20th September 2018 | Valencia

Infraestructuras Científicas y Técnicas Singulares

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Universitat de València

Gobierno de España
Ministerio de Ciencia, Innovación y Universidades

RES
RED ESPAÑOLA DE SUPERCOMPUTACIÓN

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12th Users' Conference

Book of Abstracts

12th RES Users'Conference

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Programme

20th September 2018

09:30	**Registration**
10:00	**Sergi Girona** (BSC) and **José María Ibáñez** (UV): Welcome
10:10	**Institutional presentation**
10:40	**Sergi Girona** (BSC): RES updates, resources and access
11:00	**Sergi Girona** (BSC): European HPC ecosystem
11:20	*Coffee break and poster session*
11:50	**Round table: open research data.** Organised by RDA Europe. Chair: **Jesús Marco** (CSIC)
13:00	**M. Veronica Ganduglia-Pirovano** (ICP-CSIC): RES Users' Committee Presentation and open discussion
13:40	*Lunch break (sponsored by RDA Europe)*

Scientific Parallel Sessions

	Astronomy, Space and Earth Sciences Chair: **Miguel A. Aloy** (UV)	Life and Health Sciences Chair: **Salvador Capella** (BSC)	Mathematics, Physics and Engineering Chair: **Raul Payr** (UPC)	Chemistry and Materials Science Chair: **M.Veronica Ganduglia-Pirovano** (ICP-CSIC)
15:00	*AECT 1* **Elena Khomenko** (IAC): Three-dimensional simulations of solar magneto-convection including effects of partial ionization	*BCV 1* **Antonio Fernandez-Guerra** (MPI-Bremen DE): Illuminating the functional dark side of genomes and menomes	*FI 1* **Edilberto Sánchez** (CIEMAT): Global gyrokinetic simulations of stellarator plasmas	*QCM 1* **José Javier Plata Ramos** (US): Combining high-throughput and high-performance computing for the discovery of new photo-sensitized epitaxial structures
15:30	*AECT 2* **Sascha Husa** (UIB): Modelling gravitational wave signals from coalescing black holes	*BCV 2* **Ramiro Logares** (ICM-CSIC): Microbial population genomics from a metagenomics perspective	*FI 2* **Rafael Delgado** (UAM): CATCH-U-DNA: Detecting Cancer using Quartz Micro-balance Resonators	*QCM 2* **Michele Pisarra** (UAM): Understanding the modifications of the physical properties of supported graphene by means of Density Functional Theory
16:00	*AECT 3* **Valentina Sicardi** (BSC): Generation of initial conditions for the prediction of ocean carbon uptake	*BCV 3* **Jana Selent** (UPF): Membrane lipids regulate GPCR functionality	*FI 3* **Jose Maria Garcia Oliver** (CMT Motores Termicos-UPV): LES approach for near- and far-field prediction of dense sprays	*QCM 3* **Carlos Romero Muñiz** (UAM): Graphene on rhodium from first principles: Tailoring electronic, structural and chemical properties
16:30	*Coffee break and poster session*			
17:00	*AECT 4* **Gustavo Yepes** (UAM): Simulating Virtual Universes with the MareNostrum Supercomputer	*BCV 4* **Adam hospital** (IRB): Workflow atomation and efficiency for macromolecular simulations and screening	*FI 4* **Oriol Lehmkuhl** (BSC): On the use of supercomputing for the high-fidelity simulation of massive separated flows	*QCM 4* **Núria López** (ICIQ): Simulations in Catalytic materials
17:30	*AECT 5* **Martin Obergaulinger** (UV): Multi-dimensional simulations of stellar core collapse with rotation and magnetic fields	*BCV 5* **Horacio Pérez Sánchez** (UCAM): Development and application of structural bioinformatics methods in drug discovery on high performance computing architectures and its technology transfer to the biotech sector	*FI 5* **Ivette Rodríguez** (UPC): *High Performance Computing of the fluid dynamics and heat transfer of axisymmetric wakes*	*QCM 5* **Mercedes Boronat** (UPV-CSIC): Non-noble metal clusters and particles for heterogeneous catalysis
18:00	*Pause*			

18:10	Closing session by **José María Ibáñez** (UV) and **Sergi Girona** (BSC)
18:20	*End of the conference*
19:00	*Social Event*

Acknowledgments

The RES gratefully acknowledges Universitat de València for their collaboration in organising this conference, and RDA Europe for their support and sponsorship.

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

One year more, the Annual Users' Conference of the Spanish Supercomputing Network aims to be a meeting point for HPC users and technicians, the RES Access Committee and the RES Users' Committee. In this 12th edition, the plenary talks will inform about the main updates in RES infrastructure and the future plans. Also, the RES manager will provide an introduction to the European HPC ecosystem and the Spanish participation in this initiative. The plenary session will be a roundtable about Open Research Data, co-organised by Research Data Alliance Europe, and will count on the presence of research data experts from RDA at national and European level.

The programme includes four parallel scientific sessions, focused on the four scientific areas of RES activities: Life and Health Sciences; Mathematics, Physics and Engineering; Astronomy, Space and Earth Sciences; Chemistry and Materials Science and Technology. Each session will include five talks of recognised experts, who will share their experience in RES and PRACE projects. Besides, the poster session aims to disseminate the scientific results obtained using RES resources and to promote the interaction among conference attendees.

This booklet contains the conference agenda and the abstracts of oral and poster presentations. We hope that this publication is a valuable contribution to disseminate the applications of high performance computing technologies in research.

The organising committee

Plenary sessions

- ***RES updates and European HPC ecosystem***

  Sergi Girona – BSC Operations Director and RES Manager

  The Spanish Supercomputing Network has provided HPC resources for Spanish researchers since 2006. In these 12 years, the RES has given access to 2500 research activities through 38 competitive calls, contributing to the progress of excellent science and innovation in Spain. The amount of computing capacity available for RES users has increased continuously due to the updates and improvements that the RES nodes have performed in their systems. Recently, the BSC has significantly increased its contribution to the RES and, as a result, the RES is offering XX million hours for the next four-month period. In the near future, the RES is planning to develop new services for researchers related to research data management and storage.

  In a longer term, the future of HPC in Spain is closely linked to the upcoming exascale for Europe. The EuroHPC agreement, signed in 2017 initially by seven countries, aims to develop, deploy, extend and maintain in the Union an integrated world-class supercomputing and data infrastructure and to develop and support a highly competitive and innovative High-Performance Computing ecosystem. Its mission is to provide European scientists, industry and the public sector with the latest HPC and data infrastructure and support the development of its technologies and applications across a wide range of fields.

