18th - 19th September 2019 | Zaragoza

13th Users Conference

Program & Book of Abstracts

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

13th RES Users Conference

Program & Book of Abstracts

This book is available at
www.res.es/users-conference-2019

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

The **Spanish Supercomputing Network** (RES) organizes an HPC users meeting every year to disseminate information about RES updates, shared resources, and procedures. This event aims to be a discussion forum for RES users, technical staff, the access committee and the users committee. The local organizer of this meeting is the RES node **Institute for Biocomputation and Physics of Complex Systems** (BIFI) from Zaragoza and it will be hosted in Patio de la Infanta from **Fundación Ibercaja**. The objective of this event is to encourage an interactive exchange between researchers from different backgrounds, HPC experts, technical support staff, companies and organizations with the final HPC users.

The Princess's Courtyard (**El Patio de la Infanta**) holds its name because Maria Teresa de Vallabriga, widow of Prince Luis de Borbón, brother of King Charles III, lived in this unique architectural jewel in 1793. The original name of the house was Zaporta House, because Gabriel Zaporta, a Jewish convert and noble banker of Aragon, built it in 1549 as a gift to his wife Sabina de Santángel. The Princess's Courtyard was the central part and the only one remaining today of Zaporta House. Events and the people who lived in it have forged its history. For example, the School of Drawing was founded in 1784 in the ground floor rooms of the House, opening into the Courtyard, as it was believed that drawing was essential for scientific progress and artistic creation.

18th **Wednesday**

Room **Rioja**

14:00 Registration.

15:00 Inauguration and Welcome address.

15:15 RES News and Updates.
Sergi Girona

15:35 European processor.
Mateo Valero

15:50 Presentation of BIFI.
Yamir Moreno

16:00 Presentation of RES Users Committee.
Javier Junquera

16:30 Poster session and coffee

17:00 Scientific Keynote Lecture.
Natasa Przulj

18:00 Technical Keynote Lecture.
María S. Pérez

19:00 Cultural guided visit

19th **Thursday**

Room **Rioja**
Scientific Lectures

Room **Pirineos**
Technical Lectures

08:30	Registration.	
09:00	Scientific Lecture 1. ***Tanausú del Pino***	Technical Lecture 1. ***Vicent Botti***
09:30	Scientific Lecture 2. ***Carolina Estarellas***	Technical Lecture 2. ***Danilo Adagna***
10:00	Scientific Lecture 3. ***Fernando Martín***	Technical Lecture 3. ***Francisco Javier García Blas***
10:30	Poster session and coffee	
11:00	Scientific Lecture 4. ***Guilherme Vilhena***	Technical Lecture 4. ***Ander Otxoa***
11:30	Scientific Lecture 5. ***Anne Gosset***	Technical Lecture 5. ***Adriano Galano***
12:00	Scientific Lecture 6. ***Pablo G. Lustemberg***	Technical Lecture 6. ***Bruno Leconte***
12:30	Round table	
13:30	Lunch	

Room **Alcarria**

Room **Pirineos**

14:30	Workshop PyCOMPSs	Workshop Data Management Plan
15:45	Coffe break	Coffe break
17:00	Closing	Closing

Contents

1. Welcome

Dear RES HPC users,
This September, the users of the Spanish Supercomputing Network (RES) are gathering again in the annual RES Users Meeting. Each of us are working in our own specific scientific or technological field, but we all have one common feature: we all share the Spanish HPC resources for our research purposes. The main aim of the Meeting is getting together and sharing our experiences, our expectations, and to learn from each other. We have set up an interesting program with outstanding speakers and panelists, but your attendance and participation is our most valuable asset. Moreover, I want to thank one of our nodes, BIFI, for their extraordinary help in organizing this meeting and I wish all of you a fruitful and rewarding conference.

Sergi Girona, RES Coordinator

2. Registration

Please, register at the link:
https://www.res.es/es/content/13th-res-users-conference-registration-form

Registration for the 13th Users Meeting is **free**. Since there is limited availability of space and because of logistic needs, please do register on-line before **September 9th**. Registered users have access to program sessions, social activities, coffee breaks, and lunch during the conference. Please wear your personal badge at all times.

3. Travel grants

RES Users Meeting Travel Grants aim at supporting early-career researchers who present their work in the Poster session of the meeting. Applicants will usually be Masters, PhD students, or post-doctoral researchers at the beginning of their research careers. The organization pays the grantees the lodging and travel expenses to Zaragoza and back, up to a maximum of 300 € per grant. Please submit your application here (https://www.res.es/es/travelgrants) before the deadline of **September 4th**. If available, attach to your application the recommendation letter of any of the RES nodes. Each application will be judged on the excellence of the candidate and the work being presented in the poster. Only one application per poster is accepted. Travel grants will be notified before **September 6th**.

Deadline for travel grants applications: September 4th. 14:00h

4. Venue

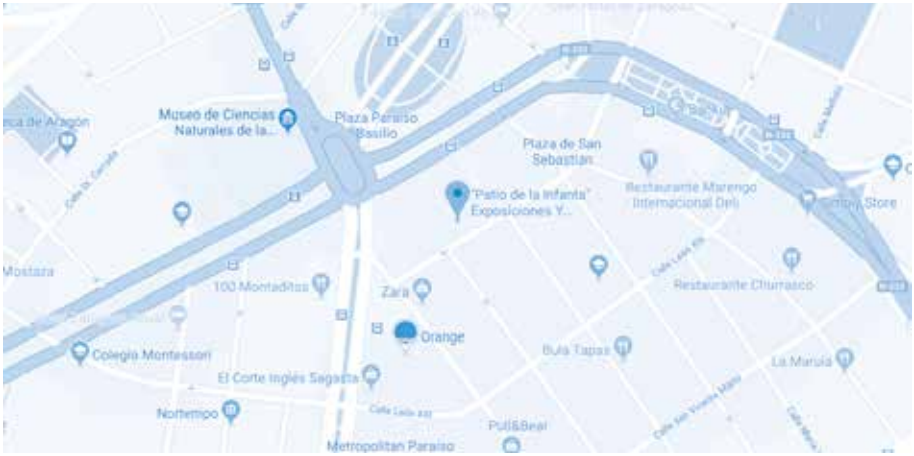
Patio de la Infanta,
C/ San Ignacio de Loyola 16, 50008 Zaragoza.

Tel. 976 97 19 26

Public transportation (bus and tram) is very convenient to move around the city, to/from the train station and the airport.

Please visit http://zaragoza.avanzagrupo.com/comoira_gt_zgz.php for instructions.

There is a nearby parking if you travel by car
(Parking Indigo, C/ San Ignacio de Loyola, 8).
https://es.parkindigo.com/es/car-park/san-ignacio



5. Program & Abstracts

Wednesday, September 18th

14:00 Registration. Hall of the Patio de la Infanta.

