB
- 16:20** *Bats as bioindicators in the North-East Iberian Peninsula (Catalonia)*
Adrià López Baucells, Museu de Granollers
- 16:40** Sponsor talk: *How metrics make the difference in HPC system design*
Solal Amouyal, HPC Group Manager, Huawei Tel-Aviv Research Center, Israel
- 16:55** CLOSING CEREMONY / RES AWARD
José I Doncel, Ministerio de Ciencia e Innovación
Sergi Girona, RES, Barcelona Supercomputing Center, BSC-CNS
José Luis González, CénitS-COMPUTAEX

TECHNICAL SESSION RES / ONLY FOR RES STAFF

During the afternoon, the support and system administration staff of the RES nodes organize a set of technical sessions related to the administration and performance of the supercomputing facilities such as security networks, new machine architectures, new data management systems and other topics related with the day-to-day work required to keep the RES HPC machines up to date and operative.

RES Awards

The Spanish Supercomputing Network (RES) offers high performance computing (HPC) resources to the scientific community to carry out analysis and simulations for their research projects. Recently, it also offers data management services to the researchers. Besides computing time and data services, the RES services offer expert advice and support for its users. As an output of the users' research projects many scientific papers are published annually by the RES users, mainly in the framework of international collaborations.

The RES Outstanding Scientific Paper Award aims at highlighting the quality of the research carried out by RES users. Candidates can participate by submitting their papers published during the last year in a peer-reviewed scientific journal. The nomination is decided by the RES Council based on the propositions of the Access Committee coordinators which will evaluate each application based on the excellence of the candidate and the work presented in the paper. The work described in the paper must have been carried out using RES HPC resources. The awarded researcher will be invited for an oral presentation during the next year edition of the Users Meeting.

In its 3rd edition the 2021 awardee will be announced during the closing session of the 15th RES Users Conference (see Program). This is an award that the RES assigns as a sign of recognition to the high-quality works that have been published using the HPC resources provided.

Past Awards:

2019 **Manuel Ortuño**, Institute of Chemical Research of Catalonia (ICIQ)

Gas reactions under intrapore condensation regime within tailored metal-organic framework catalysts

Authors: Iker Agirrezabal-Telleria, Ignacio Luz, Manuel A. Ortuño, Mikel Oregui-Bengoechea, Iñaki Gandarias, Núria López, Marty A. Lail & Mustapha Soukri.

Nature Communications (2019) 10:2076.

2020 **Ion Errea**, Donostia International Physics Center (DIPC)

Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride

Authors: Ion Errea, Francesco Belli, Lorenzo Monacelli, Antonio Sanna, Takashi Koretsune, Terumasa Tadano, Raffaello Bianco, Matteo Calandra, Ryotaro Arita, Francesco Mauri, José A Flores-Livas.

Nature (2020) 578:7793.

Abstracts (in alphabetical order of the presenter's surname)

How metrics make the difference in HPC system design

Solal Amouyal

HPC Group Manager, Huawei Tel-Aviv Research Center, Israel

Choosing the right benchmark has always been a part of HPC system design. Considerable effort has been devoted to the development and standardization of benchmarks, for different aspects of parallel computing, while the key metrics have seen relatively little change: FLOPS and GB/s still dominate system evaluation. Nevertheless, a weather forecasting system highlights different challenges than a cluster for CFD simulations or bioinformatics research. This talk will showcase Huawei's latest research on targeted optimizations of specific computational fields, and show how aligning the performance metrics with the system's goals makes a difference.

Simulations of defects and nucleobases adsorption in 2D materials by DFT-based calculations

Blanca Biel¹, Pablo Pou², Reza Rezapour¹

¹Dept. Atomic, Molecular and Nuclear Physics, University of Granada, ²Dept. Theoretical Condensed Matter Physics, Autonomous University of Madrid

The goal of our past activities was to acquire a deep knowledge of the modifications of the electronic properties of MoS₂ in the presence of defects and metallic substrates by means of advanced STM simulations. We have investigated, by means of DFT-based calculations, the effect of point-like defects (vacancies, substitutional dopants and other impurities) in 2D materials, and their characterization by means of AFM and STM techniques. On the other hand, in the search for fast, inexpensive and accurate tools for DNA sequencing and mutation recognition, we have investigated the viability of a graphene-based biosensor to recognize nucleobase mutations in DNA or RNA fragments attached to a graphene nanoribbon (GNR). To this aim, we addressed the quantum mechanical (QM) calculation of the transport characteristics of both isolated nucleobases and fragments of functionalized nucleic acids onto a GNR system in vacuum.