- ***Round table: open research data***

  Organised by RDA Europe, moderated by Jesús Marco (Vice Director/CSIC).

  This plenary session will gather research data experts at national and European level. Confirmed participants are Sara Garavelli, from RDA-EU leadership, Pierre-Antoine Bretonnière, from Barcelona Supercomputing Center on RDA adoption in Climate Modelling, Emma Lazzeri, manager of the RDA Italy node, and Fabrizio Gagliardi from RDA-EU Spain. Representatives from EOSC and HPC data are also expected. Names to be confirmed prior to the panel.

- ***Presentation of the RES User's Committee***

  Maria Veronica Ganduglia-Pirovano – Member of the CURES / Instituto de Catalisis y Petroleoquimica-CSIC, Madrid

  The purpose of CURES (Comité de Usuarios de la Red Española de Supercomputación) is to provide advice and feedback to RES (Red Española de Supercomputación) on the current state and future delivery of RES resources and services.

  CURES promotes the effective use of the high performance computing facilities at RES by sharing information about experiences in using the facility, suggesting new research and technology directions in scientific computing, and voicing users' concerns.

  In this talk I will describe how to Access to the CURES as well as present a summary of the cases attended in the last year and discuss some of the suggestions already made based on the users' comments.

Astronomy, Space and Earth Sciences

Chair: **Miguel A. Aloy** (Universitat de València)

- ***AECT 1: Three-dimensional simulations of solar magneto-convection including effects of partial ionization***

  Elena Khomenko
  Instituto de Astrofísica de Canarias

  In this contribution we are interested to study the influence of partial ionization of solar plasma into the energy balance of the solar atmosphere. Over the last decades, realistic 3D radiative-MHD simulations have become the dominant theoretical tool for understanding the complex interactions between the plasma and the magnetic field on the Sun. Most of such simulations are based on approximations of magnetohydrodynamics, without directly considering the consequences of the very low degree of ionization of the solar plasma in the photosphere and bottom chromosphere. The presence of large amount of neutrals leads to a partial decoupling of the plasma and the magnetic field. As a consequence of that, a series of non-ideal effects (ambipolar diffusion, Hall effect and battery effect) arises. The ambipolar effect is the dominant one in the solar chromosphere. We performed first three-dimensional realistic simulations of magneto-convection including ambipolar diffusion and battery effects. The simulations are done using Mancha3D code. Our results reveal that ambipolar diffusion causes measurable effects on the amplitudes of waves excited by convection in the simulations, on the absorption of Poynting flux and heating and on the formation of chromospheric structures. Thanks to the simulations with battery-excited dynamo fields we can provide a low bond on the chromospheric temperature increase due to the ambipolar effect.

- ***AECT 2: Modelling gravitational wave signals from coalescing black holes***

  Sascha Husa
  Departament de Física, Universidad de les Illes Balears

  This talk reports on recent progress of a long-term program at UIB to model the gravitational wave signals emitted during the coalescence of astrophysical black hole binary systems due to radiation reaction. The models we develop have become standard tools used to analyse the data from the LIGO and Virgo gravitational wave detectors, and have contributed to identify the sources of the first detections.

  In order to identify the sources of gravitational events, detector data need to be compared with template waveforms, which are synthesized from perturbative results and numerical solutions of the Einstein equations, which are the field equations of general relativity. The Einstein equations can be written as a set of coupled nonlinear partial differential equations, which we solve with high order finite difference methods, exploring a 9-dimensional parameter space. The talk will discuss the physical motivation for the modelling approach, computational aspects, and give an overview of the type of observational result that are obtained based on the models we develop.

AECT 3: Generation of initial conditions for the prediction of ocean carbon uptake

Valentina Sicardi, Raffaele Berbardello, Mario Acosta and Pablo Ortega
Barcelona Supercomputing Center, Earth Science Department

The recent COP21 Paris agreement ties the participating countries to reduce anthropogenic carbon emissions in order to contain global warming within 2°C by the end of this century. This translates into the necessity to estimate the compatible CO2 emissions well ahead of time to make sure targets are met. However, precision in these estimates can be achieved only if sources and sinks of carbon are known with the highest possible accuracy. The ocean represents one major sink as it takes up about 25% of the anthropogenic carbon emitted by humans. However, this estimate oscillates because natural variability and ongoing climate change could alter the capacity of the ocean to absorb carbon. Using the EC-Earth Earth System Model, we at the BSC are aiming to predict the ocean carbon uptake on timescales ranging from one month to one decade ahead. The extent to which this goal is achievable depends on the quality of both the ocean physical initial conditions and the biogeochemical initial conditions, and the initialization procedure. This presentation will show the importance of the generation of the initial conditions needed for climate prediction and in particular for ocean biogeochemical studies.

AECT 4: Simulating Virtual Universes with the MareNostrum Supercomputer

Gustavo Yepes
Departamento de Física Teórica, Facultad de Ciencias, Universidad Autónoma de Madrid

Computer simulations are becoming an indispensable research tool in many scientific disciplines where the object of study is either very risky or simply impossible to experiment with it. This is certainly the case in Astrophysics and Cosmology. The only way to do experiments and test hypotheses of theoretical models is by creating virtual universes in large supercomputer facilities. Due to the extreme non-linear physical processes responsible for the formation and evolution of structures in the universe, computational cosmology is one of the disciplines which is always pushing the technical capabilities of current supercomputing resources to their limits. Some years ago, in 2005, when the first MareNostrum supercomputer was installed at the Barcelona Supercomputer Center, a group of researchers from different countries teamed up and set up the so-called: MareNostrum Numerical Cosmology Project collaboration. The aim of this international collaboration is to simulate the formation and evolution of different cosmic structures in the Universe, ranging from the largest scales (cluster and supercluster of galaxies), to the most nearby ones (the Local Universe and the Local Group), starting from cosmological initial conditions and assuming different dark matter candidates (cold, warm, etc) and models to account for the very complex physical processes acting on the visible component (gas and stars). In my talk, I will review the work done by our collaboration in terms of the numerical experiments that have been carried out in MareNostrum since 2005 and in other european PRACE supercomputers and the most striking results that have been obtained from the analysis of these simulations. I will focus on the three main simulation projects that we are currently working on: Large Volume simulations for galaxy surveys, Simulations of the visible universe (Galaxy Clusters) and the Near Field cosmological simulations (the CLUES project).