Room **Rioja**

15:00 Inauguration and Welcome address.

- **Sergi Girona**, RES Coordinator, Operations Director, Barcelona Supercomputing Center, BSC
- **José Ignacio Doncel**, Deputy Director General of Large Scientific and Technical Installations, Ministry of Science, Innovation and Universities
- **Excma. María Eugenia Díaz Calvo**, Councilor of Science, Universities and Knowledge Society. Government of Aragón
- **Excmo. y Mgfco. José Antonio Mayoral Murillo**, Rector, University of Zaragoza

15:15 RES News and Updates in the RES. Access to available resources in RES, PRACE and EuroHPC.

- **Sergi Girona**, RES Coordinator, Operations Director, BSC

15:35 European processor

- **Mateo Valero**, Director, BSC

15:50 Presentation of the Institute for Biocomputation and Physics of Complex Systems (BIFI)-University of Zaragoza.

- **Yamir Moreno**, Director of BIFI & Head of Cosnet Lab

16:00 Presentation of the RES Users Committee (CURES) and open debate

- **Javier Junquera**, Chair of CURES, University of Cantabria.

The history, composition, main objectives, and internal rules of the Users Committee of the Spanish Supercomputing Network will be presented. Special emphasis will be made on how to contact the CURES to use this organism as the liaison between the users and the RES managers, and how to promote the use of supercomputer capabilities providing an efficient feedback. Finally, the results of the last survey about the level of satisfaction will be presented.

16:30 Poster Session (coffee will be served during the session)
Hall of Room Rioja

17.00 Scientific Keynote Lecture: Data-driven medicine.

- **Natasa Przulj,** Barcelona Supercomputing Center, BSC

We are faced with a flood of molecular and clinical data. We are measuring interactions between various bio-molecules in a cell that form large, complex systems. Patient omics datasets are also increasingly becoming available. These systems-level data provide heterogeneous, but complementary information about cells, tissues and diseases. The challenge is how to mine them collectively to answer fundamental biological and medical questions. This is nontrivial, because of computational intractability of many underlying problems, necessitating the development of heuristic methods for finding approximate solutions. We develop methods for extracting new biomedical knowledge from the wiring patterns of systems-level, heterogeneous, networked biomedical data. Our methods uncover the patterns in molecular networks and in the multi-scale network organization indicative of biological function, translating the information hidden in the topology into domain-specific knowledge. We introduce a versatile data fusion (integration) framework to address key challenges in precision medicine: better stratification of patients, prediction of driver genes in cancer, and re-purposing of approved drugs to particular patients and patient groups. Our new methods stem from novel network science approaches coupled with graph-regularized non-negative matrix tri-factorization, a machine learning technique for dimensionality reduction and co-clustering of heterogeneous datasets. We utilize our new framework to develop methodologies for performing other related tasks, including disease re-classification from modern, heterogeneous molecular level data, inferring new Gene Ontology relationships, aligning multiple molecular networks, and uncovering new cancer mechanisms.

18.00 Technical Keynote Lecture: HPC and Big Data, a marriage of convenience?

- **María S. Pérez**, Universidad Politécnica de Madrid, UPM

The areas of HPC and Big Data (BD) have followed different trajectories, due to the existence of two divergent communities and goals. However, in the last years, there has been a change in both HPC and BD applications. On the one hand, HPC applications use an increasingly high volume of data, requiring often the capacity to visualize and analyze this data. On the other hand, BD applications need more and more computational power, due to more ambitious challenges and the combination of data analysis with simulation processes. The existence of the so-called Extreme Data Analytics creates the need to combine solutions oriented to improve the access and management of data with solutions to take advantage of computing. At the storage level, we have performed a work that deals with such convergence. This constitutes a small step that could be extended to other features of computer architecture, paving the way for the desired convergence between HPC and BD.

19.00 Cultural guided visit. The tour starts at the Hall of Patio de la Infanta, walking down towards La Seo, and stopping by Plaza de los Sitios and the Roman Theatre.

Thursday, September 19th

8:30 Registration. Hall of the Patio de la Infanta.

Room **Rioja** | Scientific sessions

9:00 Solving the forward and inversion problem of polarized radiation transfer in multidimensional models of the solar atmosphere.

- **Tanausú del Pino Alemán**, Instituto de Astrofísica de Canarias, IAC

One of the key challenges in Solar Physics is to decipher and understand the magnetic activity of the solar atmosphere. To study the small-scale magnetic fields of the quiet Sun photosphere, we solved the polarized radiation transfer problem in state of the art 3D magneto-hydrodynamical models of the solar atmosphere using our PORTA code. We studied the sensitivity of the Stokes profiles to physical properties of the model and compared the results with spectroscopic-polarimetric observations. This has allowed us to confirm that in the quiet regions there is indeed a substantial amount of 'hidden' magnetic energy. We also developed a multidimensional, non-LTE inversion code. Applying sparsity regularization and the massively parallel strategy of the PORTA code, we are able to efficiently infer the self-consistent properties of chromospheric plasma structures. We obtained our first results for a relatively simple chromospheric plasma structure levitating in the solar corona.

9:30 Understanding the direct activation mechanism of AMP-Kinase: toward disclosing the isoform-binding dependency.

- **Carolina Estarellas**, Dept. of Chemistry, University College London

AMPK is a key enzyme to maintain the cellular energy homeostasis, being an important target to metabolic diseases like diabetes MT2. It is an heterotrimer formed by α, β and γ subunits. The activation mechanism of A-769662 is of particular interest, because it bounds at the ADaM binding site, located between the interfaces of α and β subunits, providing Ser108 of β-subunit phosphorylated, and enhancing the AMPK activity >90-fold. We have run MD simulations for apo, holo and holo+ATP systems with a cumulative time of 9 μs. The results indicate that the activator acts as molecular glue, making an effective connection between β- and α-subunits that pre-organizes the ATP-binding site, favoring the binding of ATP, and explaining the increase of the AMPK activity. Our next objective is to understand the molecular basis of the specific ligand-isoform interactions. Biochemically, it seems that isoform β has a crucial role in the conformational arrangement of ADaM and ATP-binding site. Which are the molecular factors that made that very similar ligands could interact with both β isoforms, while others only can specifically interact with one of the two isoforms? In order to answer these questions, preliminary results from MD simulations of α2β1 and α2β2 complex with the ligands A769662, 991, SC4 and PF-739 located at the ADaM site in presence and absence of ATP in the ATP-binding site will be presented.

10:00 Attosecond pump-probe photoelectron spectroscopy of molecules.