When portability and reproducibility also meets performance

Jordi Blasco

CTO, HPC Now! Consulting

One of the major challenges that the scientific community is facing is the portability and reproducibility required by HPC applications without sacrificing performance. Traditionally, in order to achieve portability, the optimizations levels and the exposure to advanced instructions sets were removed at the compilation stage. This strategy guarantees that the binaries and libraries can be used for old and also modern architectures. Unfortunately, this approach has a huge impact on the performance of the HPC applications. The European Environment for Scientific Software Installations (EESSI) is a collaboration between different European HPC sites & industry partners, with the common goal to set up a shared repository of scientific applications that can be used on a variety of systems. The design architecture elevates this solution to a completely agnostic shared repository from a micro-architecture and also from a Linux distribution point of view. This approach allows exposing the scientific software through a seamless user environment and enables the scientific community to use the software packages in a standard HPC cluster, a cloud environment, or a personal workstation. In this talk, HPCNow! will introduce how some clients have been able to achieve portability and long-term reproducibility without compromising performance, by adopting the EESSI architecture.

About the EESSI project: website: <https://www.eessi-hpc.org>; GitHub: <https://github.com/EESSI>; documentation: <https://eessi.github.io/docs>; Twitter: https://twitter.com/eessi_hpc

Predicting the structure and oxidation state of complex materials under reaction conditions

Jon Quinlivan, Albert Bruix

Departament de Ciència del Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona

Nanostructuring greatly expands the possibilities for designing novel materials with improved functionality, but the increased complexity hinders their characterization and understanding. The goal of our research is to tackle this complexity by combining first principles calculations, concepts from statistical mechanics and thermodynamics, multi-scale modelling approaches, global optimization algorithms, and machine learning methods. During this talk, an overview of our recent efforts to characterize complex nanomaterials will be given, focusing on a few case studies relevant for heterogeneous catalysis.

The noisy intermediate-scale quantum computing era

Alba Cervera

Computer Science and Chemistry departments, University of Toronto, Canada

A universal fault-tolerant quantum computer that can solve efficiently problems such as integer factorization and unstructured database search requires millions of quantum bits (qubits) with low error rates and long coherence times. While the experimental advancement towards realizing such devices will potentially take decades of research, noisy intermediate-scale quantum (NISQ) computers already exist. These computers are composed of hundreds of noisy qubits, i.e. qubits that are not error-corrected, and therefore perform imperfect operations in a limited coherence time. In the search for quantum advantage with these devices, algorithms have been proposed for applications in various disciplines spanning physics, machine learning, quantum chemistry and combinatorial optimization. The goal of such algorithms is to leverage the limited available resources to perform classically challenging tasks. In this talk, I will review the state-of-the-art quantum computation as well as providing a summary of some of the most used NISQ algorithms and their applications.

The role of light on the contemporary composition of the genetic material: are other alternative building blocks viable?

Inés Corral

Universidad Autónoma de Madrid, UAM

The current composition of the genetic alphabet is the result of the persistence of DNA and RNA monomers against multiple selection pressures operating on the early Earth, among which UV light exposure played a prominent role. Despite being strong UV absorbers, native nucleobases have developed extremely efficient mechanisms to dissipate the absorbed energy, preventing, this way, DNA damage. Our aim is to investigate the decay routes of non-canonical purine- and pyrimidine-derivatives to elucidate the origin of the photostability of life building blocks, and to identify potential prebiotic genetic ancestors that might have composed the primordial soup.

These results will help rationalize the relation between the functionalization schemes of purine and pyrimidine cores and their observed photophysics, which is key to determining the electronic and structural factors that established the superiority of the five contemporary DNA and RNA nucleobases against other organic chromophores.

The European Genome-phenome Archive. Why and how we keep human genomic data safe and visible at the same time

Arcadi Navarro^{1,2}, Jordi Rambla², Teresa D'Altri², Angel Carreño²

¹Universidad Pompeu Fabra, UPF, Barcelona, ²Center for Genomic Regulation, CRG, Barcelona

Thanks to the advances in DNA sequencing technologies, huge amount of human genomic data is continuously generated all around the world, providing scientists with an irreplaceable source of knowledge, and holding promises of enormous medical advances. Such data is of exceptional value for research and therefore, from an ethical point of view, must be reused as many times as possible to empower, validate or complement new studies. At the same time, human genomic sequences are considered private data and are protected by the European GDPR regulation. Therefore, access to the data must be legally controlled and restricted only to allowed researchers. The European Genome-phenome Archive provides a platform that enables both of these purposes: law compliant and secure permanent storing of private genomic data while making it searchable and thus reusable by other researchers.