AECT 5: Multi-dimensional simulations of stellar core collapse with rotation and magnetic fields

Martin Obergaulinger and Miguel A. Aloy
Departament d'Astronomia i Astrofísica, Universitat de València

Rapidly rotating stars that produce high-mass proto-neutron stars are considered potential progenitors of gamma-ray bursts that might be powered by a collapsar, i.e., a black hole surrounded by an accretion torus, or, if collapse to a black hole does not occur sufficiently early, by a long-lived proto-magnetar. Coupling special relativistic MHD, a pseudo-relativistic gravitational potential, and two-moment neutrino transport, we performed axisymmetric simulations of stars of 35 solar masses that fall into the class of potential GRB progenitors [1]. The results show explosions launched by mechanisms to which neutrino heating, rotation, and magnetic fields contribute to different degrees. The explosions occur in parallel to ongoing accretion onto the PNS, hence allowing for its growth in mass and rotational energy and, as a possible consequence, for later GRBs.

References:

[1] M. Obergaulinger, M.Á. Aloy, MNRAS 469, L43-L47 (2017)

Life and Health Sciences

Chair: **Salvador Capella** (BSC)

BCV 1: Illuminating the functional dark side of genomes and metagenomes

Antonio Fernandez-Guerra [1], Chiara Vanni [1], Pier Luigi Buttigieg [2], A. Murat Eren [3], Albert Barberan [4], Frank Oliver Glöckner [1]

[1] Max Planck Institute for Marine Microbiology, Germany, [2] Alfred Wegener Institute, Germany, [3] University of Chicago, United States, [4] University of Arizona, United States

Extensive metagenomic surveys, such as TARA Oceans and the Human Microbiome Project, have enabled in-depth ecological and evolutionary investigations of naturally occurring microbes. These studies have provided new insights into the functional capacities of microbial assemblages; however, they have also revealed many genes of unknown function that await characterization. Despite the fact that such genes constitute 40-60% of the predicted open reading frames (ORFs) found in most environments, traditional analyses often ignore them entirely. This large, uncharacterized fraction is likely to close gaps in existing organism and environment-scale metabolic models and offer novel targets for biotechnology and biomedicine. Here, we used a multi-layered computational approach to organize 322 million ORFs from 1,628 metagenomic datasets into three groups: knowns (known function, present in sequenced genomes), genomic unknowns (unknown function, present in sequenced genomes) and environmental unknowns (without any distant homology). The unknown fraction consisted of 994,878 genomic unknown components and 137,598 environmental unknown components. A subset of ubiquitous environmental unknowns (e.g. potential housekeeping genes, ORFs associated with auxiliary metabolic genes in phages) was present in all metagenomes, suggesting a significant gap in our knowledge regarding essential environmental processes. Additional sets of unknowns showed associations to environmental variations, suggesting more finely-tuned ecological roles: attributes which may assist characterization and biotechnological exploitation. To begin characterizing environmental unknowns, we used single-cell amplified and metagenome-assembled genomes to investigate their genomic context. Together, these efforts have begun to bring structure to the hidden functional potential within microbial communities, promising to fuel future discovery in the field.

BCV 2: Microbial population genomics from a metagenomics perspective

Ramiro Logares

Institut de Ciències del Mar (ICM-CSIC)

During the last five years, our capability to generate microbial metagenomes (that is, genomic fragments from multiple species in a community) from diverse environments has increased dramatically. Analysing this information requires advanced analytical approaches as well as substantial computing power. Here I will present our work where we reconstruct the genomic information of different species of ocean microbes (prokaryotes and eukaryotes) originating from large-scale metagenomic surveys. Reconstructed genomes (a.k.a. Population genomes or PGs) do not represent any single cell or individual from the population, but instead they are a consensus of the genomic information contained across multiple individuals in the population. PGs allow us accessing the genome of species that otherwise would be unavailable for research, as they are typically unculturable. Specifically, PGs allow investigating the metabolic repertoire of multiple species and their abundances across diverse spatiotemporal scales. In particular, by comparing different communities or metagenomes against PGs, it is possible to determine fine-grained genomic variation that could be associated to different populations. This opens-up multiple possibilities for understanding the spatiotemporal turnover of different variants or populations as well as to investigate adaptive or non-adaptive evolution. Together with standard shotgun DNA sequencing from cultured microbes and Single-Cell Genomics, PGs can now be added to the toolbox of molecular biologists that seek to understand the functional repertoire of environmental microbes as well as their spatiotemporal distributions, gene expression and microevolution.

BCV 3: Membrane lipids regulate GPCR functionality

Jana Selent

GPCR Drug Discovery Lab, Research Programme on Biomedical Informatics (GRIB), IMIM-UPF

Cell membranes have significant influence over signaling proteins that are embedded within them. One important class of such proteins are G protein coupled receptors (GPCRs). GPCRs are abundantly distributed in the central nervous system (CNS) where they sense molecules outside the cell and activate diverse signal transduction pathways inside the cell yielding a distinct cellular response.

Extensive computational characterization of GPCRs by means of all-atom and coarse-grained molecular dynamics simulation help shedding light into the molecular details of the intimate relationship between receptors and cell membranes. This lecture will focus on regulatory mechanisms of individual cell membrane components such as the poly-unsaturated fatty acid DHA and cholesterol that involve receptor lubricating [1] and tunneling effects [2]. Experimental validation highlights the importance of cell membrane composition for proper receptor signaling. This has important implications for CNS related disease and creates new opportunities to explore the use of membrane lipids as a therapeutic tool for major CNS conditions.

References:

[1] Guixà-González R, Javanainen M, Gómez-Soler M, Cordobilla B, Domingo JC, Sanz F, Pastor M, Ciruela F, Martinez-Seara H, Selent J. Membrane omega-3 fatty acids modulate the oligomerisation kinetics of adenosine A2A and dopamine D2 receptors. Sci. Rep. 6, 19839 (2016).