- **Fernando Martín**, Universidad Autónoma de Madrid, UAM, and IMDEA Nanociencia

The results of attosecond pump-probe theoretical simulations in which several molecules are ionized with a single attosecond pulse (or a train of attosecond pulses) and are subsequently probed by one or several infrared or xuv few-cycle pulses will be presented. Electron dynamics in the photo-excited molecule or remaining molecular ion is revealed by varying the pump-probe delay with attosecond time resolution.

Room **Pirineos** | Technical sessions

9:00 Artificial Intelligence vs HPC.

- **Vicent Botti**, Valencian Research Institute for Artificial intelligence, VRAIN, Universidad Politécnica de Valencia

Artificial Intelligence (AI) is about computer systems that show intelligent behavior, doing things that traditionally require human intelligence, perceiving their environment and determining, autonomously, which actions to perform (among a limited number of them) to achieve specific objectives based on their perceptions. It is very frequent the use we make of AI, when we enter in a garage and the license plate of our vehicle is recognized, when we use our mobile to find the best route to reach a destination, when we talk to our virtual assistant, when our mobile recognizes our fingerprint or our face, and so we could continue enumerating many more daily activities where the IA intervenes. The greater computing power of computers, the accessibility to data through the Internet and the advances that have taken place in artificial intelligence algorithms have resulted in AI being one of the most important technologies of the 21st century. Just as the steam engine or electricity once produced great changes in society, AI is transforming the world.

9:30 Performance prediction of GPU-based deep learning applications.

- **Danilo Ardagna**, Politecnico di Milano

Recent years saw an increasing success in the application of deep learning methods across various domains and for tackling different problems, ranging from image recognition and classification to text processing and speech recognition. In this talk I'll discuss the use of machine learning methods to predict the execution time required for training convolutional neural networks (CNNs), with a particular focus on deployments on general purpose graphics processing units (GPGPUs). I'll demonstrate that our approach is generally applicable to a variety of CNN models and different types of GPGPUs with high accuracy. The proposed models can support with great precision (within 11% average percentage error) the prediction on unseen hardware configurations. These models have been also integrated within an on-line scheduler that allows reducing cloud operation costs between 40 and 70% with respect to first principle policies based on FIFO, earliest deadline first and priority scheduling.

10:00 Towards data intensive aware programming models for Exascale systems.

- **Francisco Javier García Blas**, Universidad Carlos III de Madrid

Extreme Data is an incarnation of Big Data concept distinguished by the massive amounts of data that must be queried, communicated and analyzed in (near) real-time by using a very large number of memory/storage elements and Exascale computing systems. Immediate examples are the scientific data produced at a rate of hundreds of gigabits-per-second that must be stored, filtered and analyzed, the millions of images per day that must be mined (analyzed) in parallel, the one billion of social data posts queried in real-time on an in-memory components database. Traditional disks or commercial storage cannot handle nowadays the extreme scale of such application data. The ASPIDE project will contribute with the definition of a new programming paradigms, APIs, runtime tools and methodologies for expressing data-intensive tasks on Exascale systems, which can pave the way for the exploitation of massive parallelism over a simplified model of the system architecture, promoting high performance and efficiency, and offering powerful operations and mechanisms for processing extreme data sources at high speed and/or real-time.

10:30 Poster Session (coffee will be served during the session)
Hall of Room Rioja

Room **Rioja** | Scientific sessions

11:00 Single molecule nanotribology: understanding friction and adhesion at a single molecule level.

- **Guilherme Vilhena**, University of Basel, Switzerland

Understanding the motion of a single molecule over a surface is a problem of a paramount importance in the design of advanced molecular nanostructures. To date, the interplay between molecule mechanics and surface displacements is a highly challenging task as it requires knowing not only the forces needed to manipulate but also to relate them with particular molecular motion. Here we bridge this gap by combining MD, and force spectroscopy to investigate the manipulation of two different molecules (ssDNA and poly-pyrene) over a Au surface in UHV at 5K. Our experiments/simulations revealed a contrasting on-surface dynamics of these molecules. The high ssDNA adhesion allowed to quantify for the first time the stretching stiffness of a single DNA nucleotide. The poly-pyrene revealed a complex on-surface dynamics governed by its superlubric sliding. Overall our results unravel the importance of a dynamic balancing between the intra-molecular mechanics and surface interaction.

11:30 High-fidelity CFD simulations to understand the physics of the jet wiping process in galvanization.

- **Anne Gosset**, Universidad de la Coruña

This work deals with the 3D two-phase simulations of the jet wiping process, conducted with the OpenFOAM CFD libraries. In this coating process, a plane gas impinging jet is used to reduce and control the thickness of a liquid film withdrawn from a bath by a substrate moving upwards. This process is inherently unsteady, leading to the formation of large amplitude waves on the final coating. Because these non-uniformities are suspected to originate from large-scale oscillations of the gas jet, the vortical structures dominating the gaseous flow have to be accurately computed. Four test cases are simulated with the two-phase flow solver interFoam, using the Smagorinsky Large Eddy Simulation model and the Volume of Fluid method for the tracking of the interface. The unsteady characteristics of both the jet and the liquid are analyzed and the results are validated against experimental data. They confirm the existence of a hydrodynamic feedback between the runback waves and the gas jet.

12:00 HPC applied to methane dissociation and conversion and HCl interaction on CeO_2 based catalyst.

- **Pablo G. Lustemberg,** Instituto de Catálisis y Petroleoquímica, ICP-CSIC, Instituto de Física Rosario, IFIR-CONICET, Santa Fe, Argentina

This talk will show three examples of HPC applied to systems of catalytic interest. Recent results on ceria-supported Ni, Co and Cu model catalysts will be discussed, as examples of catalysts for methane dry reforming (DRM). The ability of ceria to stabilize oxidized species (Co^{2+}, Ni^{2+}) on the stoichiometric CeO_2 surfaces, and metallic ones (Co^0, Ni^0) on the reduced CeO_2-x support, is essential for catalytic activity for DRM. Methane dissociation occurs already at room temperature, whereas CO_2 dissociation occurs at the oxygen vacancies formed at higher temperatures; the Co/ceria system is the most active with a barrier for methane dissociation becoming negligible with increasing temperature. Also, the Ni/CeO_2 system is considered for the direct methanol synthesis from methane in the presence of water. Water plays a crucial role in the C-H bond breaking and the selectivity towards methanol formation. Finally, results of the interaction of HCl on CeO_2 will be shown, where I will show the impossibility of Cl_2 formation.

Room **Pirineos** | Technical sessions

11:00 Open architectures for AI and HPC

- **Ander Otxoa**, Systems Architect, IBM

11:30 Japan and the way towards Exascale.

- **Adriano Galano**, Chief Technology Officer, Fujitsu

Building on our long-standing history of innovation, 30 years of experience in the development of supercomputers and the exceptional depth and breadth of our offering, we provide the enabling technologies and services for a wide range of aerospace, meteorology, astronomy, healthcare and industrial projects. We have also teamed up with numerous prominent research agencies to design bespoke solutions for the most varied and challenging technical computing applications.

