RED ESPAÑOLA DE
SUPERCOMPUTACIÓN

11th Users' Conference

28th September 2017 - Santiago de Compostela (Spain)

Book of Abstracts

11th RES Users'Conference

28th September 2017 - Santiago de Compostela (Spain)

Book of Abstracts

This book is available at
www.res.es/users-conference-2017

Published by:

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Supported by:

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

Programme

28th September 2017

11:00	**Javier García Tobío** (CESGA) & **Sergi Girona** (BSC): *Welcome and Agenda Presentation*
11:10	**Sergi Girona** (RES Manager, BSC): *MareNostrum 4 and updates in the RES*
11:30	**Oriol Pineda** (BSC): *Access to PRACE HPC resources*
11:50	*Coffe Break*
12:15	**Ulises Cortés** (BSC): *AI@BSC: View and challenges*
13:00	***Institutional Presentation*** **María Carmen Vela** (Secretaria de Estado de Investigación, Desarrollo e Innovación) **Francisco José Conde** (Conselleiro de Economía, Empleo e Industria, Xunta de Galicia)
13:30	**Javier Junquera** (UC): *RES Users' Committee Presentation*
14:00	*Lunch and poster session*

Parallel sessions

	Chemistry and Materials Science Chair: **Francesc Illas** (UB)	Life and Health Sciences Chair: **Vicente Galiano** (UMH)	Mathematics, Physics and Engineering Chair **Xavier Trias** (UPC)	Astronomy, Space and Earth Sciences Chair: **Manuel Ruiz** (IEO)
15:30	QCM 1 **Sílvia Osuna** (UdG): *The role of conformational dynamics in the evolution of novel enzymatic activities*	BCV 1 **David Torrents** (BSC): *The computational analysis of genomic data...more complex than big*	FI 1 **Linda Angela Zotti** (UAM): *Electron transport through nanostructures and proteins*	AECT 1 **Manuel Ruiz** (IEO): *HPC and modeling in the marine sciences: marine and climate services*
16:00	QCM 2 **Annapaola Migani** (IQAC): *An excited-state perspective on the photocatalytic water oxidation on TiO2 under UHV*	BCV 2 **Nicola GA Abrescia** (CIC bioGUNE): Assembly of *vertical single beta-barrel membrane-containing viruses by high-resolution cryo-EMcryo-EM*	FI 2 **Maximilian Attems** (UB): *Holographic heavy ion collisions*	AECT 2 **Gonzalo Míguez-Macho** (USC): *High resolution modeling in the atmosphere and the earth*

16:30	QCM 3 **Javier Carrasco** (Cicenergigune): *Molecular modelling, high performance computing, and the pursuit of better batteries*	BCV3 **Carmen Domene** (University of Bath): *Studies of transport in ion channels using computer simulation*	FI 3 **Shimpei Futatani** (BSC): *Non-linear MHD simulations of ELM control via pellet injection in fusion plasmas*	AECT 3 **Neven Fuckar** (BSC): *On the EOS-COST ORA-IP and the BSC ocean-sea-ice data assimilation products*
17:00	*Coffe Break*			
17:30	QCM 4 **Chantal Valeriani** (UCM): *Ice nucleation: what we have learned so far, and what still needs to be understood*	BCV 4 **Pablo Dans** (IRB): *Expanding the boundaries of DNA crystal simulations*	FI 4 **Javier Honrubia** (UPM): *Integrated simulations of fast ignition of inertial confinement fusion targets*	AECT 4 **Roland Aznar** (Puertos del Estado): *HPC resources for ocean modelling: the IBI Copernicus Marine Service example*
18:00	QCM 5 **José Hugo García** (ICN2): *Charge and spin Hall Kubo conductivity by O(N) real-space methods*	BCV 5 **Daniel Lietha** (CNIO): *Structural and dynamic insights into allosteric inter-domain signalling in SHIP2*	FI 5 **Javier Jiménez** (UPM): The power of data: exploring the physics of turbulence from one to five dimensions	AECT 5 **Antonio Cofiño** (UC): *Climate simulations and services on HPC, Cloud and Grid infrastructures*
18:45	*Pause*			
19:00	Closing session by **Javier García** (CESGA) and **Sergi Girona** (BSC)			
19:30	*Social Event*			

Plenary sessions: Instituto de Investigaciones Agrobiológicas de Galicia (CSIC)

Parallel sessions: Facultad de Química (USC)

Acknowledgments

The RES gratefully acknowledges Fundación Pública Galega Centro Tecnolóxico de Supercomputación de Galicia (CESGA) for their collaboration in organizing this conference.

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 11th edition, the plenary talks will inform about the most important updates in RES infrastructure, specially the entry in production of MareNostrum 4. In addition, these talks will present the procedures to apply for PRACE (Partnership for Advanced Computing in Europe) supercomputing resources. The invited speaker Ulises Cortés from BSC will give the plenary lecture entitled 'AI@BSC: View and challenges' about artificial intelligence and supercomputing.