[2] Guixà-González R, Albasanz JL, Rodriguez-Espigares I, Pastor M, Sanz F, Martí-Solano M, Manna M, Martinez-Seara H, Hildebrand PW, Martín M, Selent J. Membrane cholesterol access into a G-protein-coupled receptor. Nat. Commun. 8, 14505 (2017)

BCV 4: Workflow atomation and efficiency for macromolecular simulations and screening

Adam Hospital [1], Pau Andrio [2], Laia Codó [2], Brian Jiménez [2], Luis Jordà [2] and Josep Lluís Gelpí [2,3]
[1] Cell Signalling and Adhesion Group, [2] Spectroscopy and Nuclear Magnetic Resonance Unit, [3] Structural Computational Biology Group, Structural Biology and Biocomputing Programme, Spanish National Cancer Research Centre (CNIO), Madrid 28029, Spain

SH2-containing-inositol-5-phosphatases (SHIPs) dephosphorylate the 5-phosphate of phosphatidylinositol-3,4,5-trisphosphate (PI(3,4,5)P3) and play important roles in regulating the PI3K/Akt pathway in physiology and disease. Aiming to uncover interdomain regulatory mechanisms in SHIP2, we combined structural, computational and biochemical studies on the 5-phosphatase and a proximal region adopting a C2 fold.

This reveals an extensive interface between the two domains, which results in significant structural changes in the phosphatase domain. Both the phosphatase and C2 domains bind phosphatidylserine lipids, which likely helps to position the active site towards its substrate. Although located distant to the active site, the C2 domain greatly enhances catalytic turnover. Employing molecular dynamics simulations on the phosphatase or phosphatase-C2 regions of SHIP2 we identify important dynamic changes induced by the C2 domain.

A helical section, which at one end contacts the C2 domain is stabilized by the C2 domain and at the other end the helices modify the dynamics of a loop close to the active site, affecting catalytic turnover. Combining the simulations with mutagenesis, enzyme kinetics and cell biology, we identify two distinct allosteric signaling pathways, emanating from hydrophobic or polar interdomain interactions, differentially affecting lipid chain or headgroup moieties of the PI(3,4,5)P3 substrate.

Together, this study reveals details of multilayered C2 mediated effects important for SHIP2 activity and points towards interesting new possibilities for therapeutic interventions.

BCV 5: Development and application of structural bioinformatics methods in drug discovery on high performance computing architectures and its technology transfer to the biotech sector

H. Pérez-Sánchez, H. den-Haan, J. Peña-García, R. Rodríguez-Schmidt, A. Pérez-Garrido, J.M. Cecilia, B. Imbernón-Tudela, A. Banegas-Luna and J.P Cerón-Carrasco.
Bioinformatics and High Performance Computing Research Group (BIO-HPC), Universidad Católica de Murcia (UCAM)

The development of new drugs is a very expensive process that can be benefited from the use of structural bioinformatics techniques (SBT). Besides, application of SBT is very costly since it requires of demanding computations and this situation has reached a plateau in the last decades due to limitations not overcome yet. In this talk we present how SBT in drug discovery can be drastically accelerated with the use of high performance computing (HPC) architectures such as supercomputers and Graphics Processing Units (GPUs) [1] and methodological advancements that our group (Bioinformatics and High Performance Computing, http://bio-hpc.eu) has developed in the last years, and which have been successfully applied to the discovery of active compounds in the context of anticoagulants [2], cancer [3], Parkinson [4], Fabry [5], nutraceuticals [6], Zika [7], etc. Finally we also show how other users can access our tools online and how we have transferred them to the biotechnology market.

References:

[1] I. Sánchez-Linares, H. Pérez-Sánchez, J.M. Cecilia, J.M. García, BMC Bioinformatics, 2012, 13(Suppl 14):S13

[2] J. Navarro-Fernández, H. Pérez-Sánchez, I. Martínez-Martínez, I. Meliciani, J.A. Guerrero, V. Vicente, J. Corral, W. Wenzel, J. Med. Chem., 2012, 55(14), 6403-6412

[3] D.K. Yadav, R. Rai, N. Kumar, S. Singh, S. Misra, P. Sharma, P. Shaw, H. Pérez-Sánchez, R.L. Mancera, E.H. Choi, M. Kim, R. Pratap, Sci. Rep., 2016, DOI:10.1038/srep38128.

[4] D. Morshedi, F. Aliakbari, A.T. Marvian, A. Fassihi, F. Pan-Montojo, H. Pérez-Sánchez, J. Food Sci., 2015, DOI:10.1111/1750-3841.1301

[5] V. Citro, J. Peña-García, H. den-Haan, H. Pérez-Sánchez, R. Prete, L. Liguori, C. Cimmaruta, M.V. Cubellis, G. Andreotti, PLOS ONE, 2016, DOI:10.1371/journal.pone.0165463.

[6] I. Navarro-González, H. Pérez-Sánchez, G. Martin-Pozuelo, J. García-Alonso, M.J. Periago, PLOS ONE, 2014, DOI: 10.1371/journal.pone.0083968.

[7] S. Yuan, J.F. Chan, H. den-Haan, K.K. Chik, A.J. Zhang, C.C. Chan, V.k. POON, C.C. Yip, W. Mak, Z. Zhu, Z. Zou, K. Tee, J. Cai, K. Chan, J. Peña-García, H. Pérez-Sánchez, J.P. Cerón-Carrasco, K. Yuen, (2017), Antiviral Research, DOI:10.1016/j.antiviral.2017.07.007.

Mathematics, Physics and Engineering

Chair: **Raul Payri** (UPV)

- ## *FI 1: Global gyrokinetic simulations of stellarator plasmas*

Edilberto Sánchez
Laboratorio Nacional de Fusión, CIEMAT

The magnetic confinement is a promising alternative for the use of thermonuclear fusion as a massive source of clean energy. However, an important issue in the magnetic fusion research is the confinement of particles and energy within the reactor, which is experimentally observed to be much worse than initially expected. The energy and particle transport exceed by orders of magnitude the expectations based on classical mechanisms and is said to be anomalous. Most of this anomalous transport in magnetically confined plasmas is considered to be due to micro-turbulence, which produces transport levels much above classical predictions, critically limiting the performance of a fusion reactor based on the magnetic confinement concept, either tokamak or stellarator.

Plasma turbulence is a nonlinear problem involving many different scales both in space and time, whose study requires the use of numerical simulations. The gyrokinetic formalism allows reducing the computational resources required for kinetic plasma simulations and makes them affordable in present supercomputers. These simulations are particularly challenging computationally in the three-dimensional configurations of stellarator devices.

In this contribution, an overview of global gyrokinetic simulations of micro-instabilities and turbulence carried out with the code EUTERPE in stellarator plasmas will be given. An effort to validate simulations by comparing them with experimental measurements is ongoing and will be presented. Simulations and experiments are carried out in the stellarators TJ-II (operated in Madrid) and Wendelstein7-X, the largest and most advanced stellarator in the world, which is in operation in Germany.