12:00 Heterogenous architecture for mixed HPC and AI workload with Jean Zay.

- **Bruno Leconte**, Solution Architect Manager, HPC & AI, France, Southern & CEEMA, Hewlett Packard Enteprise

At Hewlett Packard Enterprise, we continue to fuel the next frontier and unlock discoveries with our end-to-end HPC and AI offerings. These developments include the HPE Artificial Intelligence Marketplace, a first-of-its-kind ecosystem in France of AI hardware and software solution providers for start-ups and enterprises, and the HPE HPC and AI Center of Excellence in Grenoble, a center of HPC and AI experts and tools to accelerate time-to-market of new products. Supercomputing has tremendous potential to accelerate innovation in AI for public and private sectors here in France and we are building a fast, powerful machine for GENCI to become France's leading supercomputing research and development center for AI. The talk will be about heterogenous architecture for mixed HPC and AI workload for public researcher and private sectors. Topic will cover Jean Zay design, performance and usage for HPC and AI mixed workload.

Room **Rioja**

12:30 Round table. Snapshots of the future: data, energy and more HPC…

- **Nadia Tonello**, Head of Data Management group, Barcelona Supercomputing Center, BSC
- **Edilberto Sánchez**, National Fusion Laboratory, LNF, CIEMAT
- **Sergi Girona**, representative of Hosting Entity EuroHPC, Barcelona Supercomputing Center, BSC
- *Chair:* **Antonio Sánchez**, Deputy Directorate-General of Large Scientific and Technical Installations, Ministry of Science, Innovation and Universities

13:30 Lunch and visit to the Patio de la Infanta, offered by Fundación IberCaja. During lunch the RES Awards will be announced.

Room **Alcarria**

14:30 Workshop “Parallel programming with PyCOMPSs”.

- **Javier Conejero, Rosa Ma Badia**, Barcelona Supercomputing Center, BSC

PyCOMSs is a task-based programming model developed by the BSC that enables the parallel execution of sequential Python applications in distributed computing platforms. PyCOMPSs can be used to parallelize applications written entirely in Python, and also for the development of workflows that involve calls to external binaries (including MPI ones). The dislib is a machine learning library parallelized with PyCOMPSs that follows the scikit-learn syntax. The tutorial will focus in the use of PyCOMPSs in the RES supercomputers through examples, including a hands-on in MareNostrum 4. One of the exercises will be based in the dislib.

14:30 Introduction

14:40 PyCOMPSs syntax

15:20 Overview of COMPSs runtime

15:30 Introduction to dislib

15:40 Break

15:55 Hands-on in MN4:
· PyCOMPSs simple use case in Python
· Use case calling external binaries
· dislib use case

17:00 Closing

Room **Pirineos**

14:30 Workshop “Your Data Management Plan: a gateway to good, reproducible research.”

- **Nadia Tonello,** Barcelona Supercomputing Center, BSC
- **Cees Hof,** Data Archiving and Networked Services, DANS

This training will offer an introduction to the practice of preparing and writing a good Data Management Plan (DMP) when planning your research. The data and software that you produce in your research are the assets of your work and valuable to you, your peers and your funder. How to capture, preserve and share this information is the focus of a good DMP. In this training we will provide a generic introduction and exercises, including some examples form different information domains. After a generic session there will be a session focusing on information and exercises related to data from and for high level computing facilities. The training will teach you that a DMP is not just an administrative burden, but the gateway to good (future) research. The training will be a combination of presentation(s) and hands-on exercises

14:30 Introduction by Nadia Tonello

14:45 Data Management Plan (DMP) training session by Cees Hof

16:30 Open discussion: sharing experiences in Research Data Management

17:00 Closing

Room **Rioja**

14:30 Technical session "RES technical meeting" (for invitation only, reserved to RES staff).

Chair: **David Vicente,** Barcelona Supercomputing Center, BSC

- **Jorge Rodríguez**, Barcelona Supercomputing Center, BSC
- **Ubay Dorta**, Instituto de Astrofísica de Canarias, IAC
- **Pablo Sanz**, Universidad Autónoma de Madrid, UAM
- **Sergi Moré**, Barcelona Supercomputing Center, BSC
- **Miguel Pascual**, Green Revolution Cooling, Inc.

6. Poster sessions

List of posters

#1 Numerical simulation of non-premixed swirling flames

Teresa Parra, *ITAP, University of Valladolid*

Rubén Pérez, *Dept. of Mechanical Engineering. Universidad Pontificia de Comillas ICAI*

The major aim of the research is to improve the stabilization of flames of poor stoichiometries by means of a swirling flow. This provides saving of fuel as well as a reduction of contaminant emissions. Swirling burners have some advantages when compared with bluff bodies and cross flows. These are lower head losses and soot, less maintenance tasks. This work is devoted to gain an insight of flow pattern associated with different swirl numbers and diffusers. Axial swirl injector is composed by a certain number of fixed vanes in the annular nozzle. The Swirl number is associated with the angle of the trailing edge of the vanes. Besides, the influence of conical diffusers in the flame performance is analysed. To sum up, the strong swirl number had the lead stagnation point near the discharge of the nozzles and provided a reaction length lower than half diameter of the chamber. Intermediate swirl number have bigger Outer Recirculation Zones and the reaction length is more than one diameter. Finally the low swirl number do not have any vortex breakdown and the reaction length has several diameters. Bearing in mind the influence of conical diffusers, it is more important in the case of intermediate swirl numbers since the diffuser reduces the reaction length. These models were tested at a temporal resolution of 10-6 s/timestep, with spatial resolution 5 times larger than the Kolmogorov scale. It was found that for a mesh of 10 million cells without multigrid, the optimum is 360 processors. The authors acknowledge PRACE for awarding us access to the resource Curie-GENCI@CEA based in France and MareNostrum@BSC based in Spain. Ref. 2010PA1766. We acknowledge that the results of this research have been achieved using the DECI resource ARIS based in Greece at GRNET with support from the PRACE aisbl (ref. SWIRLLES Tier-1, DECI-14).

#2 Pressure induced effects of β-As_2Te_3

E. Lora da Silva, R. I. Vilaplana, *Instituto de Diseño para la Fabricación y Producción Automatizada, Universitat Politècnica de València*

The A2B3 compounds, with R-3m symmetry, have stimulated enormous research activity, because of their exceptional thermoelectric properties. More specifically, As_2Te_3 has shown some interesting properties and applications, which include memory devices, thermoelectric properties, conduction mechanism, and pressure-induced amorphisation to crystalline transition. β-As_2Te_3 is an isostructural form to layered Bi_2Te_3 and is known for displaying good thermoelectric properties. Moreover, the interest evidenced in such systems is the possibility of pressure-inducing electronic topological transitions (ETT) which can result in significant enhancements of their thermoelectric properties.