This year edition consolidates the new extended format including 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 recognized experts, who will share their experience as RES and PRACE users. 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, the abstracts of oral presentations and the list of poster presentations. We hope that this publication is a valuable contribution to disseminate the applications of high performance computing technologies in research.

The organizing committee

Plenary sessions

- ***MareNostrum 4 and updates in the RES***
  Sergi Girona – BSC Operations Director and RES Manager

  After a long process of planning and installation, the new MareNostrum4 is in production since July 1st, 2017. Its overall technical specifications have been notably improved, being the most remarkable feature the increase of power with respect to MareNostrum3, being now able to reach a peak performance of 13,7 Pflops. Its forerunner, MareNostrum3, has been dismantled and distributed among other RES nodes to help improve their respective capacities: Universidad Politécnica de Madrid, Universitat de València, Instituto Astrofísico de Canarias, Universidad de Cantabria, Universidad de Málaga, Universidad Autónoma de Madrid and CénitS.

  Besides this, some nodes have also performed -or are about to perform- different improvements in their respective systems, such as higher storage capacity, new sites for hosting the CPD, or even new machines or CPD's.

  As a summary, the RES shows nowadays an excellent health and a promising future of steady progress.

- ***Access to PRACE HPC resources***
  Oriol Pineda – PRACE Peer Review Director and Research Project Manager **in BSC**

  The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. PRACE provides persistent world-class high performance computing services for scientists and researchers from academia and industry in Europe.

  The computer systems and their operations accessible through PRACE are provided and funded by 5 PRACE members (BSC representing Spain, CINECA representing Italy, CSCS representing Switzerland, GCS representing Germany and GENCI representing France).

  The services of PRACE include access to Tier-0 systems for large-scale projects, preparatory and support programmes to promote access to Tier-0 systems, and advanced training programmes. PRACE also coordinates part of the national HPC capacities through the DECI joint programme.

- ***AI@BSC: View and challenges***

  Ulises Cortés – Academic Programs Coordinator of BSC

  El objetivo de esta plática es dar a conocer la actualidad de la actividad investigadora y docente que se hace en el Barcelona Supercomputing Center (BSC) relacionada con la Inteligencia Artificial desde tres puntos de vista:

  - El uso de la Inteligencia Artificial para mejorar la arquitectura y la eficiencia de los chipsets para la computación de altas prestaciones;
  - La investigación básica en Inteligencia Artificial, y
  - El uso de la Inteligencia Artificial para resolver problemas de impacto para la sociedad (e.g., ciencias de la vida, ciencias medioambientales) usando recursos y herramientas de supercomputación.

  En la plática se repasa toda la actividad relevante y la organización de un grupo de Inteligencia Artificial en el la Supercomputación (HPAI).

  El objetivo del BSC, en esta área, es el de convertirse en el principal referente a nivel nacional en la investigación, desarrollo e implementación de técnicas de Inteligencia Artificial usando la Supercomputación.

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

  Javier Junquera – Chair of the CURES / Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria

  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 user concerns.

  In this talk I will describe how to Access to the CURES, a summary of the cases attended in the last year, and some actions that have been taken or are in perspective for the near future.

Chemistry and Materials Science and Technology

Chair: **Francesc Illas** (UB)

• *QCM 1: Evolution of novel enzymatic activities*

Adrian Romero-Rivera[1], Marc Garcia-Borràs [1,2] and Sílvia Osuna[1]
[1] Institut de Química Computacional i Catàlisi (IQCC) and Departament de Química, Universitat de Girona, Carrer Maria Aurèlia Capmany 6, 17003 Girona
[2] Department of Chemistry and Biochemistry, University of California, Los Angeles (UCLA), 607 Charles E. Young Drive, CA 90095

Enzymes exist as an ensemble of conformations important for their function. By introducing mutations to the enzyme sequence, the populations of the different conformational states can be gradually tuned for allowing novel function

In this talk, the population shift induced by distal and active site mutations introduced along a series of laboratory-evolved enzymes (1-4) is presented. Microsecond time-scale Molecular Dynamics simulations, coupled to correlation-based analysis, are used to elucidate the changes in the conformational landscape of evolved variants.

Most importantly, our new tools based on inter-residue correlations observed along the microsecond-scale MD simulations provides a strategy to identify the amino acid positions that influence the dynamic properties of laboratory-evolved enzymes (5). Our method is therefore able to rationalize, but most importantly to predict which residues situated far away from the active site can have a large impact on the enzyme catalytic activity (5, 6).

References:

(1) Giger, L.; Caner, S.; Obexer, R.; Kast, P.; Baker, D.; Ban, N.; Hilvert, D. Nat. Chem. Biol. 2013, 9, 494.

(2) Obexer, R.; Godina, A.; Garrabou, X.; Mittl, P. R. E.; Baker, D.; Griffiths, A. D.; Hilvert, D. Nat. Chem. 2017, 9, 50.