- ## *FI 2: CATCH-U-DNA: Detecting Cancer using Quartz Micro-balance Resonators*

Rafael Delgado Buscalioni
Dept. Física Teórica de la Materia Condensada, Univ. Autónoma de Madrid

In this talk I will provide an overview of an ongoing FET-OPEN project which combines expertise to detect cancer at premature stages. The objective is to detect mutant DNA strands of the serum of the patient using a quartz microbalance, which selective attachment to its surface. To improve the mass sensitivity, liposomes are used as dissipative particles. In the talk I will provide the theoretical and numerical approach to this problem, which combines different spatio-temporal techniques: from all-atom molecular dynamics to fluctuating hydrodynamics implemented with the immersed boundary technique to resolve the DNA and the liposome.

- ## *FI 3: LES approach for near- and far-field prediction of dense sprays*

J.M. Desantes, J.M. García-Oliver, J.M. Pastor and R. Novella
CMT Motores Térmicos, Universitat Politècnica de València

Fuel injection and subsequent spray development are critical factors for charge preparation, combustion development and pollutants formation in engines. The liquid atomization process occurs at extremely small length scales and high speeds in current injection systems, which complicates both the investigation and modelling of spray flow, especially in the near-nozzle dense region. Simulation techniques devoted to capturing the liquid-gas interface have been successfully applied to simulate initial spray development, but the computational requirements can make those calculations impractical for spray applications in combustion systems due to high Reynold and Weber numbers. Downstream from the primary atomization region, a dispersed flow is formed, where well-stablished modelling approaches are based on Lagrangian particle tracking. A complete spray simulation with those methods relies on empirical correlations or low-order models in order to include atomization outcomes.

To overcome those limitations, the Eulerian diffuse interface model known as Σ-Y arises as a single framework for spray simulations. Large scale liquid dispersion is modelled as the turbulent mixing of a variable density fluid. For atomization, the surface density concept is introduced in order to evaluate the mean size of liquid fragments, assuming that interfacial details are smaller than the mesh size. This model is also capable of capturing the far-field mixing process. In the present work, an implementation of the Σ-Y model in the OpenFOAM CFD library has been developed for LES turbulent modeling approach. Assessment is performed with different experimental diagnostic techniques from Engine Combustion Network, applied for spray near-and far-field spray characterization.

- ## *FI 4: On the use of supercomputing for the high-fidelity simulation of massive separated flows*

Oriol Lehmkuhl
Dpt. Computer Applications in Science and Engineering, Barcelona Supercomputing Center (BSC-CNS)

This talk will explain the basic HPC strategy for the simulation of flow over a realistic aircraft geometry by means of large-eddy simulation (LES). Experience from different RES and INCITE projects will be shared with the conference participants, focusing in numerics, modelling and HPC challenges.

The final objective is to demonstrate the predictive capability of low-dissipation LES methodologies for practical external aerodynamics configurations with SoA supercomputing facilites. To this day, the major bottleneck in accomplishing this goal has been the presence of the energetic near-wall eddies whose length scale diminishes toward the wall. We aim to address this issue by modeling the effect of the small-scale near-wall turbulence on the large-scale resolvable fluid motion in the outer portion of the boundary layer (WMLES). To address this technical bottleneck, WMLES of the NASA Common Research Model at four angle of attacks (AoA=4;6;10;18),Re_c=11M and Ma=0.25 have been carried out recently at MN4. Comparisons with the lift and drag predicted by WMLES to the experimental data will be given.

- ***FI 5: The power of data: exploring the physics of turbulence from one to five dimensions***

Ivette Rodríguez[1], Oriol Lehmkuhl[2], Manel Soria[1], Samuel Gomez[2], M. Domínguez-Pumar[3] and L. Kowalski[3]
[1] Turbulence and Aerodynamics Research Group (TUAREG), Universitat Politècnica de Catalunya, [2] Barcelona Supercomputing Center, [3] Departamento de Ingeniería Electrónica (DEE) Grupo Micro NanoTecnología (MNT). Universitat Politècnica de Catalunya

The knowledge about fluid dynamics and heat transfer from spherical axisymmetric bodies such as spheres is of key importance in many engineering applications and science, such as dispersed particle-laden, sprays, etc. The turbulent wake and the unsteady shedding of vortices from a sphere have been subject of many experimental investigations and in less extent of numerical simulations. Regarding the heat transfer, measurements of the local and overall Nusselt number have been extensively reported in the literature, yet, there is a large scattering partly attributed to the influence of the free-stream turbulence and its length scale. The present work is motivated for the development of a spherical wind sensor for Mars atmosphere, intended for future missions after Rover 2020. However, the extend of the present research aims at shedding light not only on the heat transfer and boundary layer development from the sphere, but also on the axisymmetric wake dynamics, the formation of coherent structures and how the temperature is transported by the turbulent wake. Moreover, the influence of the free-stream turbulence, which might alter these characteristics and the wake behavior, is also considered. In order to carry out the present study, direct and large eddy simulations of the turbulent flow behind a heated sphere are performed at two Reynolds numbers of 1000 and 104, free-stream turbulence levels up to 20% (which corresponds to extreme atmospheric phenomena) and turbulence length scale in the order of the sphere diameter. All simulations have been performed on Marenostrum supercomputer.

Chemistry and Materials Science and Technology

Chair: **M.Veronica Ganduglia-Pirovano** (ICP-CSIC)

- ***QCM 1: Combining high-throughput and high-performance computing for the discovery of new photo-sensitized epitaxial structures***

J. J. Plata, J. Amaya Suárez, A. M. Márquez and J. Fdez. Sanz
Universidad de Sevilla, Department of Physical Chemistry, Faculty of Chemistry

The application of ferroelectric materials in solar cells has recently attracted the attention of the scientific community because of the coupling of light absorption with other functional properties. In conventional solar cells, the solar cell power conversion efficiency (PCE) is constrained by the Shockley-Queisser limit, in which the excited carriers are separated by the internal electric field at a p-n junction or other material interface. However, ferroelectrics present an intrinsic spontaneous polarization that is an alternative way to separate charge by the bulk of the material defined as bulk photovoltaic effect. Ferroelectric oxides, as perovskites, are stable in a wide range of mechanical, chemical and thermal conditions and can be synthesized using low-cost techniques. On the other hand, these oxides usually present band gaps located higher in energy that the solar spectrum. However, new promising perovskites oxides based materials have been designed absorbing in the solar spectrum using doping techniques or applying strain. For instance, the growth of a thin layer of a perovskite on top of a substrate with different lattice parameters creates a strain that modifies its electronic properties. However, the epitaxial growth of a material on top of a substrate is not trivial and presents different requirements. Formation energies, elastic strain energy or topological information are some of the properties that should be evaluated to discern what material and plane is an optimal candidate to be the substrate of another material. Here, we present a high-throughput search of potential substrate-ferroelectric systems and the study of their electronic properties using RES high-performance resources.