#3 Learning by doing on computational fluid dynamics

Maria T. Parra, *University of Valladolid*

José M. Molina Jordá, *University of Alicante*

This work involves the methodology used in the University of Valladolid for Mechanical Engineering students to learn Computational Fluid Dynamics playing an active role. Students carry out a fluid mechanics down scaled projects with the steps of sensibility of mesh, convergence of numerical algorithm, validation of turbulence model and description of flow patterns. Students pretend to be engineers in a consulting or design office carrying out a fluid mechanics scale down projects. Later they act as reviewers evaluating a project from a colleague. The offer of benchmark test cases ranges from head loses, driven cavities, swirling flows, to external aerodynamics. A review of the offer of workshops is supplied, such as the Ahmed car, the Roback and Johnson burner, aerodynamics of different NACA airfoils, and different geometries of driven cavities. These are classical test cases of numerical research and a sample of applications in wind energy, industrial furnaces, and lubrication. There is a deeper understanding of the topic when they need to discuss the strategies to accomplish the project, to write a technical report and finally to justify the evaluation of other works. Furthermore, they develop their critical thought, writing skills and synthesis capacity.

#4 Selective ethylene dimerization under intrapore condensation regime with defect-engineered Ru-HKUST-1 catalysts

Manuel A. Ortuño, *Institute of Chemical Research of Catalonia, Spain*

Iker Agirrezabal-Telleria, *University of the Basque Country, Spain*

Ignacio Luz, *RTI International, USA*

The production of 1-butene, a major monomer in polymer industry, is mostly dominated by ethylene dimerization processes. Although homogeneous catalysts are quite selective, they usually lack the robustness and recyclability of heterogeneous materials. In this scenario, metal–organic frameworks come into play to bridge the gap between these two worlds.

#5 Analysis of hybrid quantum-classical algorithms for optimization

Pablo Diez-Valle, *Consejo Superior de Investigaciones Científicas*

Juan José García-Ripoll, *Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas*

A promising paradigm for the resolution of optimization problems using quantum techniques is the known as hybrid quantum-classical algorithm. This kind of algorithms combines quantum computing via the variational method, and classical computing to optimize the variational parameters. In this work we focus on the resolution of Quadratic Unconstrained Binary Optimization problems (QUBO) since a broad spectrum of combinatorial optimization problems can be represented as a QUBO. The efficiency of the hybrid algorithms depends on several variables as the depth of the quantum circuit, the chosen ansatz, the classical method used to optimize the variational parameters, the entanglement etc. Our goal is to study how the mentioned conditions affect the performance in order to design more efficient optimization algorithms based on the variational method. We use the supercomputer Altamira Supercomputer at the Institute of Physics of Cantabria (IFCA-CSIC), member of the Spanish Supercomputing Network, to perform simulations which emulate a fully fault-tolerant quantum computer before running our algorithms on a real noisy quantum device. This research shall prepare for the Noisy Intermediate-Scale Quantum (NISQ) technology which will be available in the near future.

#6 Self-assembly of polymers interacting with the square well potential

Miguel Herranz, Manuel Santiago, Nikos Karayiannis Manuel Laso, *Departamento de Ingeniería Química y Medio Ambiente, ETSII, Universidad Politécnica de Madrid, UPM*

Self-assembly and crystallization of polymeric systems are closely related to processes and applications in engineering, biology, material, polymer and colloidal science. The aim of the present work is to study, through extensive simulations, how attractive interactions affect the ability of polymers to form clusters and eventually crystallize. We consider polymers as linear, freely-jointed chains of spheres of uniform size. The monomeric pair-wise interaction is a short-range potential of the “square well/shoulder” type. This model is defined by two parameters: σ_2, the range of interaction, and ε, the strength of the interaction. If ε is positive, it corresponds to repulsion (square shoulder); whereas negative values of ε lead to attraction between the monomers (square well). Simulations are carried out with a Monte Carlo scheme based on local and chain-connectivity-altering moves. Given the wealth of simulation results, we are able to con struct the phase diagram as a function of intensity and range of potential. If the strength of the attraction reaches a threshold value (ε<-0.6), polymeric chains self-assemble into clusters. Depending on the interaction strength these clusters may remain amorphous or transit to a stable, crystal phase. The higher the value of the interaction range, the more spherical and stable is be the cluster and the easier for the cluster to crystallize. We also study the bond gap effect and compare it against the strict tangency condition. Three different ordered morphologies are observed: random

hexagonal close packing, sectors of mixed fcc/hcp character randomly meeting at twin axes occupied by sites of fivefold local symmetry and pure hcp/fcc crystals. Authors acknowledge support through project "MAT2015-70478" of MINECO. We thankfully acknowledge the computer resources and technical expertise and assistance provided by the Centro de Computacion y Visualizacion de Madrid (CeSViMa) through projects "p208" and "q373" and the Barcelona Supercomputing Center (BSC) through project "FI-2019-2-0014".

#7 DFT calculations approach for PbMoO4 and Pb1-2XCaXSrXMoO4 (x= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions

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Lourdes Gracia, *Department of Analytical and Physical Chemistry, University Jaume I, and Department of Physical Chemistry, University of Valencia, UV*

Fabiana V. Motta, Mauricio R. D. Bomio, *LSQM – Laboratory of Chemical Synthesis of Materials – Department of Materials Engineering, Federal University of Rio Grande do Norte – UFRN, Brazil*

Juan Andrés, *Department of Analytical and Physical Chemistry, University Jaume I, and Department of Physical Chemistry, University of Valencia, UV*

First-principles calculations were performed to provide a deep understanding of the local structures, bonding, morphologies, band gaps, and electronic and optical properties and open the door to exploit the electrical, optical and photocatalytic activity of this very promising family of materials. The geometries, electronic structures, and morphologies of as-synthetized of the $PbMoO_4$ and Pb1-2XCaXSrXMoO4 (x= 0.1, 0.2, 0.3, 0.4 and 0.5) solid solutions samples were characterized by first-principles quantum-mechanical, based on the density functional theory [1]. By using Wulff construction and the values of the surface energies for the (001), (100), (110), (111), (011) and (112) crystal surfaces, a complete map of the available morphologies for $PbMoO_4$ were obtained [2]. Good agreement between theoretical and experimental morphologies obtained from FE-SEM images is achieved [3].

[1] Andrés, Juan. et al. 2015. "Effects of Surface Stability on the Morphological Transformation of Metals and Metal Oxides as Investigated by First-Principles Calculations". Nanotechnology **26**(40):405703.

[2] Oliveira, Marisa. C. et al. 2016. "On the Morphology of $BaMoO_4$ Crystals: A Theoretical and Experimental Approach." Crystal Research and Technology **51**(10): 634–44.