Structural analysis by cryo EM of SARS Cov-2 spike

Laura del Caño, José María Carazo

Centro Nacional de Biotecnología, CSIC

The biocomputing unit in the Centro Nacional de Biotecnología has expertise in processing CryoEM data which has been widely used during the COVID19 outbreak to access the three dimensional structure of the Sars-Cov2 virus. In collaboration with Prof McLellan, from U. Texas at Austin, we reprocessed their data on the infective Spike in the prefusion state with our own workflows, reaching a substantially higher resolution, specially in the most variable and complex parts of the map. We also received several new samples of complexes of the Spike with neutralizing agents, providing us with vital insight on ways to prepare new generations of anti virals. These computational workflows were executed using Scipion, a software framework that integrates several EM packages allowing full traceability and reproducibility. Some of the workflow processing steps required powerful hardware to run and were executed in the Minotauro cluster at BSC.

The quest for room-temperature superconductivity guided by first-principles calculations

Ion Errea^{1,2,3}

¹Departamento de Física Aplicada, University of the Basque Country (UPV/EHU), ²Centro de Física de Materiales (CSIC-UPV/EHU), ³Donostia International Physics Center, Donostia

Reaching room temperature superconductivity is one of the greatest challenges in physics. In the last few years, new superconducting compounds based on hydrogen have been discovered experimentally at record temperatures, even at room temperature. However, a pressure larger than one million atmospheres is required to synthesize these new hydrogen-based superconductors. The challenge now is to reduce the pressure needed to form these magnificent superconductors. In this talk I will review how first-principles calculations performed in modern and advanced high-performance computing facilities have been crucial in the discovery of these new high-temperature superconductors. I will argue that new and advanced theoretical methods that incorporate the effect of atomic quantum fluctuations will be crucial for discovering new hydrogen-based compounds that superconduct at such high temperatures also at low, eventually ambient, pressure.

Structural basis of the selective direct activation of AMPK: β_1 - versus β_2 -isoform dependent complexes

Carolina Estarellas, Katerina Barmpidi, Alessia Forte, Elnaz Aledavood, F. Javier Luque

Department of Nutrition, Food Science and Gastronomy. Faculty of Pharmacy and Food Science. Institute of Computational Chemistry (IQTC-UB). University of Barcelona

AMPK is a key energy sensor regulating the cell metabolism and the evolutionary adaptation to different tissues is accomplished through the expression of distinct isoforms that can form up to 12 complexes with notable differences in the sensitivity to allosteric activators. To understand the allosteric regulation of this enzyme, we have assessed the structural and dynamical properties of $\alpha_2\beta_1$ and $\alpha_2\beta_2$ AMPK complexes formed with small ligands such as A-769662, SC4, PF739, and MT47-100.^{1,2} The MD simulations reveal the mechanical sensitivity of the $\alpha_2\beta_1$ complex, in contrast with a larger resilience of the $\alpha_2\beta_2$ species. These findings are discussed considering the changes in the residue content of b-subunit isoforms, particularly the $\beta_1\text{Asn111} \rightarrow \beta_2\text{Asp111}$ substitution is considered a key factor in modulating the mechanical sensitivity of $\alpha_2\beta_1$ and $\alpha_2\beta_2$ complexes.

¹Aledavood, E. et al. *J. Chem. Information Model.*, **2019**, 59, 2859-2870. ²Aledavood, E. et al. *Comput. Struct. Biotechnol. J.*, **2021**, 19, 3394-3406.

The Road to Exascale

Adriano Galano

Head of HPC and Artificial Intelligence for Southern Europe, Hewlett Packard Enterprise (HPE)

The evolution towards the Exascale era leads us to address a large number of technological challenges: the changing explosion in the world of computing, new storage models, interconnection systems, new software paradigms and the energy efficiency implied by these levels of scalability. In this lecture we will talk about: (i) the current state of the "Exascale race" globally; (ii) how HPE CRAY is approaching the different Exascale projects in the USA; (iii) The innovations in both hardware and software of these infrastructures: evolution of processors, accelerators, storage systems and software; (iv) The challenge of adapting and adapting software experiences for the Exascale era.