- ***QCM 2: Understanding the modifications of the physical properties of supported graphene by means of Density Functional Theory***

Michele Pisarra[1,2], Cristina Díaz[2,3,4] and Fernando Martín[1,2,3]
[1] IMDEA-Nanociencia, [2] Dep. de Química, Universidad Autónoma de Madrid, [3] Condensed Matter Physics Center IFIMAC, Universidad Autónoma de Madrid, [4] Institute for Advanced Research in Chemical Science (IAdChem), Universidad Autónoma de Madrid

Graphene has been the focus of huge scientific efforts because of its physical properties which make it very promising for technological applications. A keyword in this field is tunability, which means modifying in a controlled way the properties of graphene using external factors. A fundamental role in this respect is played by Density Functional Theory (DFT) because it helps in predicting new effects and it is used to rationalize experimental findings. In this talk I will show two studies, in which DFT calculations are key in clarifying experimental results on supported graphene.

In the first one, we studied how the electronic and mechanical properties of graphene

deposited on amorphous SiO2 are modified by the action of ultrahigh pressure. In the experiments we observed a pressure-dependent, irreversible change in the graphene-substrate distance and in the effective doping of the graphene flake. By means of periodic DFT calculations, we determined that both modifications are due to the formation of a limited number of covalent C-O bonds, induced by the action of the ultrahigh pressure, that keep the graphene strongly coupled to the substrate and facilitate the charge transfer that induces the doping.

In the second case, we studied the role of supported nanostructured graphene as a catalyst, using periodic DFT calculations to understand Scannig Tunneling Microscopy measurements. The graphene ruthenium interface promotes the formation of a C-C covalent bond between two organic molecules, which would hardly take place in non catalyzed conditions. The DFT calculations clarify that the catalytic role of graphene is multifaceted: it holds the reactants in place, it allows for an efficient charge transfer between the ruthenium substrate and the reactants thus favoring changes in carbon hybridization, and finally it adsorbs the reaction product.

- ## *QCM 3: Graphene on rhodium from first principles: Tailoring electronic, structural and chemical properties*

C. Romero-Muñiz[1], A. Martín-Recio[2], P. Pou[2,3], J. M. Gómez-Rodríguez[2,3] and R. Pérez[1,3]

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In this work, we show the possibility of modeling recent experiments in complex graphene-metal (G-M) systems by means of Density Functional Theory (DFT) calculations. Since different modification techniques are currently applied on G -and related materials- to get new functionalities, our work does not restrict to the mere description of the G-M interface but we have to reproduce all these surface modifications. In particular, we reveal the multi-domain structure of G grown on Rh(111), an archetypical strongly interacting substrate, in which G adopts a rippled structure with corrugations larger than 1 Å [1]. Additionally, we will present different examples of surface modification; like the evolution of G properties as a function of the oxygen coverage in the interface [2]; the atomistic mechanisms involved in this intercalation process [3]; and the tailoring of the electronic properties by means of ion implantation nitrogen doping [4,5]. Finally, we will briefly discuss about some methodological aspects of DFT calculations in this kind of G-M systems and their current limitations when dealing with very large systems (like grain boundaries, G-covered metallic steps or under-cover chemical reactions).To overcome this issue, we present preliminary results of a new approach based on highly optimized localized orbital basis set to reach high-accuracy descriptions at quantum level of systems with thousands of atoms.

References:

[1] A. Martín-Recio et al. Nanoscale 7 (2015) 11300
[2] C. Romero-Muñiz et al. Carbon 101 (2016) 129
[3] C. Romero-Muñiz et al. Phys. Chem. Chem. Phys. (In press, 10.1039/C8CP01032C)
[4] A. Martín-Recio et al. Nanoscale 8 (2016) 17686
[5] A. Martín-Recio et al. Carbon 130 (2018) 362Sánchez, J.P. Cerón-Carrasco, K. Yuen, (2017), Antiviral Research, DOI:10.1016/j.antiviral.2017.07.007.

- ## *QCM 4: Simulations in Catalytic materials*

Núria Lopez
Institute of Chemical Research of Catalonia, ICIQ, The Barcelona Institute of Science and Technology

In the talk I will revise different aspects at the frontier of Catalysis. Our results showing the possibility to merge homogeneous and heterogeneous catalysis concepts through single atom catalyst and the implications in terms of atom economy and continuum processing will be discussed at length.

- ## *QCM 5: Non-noble metal clusters and particles for heterogeneous catalysis*

Mercedes Boronat, Estefanía Fernández and Reisel Millán and Avelino Corma
Instituto de Tecnología Química, Universitat Politècnica de València – Consejo Superior de Investigaciones Científicas

One of the main current challenges for the chemical industry is to develop new catalysts for more efficient, environmentally friendly and less energy demanding processes. Noble metals are widely used as catalysts in a large number of processes, but due to their high cost there is an increasing interest to replace them with cheaper and more abundant non-noble metals. Two examples on how DFT modelling directs the design of non-noble metal catalsts are presented.
In the first example, Ni particles have been identified as an alternative to Pt catalysts for the selective hydrogenation of substituted nitroaromatics to anilines. At difference with noble metals, the oxophylic character of non-noble metals strongly facilitates the rupture of the N-O bonds, and a direct pathway involving successive dissociation of N-O bonds followed by two hydrogenation steps, Ph-NO2 > Ph-NO > Ph-N > Ph-NH > Ph-NH2, has been found as most favorable on Ni catalysts. Calculations suggest that both catalytic activity and selectivity of Ni and, possibly, other non-noble metals can be tuned by controlling the degree of oxidation of the metal surface.
In the second example, the possibility to control the oxidation state of copper by adjusting cluster atomicity is theoretically proposed and experimentally demonstrated, and the influence of the support used to stabilize these clusters is further analyzed. Copper nanoparticles show good initial catalytic activity in oxidation reactions, but deactivate due to irreversible oxidation to CuO. Small planar Cu5 clusters are more resistant to oxidation and more easily reduced than three-dimensional Cu8 and Cu13 systems, but these properties might change when these clusters are deposited on a solid support. DFT calculations are used to understand the changes in the electronic structure, stability and catalytic activity of copper clusters supported on modified graphenes, metal oxides, or zeolites.