[3] Oliveira, Fernanda. K.F. et al. 2018. "Experimental and Theoretical Study to Explain the Morphology of $CaMoO_4$ Crystals." Journal of Physics and Chemistry of Solids **114**(June 2017): 141–52.

#8 An atomistic understanding of the 2DEG at the LaAlO3-SrTiO3 interface

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Research involving new integration of semiconductor thin films is of interest, and has led to renewed research because such devices may exhibit innovative properties [1,2]. The two-dimensional electron gas (2DEG) at the interface of two otherwise insulating metal oxides, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), the LAO/STO heterostructure, has been investigated. The calculations were carried out by using density functional theory (DFT) as implemented in the Vienna Ab-initio simulation package (VASP) program [3]. The interfaces made by the co-exposed surfaces at LAO/STO were calculated by using an explicit atomistic model. The interaction between (LaO)+−(SrO)0, (LaO)+−(TiO_2)0, (AlO_2)−−(SrO)0, and (AlO_2)−−(TiO_2)0 layers in function of termination type, excess O anions on the upper part of the heterostructure, and interatomic distance at interface was evaluated. Interaction composed of the (AlO2)−−(TiO2)0 layers increase the interatomic distance, and when is formed by the (LaO)+−(SrO)0 interface exhibits a negative charge, implies that there is a repulsive force between them, and the electrons can be repelled. Excess of O-anions in the upper part of the heterostructure is able to eliminate the oxygen vacancies present; then, a complete local coordination, [AlO_6] and [LaO_12] cluster, are formed. The excess of O anions in the [TiO_5]-[AlO_5] model does not significantly affect the values of the Mulliken charge of these clusters, despite an increase occurring in the interatomic distance between the STO and LAO (100) surfaces. Our study introduces the possibility of defect engineering through the manipulation of oxygen vacancies and facet control at the interface and surface of materials, which can be ultimately be helpful in understanding the formation mechanisms of 2DEG at metal oxide interfaces.

[1] A. Brinkman, et al. Nat. Mater. 6 (2007) 493–496.

[2] E. Lesne, et al. Nat. Mater. 15 (2016) 1261.

[3] G. Kresse, et al. Comput. Mater. Sci. 6 (1996) 15–50.

#9 HPC based study: Analysis on two systems: wild-type Kras4B and phosphorylation at S-181 of G12D bounded K-ras4B anchored into negatively charged cholesterol/ DOPC/DOPS(15:28:7) plasma membrane

Huixia Lu, Jordi Martí, *Physics Department, UPC Barcelona Tech*

All Ras proteins family members belong to a class of protein called small GTpase. It plays an essential role in signal transduction pathways which ultimately turn on genes involved in cell growth, differentiation and survival so that overactive Ras signalling can lead to cancer. At normal levels, cholesterol is an essential substance for the body and it is present in every cell of the body and has important natural functions. Taking cholesterol into consideration could help us simulate more life-like cell membrane systems than those without cholesterol. Here in my study, I choose two systems: wild-type and oncogenic Kras4B anchored in a negatively charged membrane consists of cholesterol (30 mol%), DOPC (56 mol%) and DOPS (14 mol%), in which the ratio of DOPC:DOPS is 4:1. After running standard molecular simulation for both systems for 400 ns, short well-tempered metadynamics simulations were started for testing better parameters of selected collective variables. Also standard molecular simulations were continued until 700 ns for collecting and averaging data. Interesting and novel results are presented in the conclusion part.

#10 PyCOMPSs - An Efficient Programming Framework for large scale data analytics for HPC

Daniele Lezzi, Javier Alvarez, Pol Alvarez, Javier Conejero, Marc Domínguez, Jorge Ejarque, Hatem Elshazly, Francesc Lordan, Cristian Ramon-Cortes, Sergio Rodríguez, Salvi Solà, Rosa M. Badia, *Barcelona Supercomputing Center*

This poster presents the latest updates on PyCOMPSs, a programming framework well suited for the scalable execution of scientific applications on distributed infrastructures including clouds and supercomputing clusters. In particular, we present the dislib library, a distributed machine learning library built on top of PyCOMPSs that addresses the issues of implementing and efficiently running machine learning algorithms on HPC resources. The dislib library not only eases the implementation phase, providing out of the shelf parallel implementations fo ML algorithms, but also demonstrates to scale the execution with large data sets overperforming other popular distributed machine learning libraries, such as MLlib.

#11 Toxicity prediction: HPC simulation meets machine learning

Daniel Soler, Robert Soliva, Lucía Díaz, Suwipa Saen-Oon, Nostrum Bio Discovery, NBD

The attrition rate of drug candidates amounts to up to 96% (Paul et al., 2010): Drug safety accounts for 30% of drug failures (Giri and Bader, 2015). Reliable methods to assess compound toxicity early on in drug discovery are thus needed. However, published studies on predicting small molecule toxicity are almost exclusively ligand-based. Most tools incorporate some means of molecular similarity, functional group propensities, molecular descriptors, QSAR or machine learning (ML). Therefore, we have concentrated our efforts on the High Risk-Off Target (HROT) set published by the Altman group at Stanford. These are 83 proteins that are predicted to bind low-dose drugs more frequently than high-dose drugs, i.e. proteins that are related to drugs which are administered at very low doses, because high doses lead to adverse events. Assessing whether small molecules interact with HROTs is useful in all phases of drug discovery. We are in the process of building a user-friendly plat form to discriminate in a high-throughput manner whether compounds are toxic (binding to HROTs) or not. The workflow consists in extracting 10 representative clusters from each molecular dynamics. Next, a curated dataset of active and decoy compounds are docked into these clusters. The docking scores are then used to train different machine learning models, so as to obtain a consistent and robust classifier that can predict whether a given compound hits an HROT target. We have so far tested this approach on three systems: The androgen receptor (394 actives/404 decoys), CYP3A4 (168 actives/168 decoys), and the beta-2 adrenergic receptor (230 actives/230 decoys) with successful results. In the near future, we plan to apply our methodology to a subset of the most important cytochromes and many more systems.

7. RES awards

For the first time, the RES is organizing the RES Awards program, aiming at recognizing the task performed by the RES users in their own fields of research.

The RES Awards acknowledge:

- The **RES Poster Award** is awarded to the first author of the most meritorious poster presented at the annual Users Meeting. The work described in the poster must been carried out using RES HPC resources. The award will be decided during the conference; conference attendees will vote, and the awardee will be announced during lunch on Thursday. The awarded researcher is entitled for a travel grant for the next year Users Meeting.
- The **RES Outstanding Scientific Paper** published during the last 3 years by RES users. Candidates should submit their published papers during the registration process. 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. The awardee will be announced during lunch on Thursday.
- The **RES Outstanding Career** is meant to be the highest distinction within the HPC field in Spain. The award is conferred on a distinguished person or institution for an outstanding contribution to the research, development or dissemination of HPC in Spain. The nomination is decided by the RES Council based on the accumulated merits of the person or institution. The awardee will be announced during lunch on Thursday.