(3) Jiménez-Osés, G.; Osuna, S.; Gao, X.; Sawaya, M. R.; Gilson, L.; Collier, S. J.; Huisman, G. W.; Yeates, T. O.; Tang, Y.; Houk, K. N. Nat. Chem. Biol. 2014, 10, 431.

(4) Osuna, S.; Jiménez-Osés, G.; Noey, E. L.; Houk, K. N. Acc. Chem. Res. 2015, 48, 1080.

(5) Romero-Rivera, A.; Garcia-Borràs, M.; Osuna, S. submitted for publication 2017.

(6) Romero-Rivera, A.; Garcia-Borràs, M.; Osuna, S. Chem. Commun. 2017, 53, 284.

- ***QCM 2: An excited-state perspective on the photocatalytic water oxidation on TiO2 under UHV***

Annapaola Migani[1] and **Lluís Blancafort**[2]
[1]Departament de Química Biològica i Modelització Molecular, (IQAC-CSIC), Jordi Girona, 18-26, E-08034 Barcelona, Catalonia, Spain
[2]Institut de Química Computacional i Catàlisi and Departament de Química, Facultat de Ciències, Universitat de Girona, C/ M. A. Capmany 69, 17003 Girona, Spain

The photocatalytic oxidation of water adsorbed on titania (TiO2) is one of the most important photocatalytic processes. It is relevant for the oxygen evolution reaction, which is one of the two half reactions in water splitting, and the degradation of organic pollutants. Its potential in solar-to-fuel and environmental remediation technologies has made heterogeneous photocatalysis a focus of attention covering a broad range of disciplines including chemical synthesis, materials and surface science, spectroscopy, and theory.

Although a detailed knowledge of the functioning principles would greatly help to develop its applications, the mechanism of the first elementary steps is still poorly understood because of its great complexity, and the nature of the active species has not been definitively determined yet.

In this talk, I provide a comprehensive mechanistic picture of the photocatalytic oxidation of water on the (110) surface of rutile TiO2 under ultra-high vacuum conditions, which has been recently studied experimentally by scanning tunnelling microscopy in combination with UV irradiation (1,2). I show that a theoretical approach from molecular photochemistry which treats the excitonic character explicitly is very successful to understand the mechanism and efficiency of interfacial photochemical processes between solid-state photocatalysts and organic molecules (3). I show how the different products observed experimentally, free hydroxyl radicals or diffused hydroxyl anions, are formed depending on the irradiation wave length and nature of the initially generated exciton.

Although the calculations are directly related to the experiments under UHV conditions, they also provide some important insights on the water photooxidation mechanism in aqueous environment (4).

References:

(1) Tan, S. et al. J. Am. Chem. Soc. 2012, 134, 9978–9985.

(2) Yang, W. et al. J. Phys. Chem. Lett. 2016, 7, 603–608.

(3) Migani, A.; Blancafort, L. J. Am. Chem. Soc. 2016, 138, 16165–16173.

(4) What controls photocatalytic water oxidation on TiO2(110) under ultra-high vacuum conditions? Migani, A.; Blancafort, L. Submitted.

- ## *QCM 3: Molecular modelling, high performance computing, and the pursuit of better batteries*

Javier Carrasco* CIC Energigune, Albert Einstein 48, 01510 Miñano, Álava, Spain

The rechargeable Li-ion battery - with higher energy density than its predecessors- has been a key technological enabler for the rise of portable electronics. But most importantly, looking ahead, battery technology offers broad potential to enable a future world actuated by clean energy sources. From the electrification of transportation (e.g., electric vehicles) to the support of smart grids (e.g., storing wind and solar energy produced during off-peak hours), rechargeable batteries are called to create a new energy paradigm. However, for such foreseen scenario to materialize, advances in battery performance, safety, and cost beyond current state-of-the-art are mandatory. A salient aspect of research in batteries is the discovery of new materials or novel properties of existing compounds. Yet trial-and-error exploratory research based on extending known compounds into new compositional spaces implies long-lasting work of synthesis and characterization. To mitigate this issue and accelerate the process of materials discovery, computational modelling is emerging as a powerful complementary tool.

Based on quantum chemistry grounds together with the spectacular growing of computational resources, computer molecular modelling is able nowadays to bring valuable insight in understanding the structure, properties and function of technological materials (1). Indeed, computational predictions of the performance of energy materials are now sufficiently mature to be applied successfully in many cases. Here we discuss a selection of our most exciting examples of recent work in this area. In particular, we will focus on general concepts that emerge about how density functional theory calculations (2-6) can provide valuable understanding into key thermodynamic and kinetic properties for a range of systems and processes such as phase stability and ion diffusion using the RES supercomputing facilities.