Poster presentations

1. *gvSIG Suite, a complete catalog of open source software to manage geographic information*

Carrera, Mario[1] and Anguix, Alvaro[1]
[1] gvSIG Association

gvSIG Suite is a catalog of open source solutions for geomatics. The gvSIG Suite is composed of 'horizontal' products, that are gvSIG Desktop, gvSIG Online and gvSIG Mobile, and sector products, like gvSIG Crime. At this presentation we will speak about them, and how they are integrated with the rest of the products.

gvSIG Desktop is an open source desktop geographic information system (GIS) for capturing, storing, handling, analyzing and deploying any kind of referenced geographic information in order to solve complex management and planning problems. gvSIG is known for having a user-friendly interface, being able to access the most common formats, both vector and raster ones. It features a wide range of tools for working with geographic-like information (query tools, layout creation, geoprocessing, networks, etc.), which turns gvSIG into the ideal tool for users working in the land realm. It's easily extensible, and it's available for Linux, Windows and Mac OS X platforms.

In addition, gvSIG Mobile is a powerful, easy-to-use and interoperable solution for field data gathering on Android devices and recommended for inventory projects, census, revisions, inspections.... It's integrated directly with gvSIG Desktop and gvSIG Online . It is oriented to the data field collection

The other main product of the gvSIG Suite is gvSIG Online, the integral platform for the implementation of Spatial Data Infrastructures (SDI). It is a fast and powerful solution to implement the necessary infrastructure to manage the spatial data of an organization efficiently. It allows to share geographic information in the cloud, generate maps and 2D and 3D applications easily, thanks to simple and powerful management tools.

2. *Numerical simulation of non-premixed swirling flames*

Pérez, Rubén[1] and Parra-Santos, Maria-Teresa[2]
[1] ICAI, Dpto. Ingeniería Mecánica; [2] Universidad de Valladolid, Dpto. Ingeniería Energética y Fluidomecánica

The present work focuses on the numerical simulation of diffusive flames in a confined swirl burner. The background motivation for the project arises from the greenhouse gas emissions. The methane slip due to incomplete combustion is a problem since methane is a harmful greenhouse gas. Lean flames produce less contaminant emissions and reduce fuel consume, however they are unstable. The swirling flow is a stabilizer of the flame so that poor mixtures can be burned.

The governing equations for 3D, transient, reactive flow are solved with a second order scheme. The 3D mesh has 4 million hexahedral cells. The temporal resolution must be around 1E-7 s/timestep, because of the stiffness of the reactive case.

Numerical model for no swirl and high swirl burners have been carried out using heat and mass transfer for non reactive cases and a simplified mechanism of reaction for the reactive case.

Contrasting non reactive and reactive cases, the last one produces higher axial velocities to keep the mass balance. Hence, it is a precursor of smaller Inner Recirculation Zones (IRZ) in the case of strong swirls. Besides, the hot products of reaction of the IRZ help to warm the fresh mixture. Contrasting flames with swirl number null, 0.6 and 1 it is possible to conclude the decrease of the flame front thickness while increasing the swirl number.

Contrasting different stoichiometries, lean mixtures have lower equilibrium temperature and therefore, the thermal emission of nitrogen oxides is lower.

However, strong swirls are needed for very poor mixtures in order to be burn in a stable way.

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).

3. *Intermittency and Multi-Fractal Structure of Rayleigh-Taylor and Richtmyer-Meshkov Shocks Driven by Laser Ablation Fronts on Plastic-Metal interfaces.*

Redondo, Jose M.[1], Tarquis, Ana[2], Cantalapiedra, Inma R.[3], Kharchi, Razika[1],[4], Rozanov, Vladimir B.[5] and Gushkov, Sergey[5]

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Different layers of metals with different density and plastic layers of different thickness were subject to short Laser pulses of microstructure, particularly the porosity and grain size. Their transport properties were characterized by measuring Seebeck coefficient, electrical and between 200 and 800 M Jules. Thermal conductivities and structure analysis from X ray and IR measurement were used. It has been observed that the measurement data of transport properties had a significant dependence upon the grain size of the samples as it reduced toward the nano-scales. The thermal conductivity data and the annealed structure of the Laser ablation demonstrated the significant size dependence, with a decrease of about one order of magnitude for the whole range of micro to nano-grained samples, Differences to other values of /spl kappa/ = 10 W/m.K for highly annealed sample with micron grain size were observed. The electrical conductivity has shown a similar reduction, but to a less extent, upon decreasing the grain size. On the other hand, the size dependence of Seebeck coefficient in those pairs of substrates capable of Thermoelectric currents is not so high. As a result, ZT value is still enhanced in some ablation samples, providing the grain size decrease. The highest ZT value obtained at 611 K was 0.17, much higher than the literature value of 0.1 for a single crystal samples.

Experimental results on the fractal structure of the laser driven fronts occurring at a initially smooth metal density interface due to the sudden acceleration and plasma formation of a 5 Mw collimated laser beam impinging on a plane 1cm2 section are analyzed considering the fractal and spectral structure of the final condensed surface. The experiments were performed at the laser facility of the Physics institute FIAN

4. *Quantum Chromodynamics on the Lattice*

Romero-López, Fernando[1] and Hernández, Pilar[1]

[1] IFIC, UV-CSIC

Quantum Chromodynamics (QCD) is the theory behind the strong interaction of quarks and gluons. It is responsible of binding quarks into hadrons (among them protons and neutrons), that build up most of the visible matter of the universe. An approach to solve the dynamics of this theory is Lattice QCD, where physical observables are calculated in a discrete space-time lattice. In this context, high-performance computing is necessary to deal with extremely high-dimensional numerical integrals. Our goal for this poster is to introduce our project within Lattice QCD and its computational challenges.