HPC simulations of hybrid Quantum algorithms

Artur Garcia

Barcelona Supercomputing Center (BSC-CNS)

In this talk we present our approach to the simulation of Quantum algorithms on supercomputers. Our method is based on Tensor Networks. This numerical technology allows the simulation of large Quantum circuits, and it is a convenient description to an implementation and execution in HPC systems. With these tools, one can simulate hybrid systems performing optimization tasks using classical and Quantum resources. As an example, we show how to optimize the celebrated QAOA method using classical tools borrowed from classical Reinforcement Learning.

Investigating the practical complexity of quantum computations

Juan José García-Ripoll

Consejo Superior de Investigaciones Científicas, CSIC

In this brief talk, I will summarize our lines of research on quantum optimization, quantum simulation and machine learning at the Quinfog group in IFF-CSIC. In particular, I will focus on different works, where we analyze the added value of entanglement in these tasks, showing that it is not just the amount of entanglement, but also the adaptation and expressive power of a quantum algorithm what seems to determine the actual performance.

Refs.: P. Díez-Valle et al, arXiv:2103.14479; S. Altares-López et al, arXiv:2105.12626

Early perturbation of the A β 42 conformational landscape by novel curcumin azobioisosteres

Tiziana Ginex

Centro de Investigaciones Biológicas, CIB-CSIC

Recently, we reported some azobioisosteric analogs of curcumin and taxifolin with anti-amiloidogenic properties that exceed the parent compounds in activity against A β 42 aggregation inhibition, intracellular oxidative stress and neuroinflammation. [1] The interaction with full-length A β 42 peptide was thus studied by means of replica-exchange molecular dynamics simulations. Given the well-known critical impact of the chosen parameters on the IDPs conformational landscape, [2] two different force fields (Amber and CHARMM) were used to simulate the effect of a representative azobioisostere on the A β 42 peptide in a dimeric assembly. The analysis of the trajectories reveals that the presence of the azobioisostere redirects the conformational landscape of A β 42 toward off-pathway conformations, favoring the formation of aggregates that nucleate around the curcumin-taxifolin hybrid. [3] These results provide an initial basis to explore the introduction of chemical modifications that may improve the pharmacological profile of novel azobioisosteric derivatives.

1. Hofmann J, Ginex T, Espargaró A, Scheiner M, Gunesch S, Aragón M, Stigloher C, Sabaté R, Luque FJ, Decker M. Azobioisosteres of Curcumin with Pronounced Activity against Amyloid Aggregation, Intracellular Oxidative Stress, and Neuroinflammation. *Chem. Eur. J.* 2021; 27(19): 6015-6027.
2. Rauscher S, Gapsys V, Gajda MJ, Zweckstetter M, de Groot BL, Grubmüller H. Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. *J. Chem. Theory Comput.* 2015; 11(11): 5513-24.
3. Ginex T and Luque FJ. Early perturbation of the A β 42 conformational landscape by novel curcumin azobioisosteres. *ACS Chem. Neurosci.* (under revision).

In silico study of Li₆PS₅Cl Argyrodite electrolyte degradation at contact with bare and coated metallic Li anode

Andrey Golov, Javier Carrasco

Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Álava Technology Park, Vitoria-Gasteiz

We present results of interfacial properties predictions based on *ab initio* molecular dynamics simulations of 12 Li/Li₆PS₅Cl and 4 Li/coating/Li₆PS₅Cl interface models with Li₂Sn₅, MoS₂, LiF, and Li₃P thin-film coatings. We found that Li₆PS₅Cl is not compatible with metal Li anode due to a chemical reaction between them. The coatings significantly decrease the degradation rate, while only MoS₂ fully prevents the reaction. Evaluation of ionic conductivity based on topological analysis of procrystal electron density distribution shows that Li diffusion through the MoS₂, LiF, and Li₃P to be hindered by a factor of 7.5, 3, and 2 with respect to bulk Li₆PS₅Cl. In contrast, the presence of Li₂Sn₅ almost does not affect interfacial resistance. These results provide useful information about properties and atomic-scale processes at solid-electrolyte interfaces for design of sulfide-based all-solid-state batteries.