8. List of speakers (in alphabetical order)

Danilo Ardagna, Associate Professor, Politecnico di Milano, Italy

Received his Masters degree and PhD in Computer Science from Politecnico di Milano where he is currently an Associate professor. He was a visiting researcher at IBM TJ Watson Research Center and at the Basque Center for Applied Mathematics. His research interests are performance modelling and cloud resource management. He has developed solutions for web services compositions, optimization of virtualized systems and resource management of big data and artificial intelligence applications.

Rosa Ma. Badia, director of the Workflows and Distributed computing group, Barcelona Supercomputing Center, BSC

She holds a PhD from the UPC (1994). She is a Scientific Researcher at the Spanish National Research Council (CSIC). She graduated on Computer Science at the Facultat d' Informàtica de Barcelona (UPC, 1989). She was lecturing and doing research at the Computer Architecture Department (DAC) at the UPC from 1989 to 2008, where she held an Associate Professor position from 1997 to 2008; she is currently part-time lecturing again at the same department.

Vicent Botti, Full Professor of Computer Sciences and Head of the Valencian Research Institute for Artificial Intelligence, VRAIN, at the Universidad Politécnica de Valencia, UPV

He has been working in the area of Artificial Intelligence and Multi-agent systems for 30 years. His main research lines have been: Responsible Artificial Intelligence, Autonomous Agents, Multi-Agent Systems, Agreement Technologies, Agent-Based Social Simulation, Emotional Agents, Real-Time Artificial Intelligence, Real-time Systems and Softcomputing. He has over 350 international refereed publications. He has taken part in 71 research projects, having been the principal investigator (IP) in 32. He was awarded with the 2005 Prize of Research of the Spanish Association for Artificial Intelligence, the 2017 Fellow of the European Association for Artificial Intelligence, and the 2018 Spanish National Prize of Informatics (SCIE).

Javier Conejero, Senior Researcher of the Workflows and Distributed Computing research group, Barcelona Supercomputing Center, BSC

He holds a PhD on Advanced Computer Technologies (2014) from the University of Castilla-La Mancha (UCLM), Spain. During his PhD, he was awarded by the Ministry of Economy and Competitiveness (MINECO) of the Spanish Government with a FPI fellowship grant. Previously, he worked at CERN for one year (2009) into WLCG software development and management. Since 2015, he is leading the efforts on the PyCOMPSs binding at BSC. In 2016 he was awarded by the MINECO with the Juan de la Cierva grant. His current research interest are QoS, development paradigms, parallel and distributed computation, HPC and Cloud computing. He is currently participating in the NEXTGenIO EU funded project.

Tanausú del Pino Alemán, Postdoc, Instituto de Astrofísica de Canarias

Defended his PhD Thesis, titled "Radiative Transfer Modeling of the Spectral Line Polarization Produced by Optically Pumped Atoms in the Solar Atmosphere", in November 2015 at the IAC. Between 2016 and 2017 worked as an Advance Study Program Postdoc fellow at the HAO-NCAR in the USA. Since 2018 is an Advanced Postdoctoral Fellow of the ERC Advanced Grant POLMAG at the IAC in Spain.

Carolina Estarellas, Marie Curie Fellow, University College London, UCL

She obtained her PhD in 2012 at the University of Balearic Islands. As a postdoc she joined the groups of Prof. Sponer at CEITEC (Czech Republic, 1 year), Prof. Luque at UB (Spain, 4 years) and Prof. Gervasio at UCL (UK, 2 years). Her research lines are centered at the study of reaction mechanisms via quantum mechanics methods, the understanding of structure-function relationship in complex protein-ligand systems for drug design, and method development.

Adriano Galano, Chief Technology Officer, Fujitsu

Leader of the team of BDMs, CATMs and Sales Specialists with a focus on Infrastructure and Business Solutions: High Performance Computing, Big Data and Business Analytics, Data Protection, Software Defined Data Center, SAP, Workplace and Mobility Solutions, Networking and Security in addition to our Product Portfolio with very well recognized brands as: PRIMERGY, PRIMEQUEST, ETERNUS, CELSIUS, LIFEBOOK, FUTRO and PRIMEFLEX.

Francisco Javier García-Blas, Associate Professor, University Carlos III of Madrid

He received a PhD in Computer Science from University Carlos III in 2010. He has participated in several projects with researchers from various high performance research institutions such as HLRS (funded by HPC-Europe program), DKRZ, and Argonne National Laboratory. He is currently involved in various projects in topics such as parallel I/O, image processing, heterogeneous computing, and accelerators for high-performance platforms. He has been involved in six research projects funded by the European Union (such as Repara, Rephrase and ASPIDE). He currently has more than 80 international publications in journal and conference papers.

Anne Gosset, Prof. Contratado Doctor, University of A Coruña

She holds a PhD in Applied Sciences from the Université Libre de Bruxelles (Belgium) in 2007. She develops her investigation activity in the field of fluid mechanics applied to industrial processes, with a special interest in the metallurgy and naval sectors. Since April 2017, she is the director of the Centro de Investigaciones Tecnológicas, one of the 4 research centers of the UDC, which has 8 groups and 100 researchers in total.

Cees Hof, Data Archiving and Networked Services, DANS

DANS is the Netherlands institute for permanent access to digital research resources. At DANS he is responsible for project acquisition, is involved in several EOSC related projects, works together with the Netherlands eScience Center (NLeSC) on a FAIR Software Route, and acts as a DANS liaison officer for the life sciences. Cees is one of the Research Data Management (RDM) trainers within DANS and also a coach in the Essentials 4 Data Support training module, the successful (inter)national RDM course that DANS organises jointly with the national academic computing center SURFsara and the Technical University Delft. He started as an applied researcher in the field of ecology and eco-toxicology and received his PhD from the University of Amsterdam as an evolutionary biologist and palaeontologist. Before moving to DANS he was the coordinator of the European Network for Biodiversity Information (ENBI) and the Node Manager of the Dutch branch of the Global Biodiversity Information Facility (GBIF) for more than 10 years.