5. *DNS of thermal heat flux at high Reynolds numbers and low Prandtl numbers*

Alcántara Ávila, Francisco[1] and Hoyas Calvo, Sergio[1]

[1] Universitat Politècnica de València

Direct Numerical Simulations of turbulent heat transfer in a channel flow are presented for three different Reynolds numbers, namely Re_tau = 500, 1000 and 2000. Medium and low values of the molecular Prandtl number are studied, ranging from 0.71 (air), down to 0.007 (molten metals), in order to study its effect on the thermal flow. Mixed boundary conditions at both walls are used for the thermal flow. Mean value and intensities of the thermal field were obtained. Two different behaviors were observed, depending on the Prandtl and Pèclet numbers. The expected logarithmic behavior of the thermal flow completely disappears for Prandtl below 0.3. This is a direct effect of the thicker viscous thermal layer generated as the Prandtl number is reduced. Von Kármán constant was computed for cases above this Prandtl, and turbulent Prandtl and Nusselt numbers were obtained for all the cases. Finally, the turbulent budgets for heat fluxes, temperature variance and its dissipation rate are presented. As a general result, there is a scaling failure near the wall in very cases studied, which is accentuated for lower Prandtl numbers. The statistics of all simulations can be downloaded from the web page of our group.

6. *Atomistic modelling of materials for renewable energy applications*

García Muller, Pablo[1], Mayo García, Rafael[1] and Moríñigo, José Antonio[1]

[1] CIEMAT – Technology

Classical Molecular Dynamics (MD) has become a powerful tool for the simulation of the mechanical and electrical properties of different materials. Particularly, in research areas in which the simulated environment is expensive or difficult to attain, for instance the walls of fusion reactors or deposition process of photovoltaic cells. MD, either by itself or as a bridge between ab-initio and continuum methods in a multi-scale scheme 'is a must' in research programs related to the synthesis of novel nanomaterials with outstanding properties with applications to green energy programs. Some examples of the activities carried out by our group are briefly outlined here:

1. Characterisation of the embrittlement of Fe alloys due to Helium/Hydrogen bubbles formation on damaged material by neutron irradiation in fusion reactors. The formation energy of different bubble sizes are calculated by MD which are used by larger scale simulation software like Kinetic Monte Carlo.
2. Identification of dislocation and grain boundary interactions dynamics of Fe alloys under load/stress. Calculation of binding energy between dislocation and grain boundary. Investigation of transmission of dislocations across grain boundaries.
3. Simulation of the deposition and the electrical properties of hydrogenated amorphous/crystalline Silicon solar cells. Ab-initio methods are used for the electrical characterisation whereas MD can considerably speed up the simulation of the deposition and thermalisation phases.

7. Molecular simulations of athermal chain molecules under extreme confinement

Benito Piedra, Fco. Javier[1], Ramos, Pablo[1,2], Karayiannis, Nikos Ch.[1,2], Foteinopoulou, Katerina[1,2] and Laso, Manuel[1,2]

[1] Escuela Técnica Superior de Ingeniería Industrial, Universidad Politécnica de Madrid

[2] ISOM, UPM, Spain

We present results from extensive Monte Carlo (MC) simulations on athermal chain molecules under extreme confinement. Polymers are modeled as freely-jointed chains of hard spheres of uniform size. Spatial confinement is achieved by including flat, parallel impenetrable walls in one or more dimensions of the simulation box. A new algorithmic approach is implemented for the generation and successive equilibration of polymer configurations. The new technique significantly improves on the original protocol described in (Karayiannis and Laso, Macromolecules, 2008, 41, 1537). The present MC scheme allows the systematic study of the effect of chain length, polydispersity, volume fraction, bond tolerance (gap), cell aspect ratio and level of confinement on the short- and long-range structure of polymer chains near and far from the confining planes. Starting from cubic amorphous cells filled with polymer chains, the MC algorithm is able to reach quasi 2-d (plate-like) and 1-d (tube-like) states under conditions of extreme confinement and/or cell aspect ratio where the inter-wall distance approaches the diameter of beads forming the chains. A comparison with corresponding bulk packings shows the similarities and differences produced by extreme spatial confinement not only on structural polymer properties but further on the phase behavior of chains and on the primitive path network of topological constraints (entanglements).

8. PyCOMPSs/COMPSs, an efficient programming framework for HPC

Lezzi, Daniele[1], Badia, Rosa M.[1], Alvarez, Javier[1], Amela, Ramon[1], Conejero, Javier[1], Ejarque, Jorge[1], Lordan, Francesc[1], Alvarez, Pol[1], Ramon-Cortes, Cristian[1] and Rodriguez, Sergio[1]

[1] Barcelona Supercomputing Center

One of the biggest challenges in the programming of scientific application is the efficient exploitation of computing infrastructures. In the era of Big Data applications one of the pressing requirements on the researcher is to achieve a convergence between the Exascale and Big Data worlds. The issues related to such a challenge include the design of tools to easily program or migrate the code and to execute the applications on the computing infrastructures. Amongst the different paradigms for implementing distributed applications, the task-based programming has proven to be a suitable model. PyCOMPSs/COMPSs is a task-based framework which aims to ease the development and execution of applications for distributed infrastructures, such as Clusters and Clouds. A COMPSs application is composed of tasks, which are annotated methods. At execution time, the runtime builds a task graph that takes into account the data dependencies between tasks, and from this graph schedules and executes the tasks in the distributed infrastructure, exploiting the inherent parallelism and taking also care of the required data transfers between nodes. COMPSs is written in Java, and supports applications in Java, Python and C/C++. COMPSs has proven to improve the performance of the execution of the applications, achieving scalability while maintaining an easy programming model. COMPSs has been adopted by several user communities from different fields such as Life Science, Earth Science, Engineering belonging. It is daily used by BSC and RES users in Marenostrum and is also deployed in worldwide infrastructures such as the EGI Federated Cloud.

9. HPC User Portal: Job monitoring, made easy

Tripiana Montes, Carlos[1] and Menes Rouco, Martín[1]

[1] Barcelona Supercomputing Center

This poster presents the key features of the new user-oriented monitoring tool for HPC jobs at BSC-CNS, which is aimed to address the daily concerns and provide only the most relevant information to the users. This poster details the user interface and provides a small illustration of the underlying infrastructure. It is not intended as a technical poster, but as a use cases description.

10. HPC-Europa3: travel, learn, compute, network

HPC-Europa3 Consortium

HPC-Europa3 is a programme funded by Horizon2020, which offers grants to do international research visits for researchers from universities, institutes and companies using HPC technologies. Nine European leading HPC centres participate in this programme and provide computing resources and technical support to visitors.

HPC-Europa3 started in May 2017 and runs until April 2021, aiming to support 1220 international research visits through 16 competitive open calls. This poster provides detailed information about the programme and useful tips for applicants.