Study of how the eccentricity factor of elliptical nozzle affects the primary atomization using Direct Numerical Simulation

F. J. Salvador, J. Gimeno, M. Carreres, L. A. González-Montero

CMT – Motores Térmicos, Universitat Politècnica de València

The atomization process is a physical phenomenon that takes place as an essential mechanism in many industrial fields. In this context, Direct Numerical Simulations (DNS) are becoming more important as a fundamental tool to shed light on the processes that take place on the near field, where the optical access is difficult and expensive. However, the limitations of DNS prevent from accurately solving most real engineering. Thus, a more fundamental standpoint is chosen to first understand the fundamental mechanisms that drive the process. This work presents a study of the influence of the elliptical nozzle eccentricity factor shape on droplet formation and distribution, and turbulent structures by using DNS simulations performed with the Paris-Simulator code. The injection inflow conditions are obtained by mapping velocity fields from Large Eddy Simulation (LES) of two elliptic duct with eccentricity factor of 0.85 and 0.92 with a Reynolds number around 5000 for both cases.

Database generation for 2.5D borehole resistivity measurements using refined isogeometric analysis

Ali Hashemian¹, Daniel Garcia², Jon Ander Rivera^{1,3}, David Pardo^{1,3,4}

¹BCAM – Basque Center for Applied Mathematics, Bilbao, Basque Country, ²IDAEA – Institute of Environmental Assessment and Water Research, Barcelona, Catalunya, ³University of the Basque Country UPV/EHU, Leioa, Basque Country, ⁴Ikerbasque – Basque Foundation for Sciences, Bilbao, Basque Country

Borehole resistivity measurements are routinely inverted in real-time during geosteering operations. The inversion process requires a massive database that relates multiple Earth models to the corresponding borehole resistivity measurements. We often produce such a database a priori using tens of thousands of simulations by solving the dimensionally reduced Maxwell's equations with different 2D Earth models in the context of the so-called 2.5D analysis. To efficiently generate a massive database for borehole resistivity measurements, we propose to use the refined isogeometric analysis (rIGA) as a high-performance computational (HPC) method to perform rapid and accurate 2.5D simulations. rIGA decreases the computational cost of LU factorization when solving the discretized form of Maxwell's equations. Numerical results show that we can generate a synthetic database composed of 100K Earth models with the corresponding measurements in 56 hours using two CPUs on the MareNostrum4 supercomputer at Barcelona Supercomputing Center.

Impact of the COVID-19 lockdowns upon air pollution at the European level

Marc Guevara, Oriol Jorba, Albert Soret, Hervé Petetin, Dene Bowdalo, Kim Serradell, Carles Tena, and Carlos Pérez García-Pando
Earth Science Department, Barcelona Supercomputing Centre, BSC-CNS

The spread of the new COVID-19 disease forced national Governments across the world to implement extensive lockdown measures during 2020. This resulted in unprecedented reductions of anthropogenic emissions that significantly impacted air quality levels. In this talk, we will present the work aiming at quantifying the impact of the different phases of the lockdowns upon air quality. We have estimated both the actual 2020 air quality and the so-called “business-as-usual” levels that would have been observed in the absence of the lockdowns. The results of the work provide insights on the response of reactive species during the lockdowns that will be useful to design future policy-based emission reductions, and help quantifying the changes in short-term mortality attributable to changes in air pollution due to the lockdowns during 2020.

Homogeneous nucleation of NaCl in supersaturated solutions

C. P. Lamas¹, J. R. Espinosa², M. M. Conde³, J. Ramírez³, P. Montero de Hijes¹, E. G. Noya⁴, C. Vega¹, E. Sanz¹

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The Seeding method is an approximate approach to investigate nucleation that combines molecular dynamics simulations with classical nucleation theory. This technique has been successfully implemented in a broad range of nucleation studies in recent years. However, its accuracy is subject to the arbitrary choice of the order parameter threshold used to distinguish liquid-like from solid-like molecules. We revisit here the crystallization of NaCl from a supersaturated brine solution and show that consistency between Seeding and rigorous methods like Forward Flux Sampling (from previous work) or spontaneous crystallization (from this work), is achieved by following a mislabelling criterion to select such threshold (i. e. equalling the fraction of mislabelled particles in the bulk parent and nucleating phases). This work supports the use of Seeding to obtain fast and reasonably accurate nucleation rate estimates and the mislabelling criterion as one giving the relevant cluster size for classical nucleation theory in crystallization studies.

Quantum computation from zero

José I. Latorre

University of Barcelona

We review the very basic ideas on quantum computation. We also discuss the relation of quantum computers with supercomputers.