** In collaboration with Nebil A. Katcho, Oier Lakuntza, Ariel Lozano, Oier Arcelus, Unai Arrieta and others.*

References:

(1) A. Jain, Y. Shin and K. A. Persson, Nat. Rev. Mater. 1, 15004 (2016).

(2) N. A. Katcho, J. Carrasco, D. Saurel, E. Gonzalo, M. Han, F. Aguesse, T. Rojo, Adv. Energy. Mater. 7, 1601477 (2017).

(3) L. Buannic, B. Orayech, J.-M. López Del Amo, J. Carrasco, N. A. Katcho, F. Aguesse, W. Manalastas, W. Zhang, J. Kilner, A. Llordés, Chem. Mater. 29, 1769 (2017).

(4) A. Lozano, B. Escribano, E. Akhmatskaya, J. Carrasco, Phys. Chem. Chem. Phys. 19, 10133 (2017).

(5) T. Deng, W. Zhang, O. Arcelus, J.-G. Kim, J. Carrasco, S. Jo Yoo, W. Zheng, J. Wang, H. Tian, H. Zhang, X. Cui, T, Rojo, Nat. Commun. 8, 15194 (2017).

(6) U. Arrieta, N. A. Katcho, O. Arcelus, J. Carrasco, Sci. Rep. 7, 5350 (2017).

- ***QCM 4: Ice nucleation: what we have learned so far, and what still needs to be understood***

Chantal Valeriani
Departamento de Física Aplicada, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Avenida Complutense, 28040, Madrid (Spain)

The avoidance of water freezing is the holy grail in the cryopreservation of biological samples, food and organs (1).

Fast cooling rates are used to beat ice nucleation and avoid cell damage. In our group, we have recently developed a computer simulation method that thank to the use of supercomputers allows us to investigate ice nucleation within a broad temperature and pressure range (2,3,4).

Using the seeding approach, we have been able to evaluate the nucleation rate in a wide metastability range (5) and for several water models (6), estimate the ice-liquid interfacial free energy up to coexistence conditions (in reasonable agreement with the reported experimental values), and unravel the physics behind the slowing down of the nucleation rate of ice Ih at high pressure (7,8).

The versatility of our numerical technique will allow us to investigate not only nucleation of many different forms of ice from pure water, but also ice nucleation from salty solutions.

References:

(1) Morris, G. J. & Acton, E., Cryobiology 66, 85 (2013).

(2) Espinosa, J. R., Vega, C. & Sanz, E.,. J Chem. Phys. 141, 134709 (2014).

(3) Espinosa, J. R., Vega, C. & Sanz, E., The Journal of Physical Chemistry C 120, 8068-8075 (2016).

(4) Sanz, E., Vega, C., Espinosa, J. R., Caballero-Bernal, R., Abascal, J. L. F. & Valeriani, C. Journal of the American Chemical Society 135, 15008-15017 (2013).

(5) E. Sanz, C. Vega, J.R. Espinosa, R. Bernal, J. Abascal and C. Valeriani, J. Am. Chem. Soc 135, 15008 (2013).

(6) J.R.Espinosa, E.Sanz, C.Valeriani and C.Vega, J.Chem.Phys. 142, 18C529 (2014).

(7) Kanno, H., Speedy, R. J. & Angell, C. A., Science 189, 880-881 (1975).

(8) JR Espinosa, A Zaragoza, P Rosales-Pelaez, C Navarro, C Valeriani, C Vega & E Sanz. Physical Review Letters 117 (13), 135702 (2016).

- ***QCM 5: Charge and spin Hall Kubo conductivity by O(N) real-space method***

José H. Garcia
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

Modern electronics are based on the manipulation of electrical currents in devices that nowadays can reach nanoscopic scales. Spintronics, a branch of electronics that aims to use the electron's spin for the creation of faster devices operating at a fraction of the energy cost and having vastly larger memory capacities, requires the manipulation of both charge and spin currents. The conductivity determines the amount of current flowing through a system, and hence is a key piece of information for both electronics and spintronics. By using on O(N) real-space approach, we computed the conductivity and spin conductivity of systems consisting of millions of atoms, making use of a parallelization scheme that allow us to run simulations on more than one thousand cores. This approach allows us to demonstrate the potential of some graphene-based heterostructures for spintronics, electronics and valleytronics in a limit that is unattainable with standard computational techniques.

Life and Health Sciences

Chair: **Vicente Galiano** (UMH)

- ***BCV 1: The computational analysis of genomic data… more complex than big***

David Torrents[1,2]
[1]Institució Catalana de Recerca i Estudis Avançats (ICREA)
[2]Barcelona Supercomputing Centre (BSC)

The current scenario in Biomedicine is dominated by the massive generation of different types of biological data. In particular, the activity around the sequencing of disease genomes is pushing the understanding of the molecular and genetic basis of multiple pathologies at unprecedented levels and is becoming the pillar of the upcoming Medicine based on accurate diagnosis and personalized treatment protocols.