Javier Junquera, Ramón y Cajal fellow, Universidad de Cantabria

BS degree at the Universidad de Oviedo (Spain) in 1996. Ph.D. in 2001 Universidad Autónoma de Madrid. Postdoc at the Université de Liège (Belgium; 2001-2003) working with Philippe Ghosez and at Rutgers University (New Jersey, USA; 2003-2004) in Karin M. Rabe's group. His most important methodological work is the contribution to the development of the SIESTA project (http://www.icmab.es/siesta). SIESTA is both, a Density-functional Numerical Atomic Orbital (NAO) method and its computer program implementation, to perform electronic structure calculations and ab-initio molecular dynamics simulations of molecules and solids, with the capability of making the computer time and memory scale linearly with the number of atoms (order-N scaling). From the applied point of view, he has specialized in the study of ferroelectric size effects in nanostructures. Right now, he is involved in the development of "second-principles" methods. The goal is to achieve simulations of tens of thousands of atoms at operating conditions (finite temperature), describing the coupled dynamics of ions and relevant electronic degrees of freedom, and accessing scales and physical phenomena that have never been investigated so far with atomistic details and first-principles accuracy.

Bruno Leconte, Solution Architect Manager, HPC & AI, France, Southern & CEEMA, Hewlett Packard Enterprise

After 15 years at SGI (Silicon Graphics) in various HPC technical position and several years managing SGI Southern Europe team, he is leading Hewlett Packard Enterprise High-Performance Computing (HPC) and Artificial Intelligence (AI) Solution Architect

group covering France, Spain, Italy, Southern Europe, Eastern Europe, Middle East and Africa. Hewlett Packard Enterprise HPC & AI Solution Architect group is focused on solving complex problems for our customers and for our society. He holds a PhD in Science and brings with him a wealth of customer experience and depth of AI and HPC knowledge.

Pablo G. Lustemberg, Instituto de Catálisis y Petroleoquímica, ICP-CSIC, Instituto de Física Rosario, IFIR-CONICET, Santa Fe, Argentina

Since 2019 he is a Marie Curie Fellow at the Instituto de Catálisis y Petroleoquímica (CSIC), Madrid. Since 2012 he is also a Researcher at the National Council of Scientific and Technical Research (CONICET), Institute of Physics Rosario (IFIR), Argentina. In 2015 he was a PostDoc in Chemistry at Instituto de Catálisis y Petroleoquímica (CSIC), Madrid, and in 2010-2012 a PostDoc in Chemistry at Instituto de Química Física de los Materiales, Medio Ambiente y Energía (INQUIMAE), Argentina. He holds a Masters in Physics (2004) and a PhD in Physics (2010), from Instituto Balseiro, Universidad Nacional de Cuyo, Argentina. He also holds a Degree in Physics, from Universidad de Buenos Aires (2003).

Fernando Martín, Full Professor, Universidad Autónoma de Madrid, UAM

His research focuses on the interaction of laser light with atoms and molecules, and the properties of new materials and nanoobjects. In 2000, he was awarded the National Research Prize Rey Juan Carlos I, in 2010, the prize of the Spanish Royal Society of Chemistry in Chemical Physics, in 2011, the Advanced Grant from the European Research Council XCHEM, and in 2017 the Prize Rey Jaime I in Basic Research.

Ander Otxoa, Systems Architect, IBM

He has been working for IBM since year 2000 as Systems Architect, developing his professional career in different countries both in Latin America and Europe. He has taken a deep dive in High Performance Architectures as IBM POWER, focusing in Artificial Intelligence and specifically Deep Learning.

María S. Perez, Full Professor, Universidad Politécnica de Madrid, UPM

She is part of the Board of Directors of BDVA and member of the Research and Innovation Advisory Group of the EuroHPC Joint Undertaking. Her research interests include high performance and large-scale computing, storage, big data and application of AI techniques. She is the coauthor of 4 books, 7 book chapters and has published more than 100 articles in international journals and conferences.

Natasa Przulj, ICREA Research Professor, Barcelona Supercomputing Center, BSC

Elected academician of The Academy of Europe, Academia Europaea, and a Fellow of the British Computer Society. She has been a Professor of Biomedical Data Science at University College London (UCL) Computer Science Department since 2016. She received two prestigious European Research Council (ERC) grants, the ERC Consolidator grant titled “Integrated Connectedness for a New Representation of Biology” (2018-2023) and the ERC Starting Independent Researcher Grant titled “Biological Network

Topology Complements Genome as a Source of Biological Information" (2012-2017). She was awarded the British Computer Society Roger Needham Award in 2014 for a distinguished research contribution in computer science by a UK based researcher within ten years of their PhD. She held a prestigious NSF CAREER Award for the project titled "Tools for Analyzing, Modeling, and Comparing Protein-Protein Interaction Networks" in 2007-2011 at University of California Irvine. Her research has also been supported by other large governmental and industrial grants including those from GlaxoSmithKline, IBM and Google. She was previously an Associate Professor (Reader; 2012-2016) and Assistant Professor (Lecturer; 2009-2012) in the Department of Computing at Imperial College London and an Assistant Professor in the Computer Science Department at University of California Irvine (2005-2009). She obtained a PhD in Computer Science from University of Toronto in 2005 and a BSc First Class Honors in Mathematics and Computing Science in 1997 from Simon Fraser University.

Edilberto Sánchez, OPI scientist, National Fusion Laboratory of CIEMAT

He has worked in turbulence and transport in fusion plasmas and also in the development of data acquisition systems for fusion devices. Currently enrolled at the LNF Theory Unit, where he is dedicated to the simulation of turbulence in magnetically confined plasmas with gyrokinetic codes. Coordinator of the Physics panel of the Spanish Supercomputing Network (RES).

Nadia Tonello, Head of Data Management group, Barcelona Supercomputing Center, BSC

She holds a PhD from the Technical University of Munich with research work in Astro-particle Physics at the Max-Planck Institute for Physics, as part of the MAGIC collaboration. She worked as a scientific liaison in the Astrophysics and Cosmology group at Port d'Informació Científica (HTC data center, Barcelona) for two international projects: the PAU Survey and the ESA mission Euclid. She was responsible of the management of both observed and simulated data archives, the parallelization and optimization of pipelines code, and the operations of data analysis and validation. She was the deputy leader of the Spanish Scientific Data Center of the Euclid Science Ground Segment and member of the image simulations unit (OU-SIM), coordinating the code integration activities and the validation of the products. At BSC, she is responsible for data services of the Center and the collaboration with the RES Data WG. She is currently involved in projects of Open Data and Open Science such as RDA, EUDAT CDI, EOSC-hub and EOSC-synergy. She is also one of the Spanish delegates at the European Open Science Cloud Governing Board.

Guilherme Vilhena, Marie Curie fellow, University of Basel

Graduated in 2017 in Physics at the University of Coimbra (ranking best student of the promotion). In 2011 he obtained a PhD in the University of Lyon with a Portuguese fellowship awarded based on his merits. Then, he spent 7 years in Universidad Autónoma de Madrid developing methods to unravel atomic detail of Scanning Probe Microscopy Experiments. Now, he is a Marie Curie fellow (ranking top 2% in the Physics panel) in the University of Basel to unravel the molecular origins of friction at nanoscale.

9. Organizing committees

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