Bats as bioindicators in the North-East Iberian Peninsula (Catalonia)

Adrià López Baucells

Museu de Granollers

With the aim of broadening the knowledge on the distribution of the bats in Catalonia, between the years 2004 and 2009, it has been carried out an important effort of survey: 556 sessions of capture, 317 reviews of shelters, 3,336 reviews of 788 bat boxes and 2,663 sessions of bat detectors (22,683 minutes of sounds analysed) in all types of habitats situated between 0 and 2,700 meters above sea level. Information data has been obtained for 26 species of bats in 594 new grids of UTM 10x10 km. Besides, new information of the less known species like: *Nyctalus lasiopterus*, *Myotis alcathoe*, *Myotis mystacinus*, *Myotis escalerai*, *Myotis sp1*, *Myotis bechsteinii*, and *Plecotus macrobullaris*, has been updated. According to the existing datum, the study proposes a category of conservation (red list) of all the species of Catalonia and invites to follow up ecological studies for a correct management and conservation of the bats of Catalonia.

Magnetism, Topology and Optics of Novel 2D Materials

Alejandro Molina-Sánchez

Institute of Materials Science (ICMUV), University of Valencia

2D materials have become a platform to study physical paradigms and phenomena at the nanoscale. The discovery of ferromagnetic order in 2D materials have increased the interest in these materials. Using BSC, we have investigated the link between magnetism and topological properties. We have characterized the optical properties of magnetic monolayers by calculating the magneto-optic Kerr effect. Using a combination of density functional and Bethe-Salpeter theories, we calculate both the optical absorption and the magneto-optical Kerr angle spectra, including both excitonic effects. We have also investigated hybrid heterostructures $\text{MoSe}_2/\text{CrBr}_3$ and VOCl/FeOCl . Regarding the spin-charge excitation properties, we formulate the elementary excitations of 2D magnets using an itinerant fermion Hamiltonian. We obtain the magnon dispersion for 2D- CrI_3 with a gap at the Dirac points with the same Berry curvature in both valleys. For CrI_3 ribbons, we find chiral in-gap edge states.

QM/MM computational studies of the main protease of SARS-CoV-2: towards the design of new inhibitors

Kemel Arafet, Sergio Martí, Katarzyna Świderek and Vicent Moliner

Institute of Advanced Materials (INAM), Universitat Jaume I, Castelló.

Computational Chemistry techniques based on the combination of Quantum Chemistry and classical Molecular Mechanics (QM/MM) have been extensively applied to the study of enzyme catalysis. Merging these techniques with experimental methods has allowed to acquire a deep knowledge of the reaction mechanisms of these complex but highly efficient biocatalysts at the molecular level. We will focus in this communication on the study of the main protease of SARS-CoV-2 (M^{Pro}). Based on our experience on other cysteine proteases from different organisms, we started the study of the proteolysis reaction and continued with efforts oriented to the design of new inhibitors. Results obtained in our laboratory in this line of research, thanks to the computer resources at Pirineus and Mare Nostrum 4¹, and the technical support provided at by Barcelona Supercomputing Center, will be summarized in this communication.

¹QSB-2020-2-0004, QSB-2021-1-0007

DNN workload on large-scale parallel environment

Kohta Nakashima

Senior Director, Fujitsu ICT Labs, Japan

Fujitsu develop not only large scale supercomputer hardware such as Fugaku but also software technologies for large scale and heavy workload such as deep neural network. In this talk, we introduce our software technologies for DNN workload on large-scale parallel environment.

Three-dimensional models of magnetorotational core-collapse supernovae

M. Obergaulinger, M.Á. Aloy

Universitat de València

Core-collapse supernova form a diverse class of explosions produced at the end of the lives of massive stars. Studying these events is heavily dependent on supercomputing due to the complexity of the turbulent flows and the neutrino transport in dense matter. We rely on a high resolution code in a hybrid parallelisation model (OpenMP/MPI) and proper management and visualisation of large datasets. Further optimisation is planned to use GPUs for the simulations and machine learning for the data analysis. Our three-dimensional models including all relevant physics and covering unprecedentedly long simulation times demonstrate how the subset of progenitors with strong magnetic fields and high rotational energies can be responsible for producing particularly high explosion energies and for playing an important role in the chemical enrichment of early galaxies with heavy elements in ways that are not accessible to ordinary, primarily neutrino-driven explosions.