In order to meet final research and clinical standards, and fulfil upcoming expectations the design of computational approaches has to consider and combine precise algorithms with implementations consisting on efficient software- hardware integrations. Computational Biology has become a key and a central element in the study and treatment of diseases

- ***BCV 2: Assembly of vertical single beta-barrel membrane-containing viruses by high-resolution cryo-EM***

Nicola G.A. Abrescia[1,2]
[1]Molecular recognition and host-pathogen interactions programme, CIC bioGUNE, CIBERehd, Bizkaia Technology Park, 48160 Derio, Spain.
[2]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain.

Structure based approaches have revealed close relationships between viruses infecting organisms from different domains of life (1). Within the virosphere archaeal viruses constitute the least explored niche. In 2015, combining biochemical and cryo-electron microscopy (cryo-EM) techniques, we solved the structure of euryarchaeal, halophilic, internal membrane-containing Haloarcula hispanica icosahedral virus 2 (HHIV-2) albeit at ~11 Å resolution (2). HHIV-2 was isolated from the largest saltpan in Europe located in Margherita di Savoia (Foggia-Italy). We showed that the density of the two major capsid proteins (MCPs) recapitulates vertical single beta-barrel proteins and proposed that additional proteins would aid the assembly of such a large (800 Å edge-to-edge) and complex virion. However, the limited resolution caused frustration in understanding the assembly of these novel viruses with vertical single beta-barrel MCPs and belonging to the Sphaerolipoviridae family.

Capitalizing on the immense advances in high-resolution cryo-EM (3,4) and on the supercomputing resources of the Picasso node (Malaga) via the RES network, we have now visualized HHIV-2 at 4.4 Å. The near-atomic-resolution has allowed an unprecedented 3D snapshot for this type of viruses. We built the structural models of the two MCPs, spike complex proteins and ancillary proteins in the context of the internal membrane vesicle. More recently we have also determined the structure of Holoarcula californiae icosahedral virus 1 (HCIV-1) (5), a HHIV-2 related virus but discovered at more than 5,000 miles away (Samut Sakhon, Thailand) and whose 4.2 Å resolution provides a further means for structural comparison and analysis.

The unfolding picture provides the principles governing the assembly mechanism of vertical single beta-barrel viruses.

References:

(1) Abrescia, N.G., Bamford, D.H., Grimes, J.M., Stuart, D.I. Annu Rev Biochem. 81:795-822 (2012).

(2) Gil-Carton*, D., Jaakkola*, S.T., Charro, D., Peralta, B., Castaño-Díez, D., Oksanen, H.M., Bamford, D.H., Abrescia, N.G. Structure 23:1866-77 (2015).

(3) Kühlbrandt W. Science 343:1443–1444. (2014).

(4) Stuart, D.I., Subramaniam, S., Abrescia, N.G. Nat Methods 13:607-8 (2016).

(5) Demina, T.A., Pietilä, M.K., Svirskaitė, J., Ravantti, J.J., Atanasova, N.S., Bamford, D.H., Oksanen, H.M. MBio 7(4). pii: e00699-16 (2016).

BCV 3: Studies of transport in ion channels using computer simulation

Carmen Domene
Department of Chemistry, 1 South Building, University of Bath, Bath, UK.

My research is aimed at understanding the physical and chemical principles underlying ion channel function, their activation, permeation and selectivity properties. By selected examples from the work we have carried out, I will provide an overview of the current knowledge we have about this family of membrane proteins.

BCV 4: Expanding the boundaries of DNA crystal simulations

Antonija Kuzmanic, Pablo D. Dans and **Modesto Orozco**
Molecular Modeling & Bioninformatics group. Institute for Research in Biomedicine (IRB Barcelona). Barcelona Institute of Science and Technology.

Macromolecular crowding is an important factor that influences the behavior of biomolecules in cellular environments. In human cells, one-meter-long DNA has to pack into a nucleus of 5 μm in diameter, indicating that DNA molecules are highly packed. Biomolecular simulations by means of atomistic Molecular Dynamics (MD), strongly complement experiments (NMR or X-ray crystallography) in elucidating the structure and dynamics of biomolecules. However, until 2017, these simulations were restricted to single DNA molecules of small sizes, immersed in explicit solvents, mainly due to limitations in the available computational resources. With such systems, timescales of several dozens of microseconds are typically reached. These spatial/temporal limitations are even more critical for the simulations of DNA in crystals, where multiple DNA molecules are packed together generating strongly crowded conditions as in the cellular nucleus.