Numerical modeling of double-polarity subduction

Mireia Peral¹, Jonas Ruh², Manel Fernàndez¹, Sergio Zlotnik³, Jaume Vergés¹

¹Group of Dynamics of the Lithosphere, Geociències Barcelona (Geo3Bcn-CSIC), Barcelona, ²Institute of Geophysics, Department of Earth Sciences, ETH Zurich, Switzerland, ³Department of Civil and Environmental Engineering, Universitat Politècnica de Catalunya, Barcelona

Subduction occurs in many zones on Earth when one tectonic plate collides and sinks under another into the Earth's mantle. Complex subduction zones may involve more than one subducting plate showing non-unique subduction polarity. Combining numerical and analog experiments are crucial to study such tectonic processes that cannot be observed directly. In this work, we present a series of numerical models of double-polarity subduction reproducing previous analog experiments. The objective is to determine under which conditions the numerical models best reproduce the analog experiments. We also study the dynamics of such systems by combining both methodologies. Our results show that boundary conditions affect the evolution of the system at short distances allowing for a reduction of the model domain relative to the analog model increasing resolution and saving computation time. Finally, we present a numerical model resembling the complex subduction zone of the Western Mediterranean.

Leading the new era of HPC

Simón Viñals Larruga

Business Development Manager Spain & Portugal, AMD

Computational Science has never been more critical for society, and AMD is leading the new era of HPC technology which will lead us from Petascale to the Exascale Supercomputers that the society needs. This presentation will explain the three technological reasons why the next wave of Supercomputers is based on AMD technology: CPU, GPU and Software. AMD EPYC processors define the present and the future of HPC, AMD Instinct GPUs provide an accelerated platform that is unified, open and optimized for HPC. Finally, the ROCm Open Software platform provides a comprehensive environment that unlocks all the GPU power to accelerate computational tasks, delivers Deep Learning at Scale and enables Innovation, Collaboration and Efficiency. With a solid roadmap, AMD sets the path forward.

HPC National Competence Center



EuroCC Spain Competence Center (<https://eurocc-spain.res.es/>)

The EuroCC Spain project aims to create a National Competence Center (NCC) that is capable of providing a wide portfolio of Supercomputing, Big Data and Artificial Intelligence services adapted to the respective needs of the industry (especially SMEs), the the academic world and public administration in Spain.

The NCC center in Spain will be part of a network of National Competency Centers made up of 33 participating, member and associate states. In this way, use and benefit are made of the advantages, experience and resources available in Europe in the field of supercomputing, big data and artificial intelligence for the coordination of initiatives at the national level to promote these technologies.

Innovation Journey

Innovation Journey is a workshop series that aims to promote collaboration between research personnel in need of entrepreneurship management skills; and industry and SME professionals searching for new ventures in the field of High-Performance Computing, Big Data and AI. The goal is to accompany researchers as they make their first contact with the private sector and to foster the use of HPC technologies in industry and SME initiatives. The seven-session program will offer business training through interactive workshops and an approach to the implementation of practical solutions in the market, as well as mentoring and guidance by entrepreneurs, which will be established through a rigorous curriculum.



EUROCC SPAIN, RES & BSC-CNS PRESENT:
INNOVATION JOURNEY
Supercomputing for Industry and SMEs
OCT 1st - NOV 12th

DO YOU KNOW WHAT SUPERCOMPUTING CAN DO FOR YOU?
¿And Big Data or Artificial Intelligence?
Supercomputing technologies provide the means to tackle large and complex problems more effectively.

SUPERCOMPUTING & INDUSTRY
Endless applications
Many companies use supercomputing to design new products, optimise manufacturing processes, solve production problems, extract data and simulate processes in order to become more competitive, profitable and environmentally-friendly.

WHAT ARE WE OFFERING?
Your idea - A reality
Innovation Journey is a workshop series in which teams made up of researchers and professionals like you use supercomputing to take their business proposition to the next level.

WHAT CAN YOU EXPECT?
A disruptive initiative
Training in Supercomputing, Big Data and Artificial Intelligence
Working in Collaboration with highly qualified researchers
Developing projects with a high degree of Innovation

TAKE THIS GREAT OPPORTUNITY
And find out what supercomputing can do for your business
The Innovation Journey will take place during 7 full-day sessions in seven consecutive weeks
It will combine theoretical and practical sessions that will encourage collaboration between companies and researchers to develop a solution using supercomputing.

Find further details in the links below
Deadline: June 30th
Contacto: eurocc@res.es

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EuroCC SPAIN, RES, BSC-CNS, and the BSC-CNS member states: Austria, Belgium, Bulgaria, Canada, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovakia, Spain, Sweden, the United Kingdom, France, the Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro.

EUROCC SPAIN, RES & THE BSC-CNS PRESENT:
INNOVATION JOURNEY
Find your inner entrepreneur
OCT 1ST - NOV 12TH 2021

ARE YOU A RESEARCHER WITH A LOT OF POTENTIAL?
We are sure you are.
In fact, you are probably aware of that too. And you might have started thinking what of all the potential could be further developed in the private sector?

5/10 BSC-CNS SPIN OFFS WERE CREATED IN THE PAST YEAR
Tech-transfer: a reality
The transfer of technology developed inside the BSC-CNS to society and the private sector by becoming a reality, it allows researchers to develop and exploit their discoveries in a more independent and challenging, but also fruitful, way.

WHAT ARE WE OFFERING YOU?
New beginnings, a new path
In the Innovation Journey, you will be part of a multidisciplinary group of researchers. You will receive training on how to get started in the entrepreneurial world and develop your entrepreneurial muscles collaborating with companies that are already active in the market.

LEARNING BY DOING
A methodology that works
The Innovation Journey is a success story. It completely emerged after participating in the last edition. This year, you will also be able to collaborate with companies that will bring their expertise to assist you on your way to the private sector.

YOU HAVE THE SCIENTIFIC POTENTIAL
Let yourself discover your inner entrepreneur
The Innovation Journey will take place during 7 full-day sessions in seven consecutive weeks. It will combine a theoretical and practical "learning by doing" methodology, which will approach actual enterprises and businesses
It will take off on October 1st.

Find further details in the links below
Deadline: 30th June
Contact: techtransfer@hoop@bsc.es

Promoted and organized by:
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EuroCC_Spain_RES Conference

NATIONAL CENTER FOR SUPERCOMPUTATION COMPETENCES Promoting the use of HPC in business innovation



September 16, 2021



**10:00 to
14:00**



INSCRIPTION



PROGRAM

OBJECTIVES:

Make companies aware of the **National Center for Supercomputing Competencies**, as well as national strengths in high-performance computing (HPC), supercomputing, as well as High Performance Data Analysis (HPDA) and Artificial Intelligence capabilities. (AI) to increase the usability of these technologies in national companies.

SCHEDULE

- 10: 00-10: 10 **Welcome. SCAYLE, Castilla y León Supercomputing.**
- 10: 10-10: 30 Presentation of the National Center of Competence in Supercomputing.
BSC-CNS, National Supercomputing Center.
- 10: 30-10: 50 **Round table** . The map of competences in HPC, IA, Big Data in Spain.
-BIFI, Institute of Biocomputation and Complex Systems. *Mr. Alfredo Ferrer Marco , Technical and research staff hired .*
-COMPUTAEX-CénitS, Extremadura Computing and Advanced Technologies Foundation. *D. Javier Corral Garcia, Project Analyst and communication of CénitS .*
- 10: 50-11: 10 **Round table** . The acquisition of competences: Training in Spain.
-UNICAN, University of Cantabria. *Mr. Jose Luis Bosque, Associate Professor at the University of Cantabria.*
-CSUC, Consorci de Serveis Universitaris de Catalunya. *D Adrián Macía , head of scientific calculation at the CSUC.*
- 11: 10-11: 30 **Coffee break** .
- 11: 30-11: 50 **Round table**. Access to knowledge and experts.
-IAC, Instituto de Astrofísica de Canarias. *Mr. José Carlos Ruiz Luque, Postdoctoral Researcher in High Performance Computing .*
-BIFI, Institute of Biocomputation and Complex Systems. *Mr. Alfredo Ferrer Marco, Technical and research staff hired .*
- 11:50 - 12:10 **Round table. The access of companies to HPC** .
-CESGA, Galician Supercomputing Center. *Mr. Ignacio López Cabido, Technical Deputy Director .*
-BSC-CNS, National Supercomputing Center. *Mr. Alberto Antonio Gómez , Coordinator of the EuroCC project at BSC-CNS.*
- 12: 10-12: 25 **Success story 1: Bettair Cities.** *Mr. Francisco Ramírez Javega , Scientific Director of Bettair Cities .*
- 12: 25-12: 40 **Success case 2: TBD.**
- 12: 40-13: 00 **Role of CDTI in Large Scientific Facilities, grants and opportunities for Industry-Science collaboration in HPC** .
Mr. Javier Echávarri Delmás, Directorate of Space, Large Facilities and Dual Programs . Large Scientific Facilities.
- 13: 00-13: 15 Closing ceremony. SCAYLE.
- 13: 15-14: 00 Personalized interview request (for companies).

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