Since crystallographic structures have been historically used as the golden standard to compare and validate MD force-fields, crystal simulations were being attempted for long time but with little success, mainly due to their size. Given recent advances in computer speed, MD algorithms, and force-fields, crystal simulations of more realistic systems have begun to emerge. Nevertheless, in the latest and most extensive study of DNA crystal simulations published to date (2015), the authors concluded that the integrity of the crystal lattice was slowly degraded in MD simulations, disrupting the crystal structure on the microsecond timescale. With the help of millions of CPU hours obtained through PRACE calls, and our new force-field for DNA simulations (PARMBSC1, 2016), we were finally able to obtain stable crystal simulations, expanding the actual limits of the field. This allowed us to understand with unprecedented level of detail the nature of the intermolecular forces that participate in the formation of crystals in various symmetry groups and under different ionic environments, and to decipher the crucial role that chemical additives (small molecules or specific cations that are added experimentally to obtain the crystals) play in the stability of the simulated crystals.

- ***BCV 5: Structural and dynamic insights into allosteric inter-domain signalling in SHIP2***

Johanne Le Coq[1], Marta Camacho Artacho[1], José Vicente Velázquez[1], Clara M. Santiveri[2], Luis Heredia Gallego[1], Ramón Campos-Olivas[2], Nicole Dölker[3] and **Daniel Lietha[1]**

[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.

Mathematics, Physics and Engineering

Chair: **Xavier Trias** (UPC)

- ## *FI 1: Electron transport through nanostructures and proteins*

Linda Angela Zotti
Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid

The field of Molecular Electronics, which is a central pillar of Nanoscience, aims at using molecules as active elements in nanoscale devices (1). Molecular junctions fabricated with various techniques such as the Scanning Tunneling Microscope (STM) or the so-called Mechanically Controllable Break-Junctions (MCBJ) have turned out to be ideal test-bed systems to investigate quantum theories for the charge and energy transport in nanoscale systems. In this talk, I will present recent results on simulations on electronic transport through metallic nanocontacts and organic molecules. I will show how theoretical computation can help shedding light on the geometrical and electronic properties of molecular junctions throughout the stretching process which takes place in the experiments, as well as getting an insight in the electron transport mechanism and many interesting effects such as quantum interference and heat dissipation.

Finally, I will discuss our recent study on single-protein junctions, aimed at gaining an understanding of interesting conductance properties which were observed in recent experiments. This is achieved by a combined study of molecular dynamics and density functional theory which can offer crucial information about the conformation and the electronic properties of the system.

References:

(1) Scheer, Elke, Cuevas, J. Carlos. Molecular electronics: an introduction to theory and experiment. Vol. 1. World Scientific, 2010

- ## *FI 2: Holographic heavy ion collisions*

Maximilian Attems[1], Yago Bea[1], Jorge Casalderrey-Solana[2], David Mateos[1], Daniel Santos-Olivan[3], Carlos Sopuerta[3], Miquel Triana[1], Miguel Zilhao[4]
[1]University of Barcelona, [2]University of Oxford, [3]Institute of Space Sciences, [4]University of Lisbon

Understanding the properties of extreme phases of nuclear matter created in relativistic heavy ion collisions is one of the major challenges in theoretical physics. Matter under such extreme conditions was present in the very early universe and is nowadays produced both at the Large Hadron Collider and the Relativistic Heavy-Ion Collider.

In this talk we address questions that are central to the understanding of the very early stages of such collisions: What is the time-scale of the thermalization and why does it happen so fast? We will study these questions in the strongly coupled setup via the gauge/gravity duality by utilizing numerical relativity techniques to describe black hole formation in the gravity side. This allows to access real-time dependent non-equilibrium dynamical quantities and will improve the understanding of pre-equilibrium flow in heavy ion collisions.

- ***FI 3: Non-linear MHD simulations of ELM control via pellet injection in fusion plasmas***

Shimpei Futatani
Department of Computer Applications in Science & Engineering (CASE), Barcelona Supercomputing Center, Barcelona, Spain

This work is dedicated to the nuclear fusion physics research in close collaboration with existing experimental fusion devices and the ITER organization (www.iter.org) which is an huge international nuclear fusion R&D project. The goal of the ITER project is to demonstrate an energy production by nuclear fusion which is the reaction that powers the sun.

One of the ideas of the nuclear fusion on the earth is that the very high temperature ionized particles, forming a plasma can be controlled by a magnetic field, called magnetically confined plasma. It is a demanding task to achieve a sufficiently good confinement for a 'burning plasma' due to various kinds of plasma instabilities.

One of the critical unsolved problems is MHD (MagnetoHydroDynamics) instabilities at the plasma boundary, called Edge Localized Modes (ELMs). ELMs leed to energy bursts onto the plasma facing components which could be damaged in future tokamak devices like ITER. The injection of pellets (small deuterium ice bodies) into the plasma to trigger small ELMs is a promising ELM mitigation method for the steady operation of ITER. Although the technique has been demonstrated to decrease ELM size successfully in existing fusion devices, experimentally, uncertainties still remain regarding the theoretical physics understanding not yet established as well as the numerical modelling point of view. The simulation of the plasma physics, which includes wide range of spatio-temporal scales, especially, the non-linear interaction of plasma particles and magnetic physics requires a significantly large computing resources within highly sophisticated numerical scheme.

In order to advance the physics understanding of ELM control by pellets, non-linear MHD code JOREK is performed using the high performance computing machines. The numerical experiment of the pellet injection studies contributes the design and the optimization of the pellet injector and the injection conditions in the fusion devices.

• *FI 4: Integrated simulations of fast ignition of inertial fusion targets*

Javier Honrubia
School of Aerospace Engineering, Universidad Politécnica de Madrid, Spain

Inertial Confinement Fusion (ICF) intends to trigger thermonuclear fusion reactions in a few milligrams of Deuterium-Tritium (DT) contained in a 1 - 2 mm radius hollow spherical microcapsule (1). In a first stage, the microcapsule is accelerated inwardly by set of laser beams. When the capsule central void is closed, the kinetic energy of the implosion is converted into DT internal energy, raising rapidly the DT temperature of a small central zone (hot spot) where ignition occurs.

Subsequently, the ignition propagates to the rest of the fuel, which remains confined over a short period of time, which is sufficient to burn-up a substantial fraction of the DT (2). Neutrons, charged particles and thermal radiation are released from the microcapsule. These radiations deposit their energy in the first wall, heating a liquid coolant to initiate a conventional thermodynamic cycle.

In 2009, the National Ignition Facility (NIF) started its operation at the Lawrence Livermore National Laboratory in Livermore (California) with the goal of demonstrating the scientific feasibility of ICF (3). So far, the NIF has achieved the record of producing more energy by fusion reactions than the energy stored in the DT (4). However, the difficulties found in achieving ignition and moderate energy gain have led to new target designs as well as to envision alternative ignition schemes (5).

One of the main scientific attractive of the ICF is the huge range of densities and temperatures found in fuel targets, which go from ideal low density plasmas in the laser interaction region to degenerate plasmas at densities higher than 103 times the solid density in the igniting fuel. In addition, the ICF target evolution implies physical phenomena with very different space and time scales, which go from femtoseconds (fs) to nanoseconds (ns). Some of these phenomena are ultra-intense laser-plasma interactions (LPI) (fs), multidimensional radiation-hydrodynamics (ns), transport of laser-driven supra-thermal electrons (ns) and fusion reactions (ps).

Fast ignition of fusion targets is a good example of the multiple time scales found in ICF. It consists in separating fuel compression from ignition. Compression is produced by laser pulses of intensities about 1014 Wcm-2 and durations of tens of nanoseconds, while the ignition hot spot is generated by ultra-intense laser pulses of 1020 Wcm-2 of 10-15 picoseconds duration. Simulations of fast ignition of fusion targets carried out at the MareNostrum and Magerit HPC facilities will be presented (6,7). They comprise multidimensional radiation hydrodynamics, Particle-In-Cell and hybrid simulations of fast ignition of imploded ICF capsules.

References:

(1) J. Lindl et al., The physics basis for ignition using indirect-drive targets on the National Ignition Facility, Physics of Plasmas 11, 339 (2004).

(2) S. Atzeni and J. Meyer-ter-Vehn, The Physics of Inertial Fusion, Oxford University Press (2004).

(3) J. Lindl, O. Landen, J. Edwards and Ed. Moses, Review of the National Ignition Campaign 2009-2012, Physics of Plasmas 21, 020501 (2014).

(4) O.A. Hurricane et al., Fuel gain exceeding unity in an inertially confined fusion implosion, Nature 506, 343-348 (2014).

(5) M. Tabak et al., Physics of Plasmas 1, 1626 (1994).

(6) J.J. Honrubia and J. Meyer-ter-Vehn, Three-dimensional fast electron transport for ignition-scale inertial fusion capsules, Nuclear Fusion 46, (2006).

(7) J.J. Honrubia and M. Murakami, Ion beam requirements for fast ignition of inertial fusion targets, Physics of Plasmas 22, 012703 (2015).

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

Javier Jiménez
School of Aeronautics. Universidad Politécnica de Madrid, 28040 Madrid, Spain

Turbulence is a chaotic motion of fluids which, in practical applications, requires a large number of degrees of freedom (109-1012) to be represented. Besides being physically challenging, it is an industrially important phenomenon that has to be addressed; approximately 5% of the energy consumption of mankind is attributable to turbulent friction. Its high dimensionality has traditionally made turbulence research dependent on the limitations of experimental data acquisition and post-processing power. Supercomputing has changed that.Today, simulations exceed in many cases the capabilities of experiments and promise, in principle, unlimited data on flows of interest.

The burden has changed from data limitations to postprocessing, and to the formulation of relevant questions. This has also began to move the limiting computational resource from raw computing power to large memories and, specially, to large archival storage capacity. Postprocessing of the data, in many cases of the order of hundreds of TBs, cannot anymore be done on-the-fly, or even by a single research group, and calls for international collaboration as an integral part of the research program. Some examples will be given of recent applications involving supercomputers and, lately, gpus.

They range from the low-order statistics required by entry-level modelling, to five-dimensional data resolved in space, time and scale, directed to physical understanding and to the formulation of control strategies. Future challenges will also be addressed.

Astronomy, Space and Earth Sciences

Chair: **Manuel Ruiz** (IEO)

- ***AECT 1: HPC y modelado en ciencias del mar: servicios marinos y climáticos.***

Manuel Ruiz
Instituto Español de Oceanografía

La supercomputación es una herramienta fundamental en las simulaciones numéricas en oceanografía. En los últimos años, el incremento de la potencia y de la capacidad de almacenamiento han permitido que se realicen simulaciones regionales de la circulación costera a alta resolución y de periodos largos.

La supercomputación está permitiendo que varios usuarios de la comunidad española mantengan servicios de predicción de corto plazo de la circulación oceánica como el servicio IBI del programa Copernicus marino (marine.copernicus.eu) o servicios de predicción regional en Galicia y otras regiones.

La financiación europea y regional de estos servicios permite el uso de supercomputación dentro de la RES (por ejemplo los servicios mencionados se ejecutan en el CESGA). Estos servicios de predicción, así como simulaciones costeras y regionales se están utilizando en el desarrollo de servicios basados en observaciones y modelados para distintos usuarios marinos (acuicultura, pesquerías, turismo...).

Otro de los campos de interés de la comunidad española en modelado oceanográfico es la generación de reanálisis de la circulación en aguas españolas. Distintos usuarios participan en la generación de reanálisis en el Atlántico y en el Mediterráneo. En este último la comunidad española es muy activa en programas como MEDCLIVAR (www.medclivar.eu) y MEDCORDEX (www.medcordex.eu). España participa en una COST Action de Evaluación de Síntesis Oceánicas EOS-COST (http://eos-cost.eu), que pretende mejorar la coordinación europea en los reanálisis marinos.

En esta presentación se realizará una revisión de los servicios marinos que se desarrollan en España y en Portugal, enmarcándolos en las iniciativas europeas de desarrollo de observaciones y servicios marinos y climáticos. Asimismo, se presentarán los retos que presenta el desarrollo y mantenimiento de estos servicios marinos para usuarios finales desde el punto de vista de la HPC.

- ***AECT 2: Modelización de alta resolución en la atmósfera y el suelo***

Gonzalo Míguez Macho
Facultad de Física, Universidad de Santiago de Compostela

Aunque los fundamentos teóricos de la dinámica de la atmosfera y del flujo de agua en el suelo son conocidos desde hace mucho, la complejidad y no linealidad de los procesos asociados ha sido una barrera para la predicción y comprensión de numerosos fenómenos en estos medios. La computación de altas prestaciones es un gran aliado en el campo de las ciencias de la Tierra, y ha estado detrás de numerosos e importantes avances en el conocimiento de cómo funciona el sistema climático. En esta presentación se muestran ejemplos de cómo una avanzada capacidad de computo permite simular con gran detalle fenómenos en la atmosfera y en el suelo, dándonos una visión y comprensión de nuestro entorno con un detalle y a escalas que no se habían visto antes

- ***AECT 3: On the EOS-COST ORA-IP and the BSC ocean-sea-ice data assimilation products.***

Neven S. Fučkar[1] and Francois Massonet[1,2]
[1]Barcelona Supercomputing Center (BSC), Earth Sciences Department, Climate Prediction Group, 08034 Barcelona, Spain
[2]Georges Lematre Centre for Earth and Climate Research, Earth and Life Institute, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

Development and proliferation of in-situ and remote sensing systems for observation of the ocean and sea ice state is indispensable for advancing our understanding of the Earth's climate system. However, we are never going to be in the position to close unavoidable temporal and spatial gaps in observations. Hence, data assimilation methods offer the best possible option of filling these gaps in a dynamically consistent manner by merging model simulations with observed data. This talk will present some of the results of an extensive multi-institutional project comparing ten state-of-the-art ocean and sea ice reanalysis products (ORA-IP) as well as some novel data assimilation activities in the Earth Sciences Department at the Barcelona Supercomputing Center.

The ocean and sea ice reanalysis products enable analyses of climate variability and changes free of discontinuity as well as observation-based initialization of climate predictions on seasonal-to-decadal timescales. This is crucial for achieving dynamical predictions with practical skill since the ocean state is the most important sources of climate predictability. The additional key sources of climate predictability on these timescales are sea ice, snow and soil moisture, and here we are also going to focus on sea ice cover.

- ## *AECT 4: HPC resources for ocean modelling: the IBI Copernicus Marine Service example*

R. Aznar[1], M. G. Sotillo[1], A. Amo Baladrón[1], P. Lorente[1], A. Pascual[1], P. Rey[2], A. Rodríguez[2], G. Reffray[3], B. Levier[3].
[1]Área de Medio Físico, Organismo Público Puertos del Estado, Madrid (Spain).
[2]Centro de Supercomputación de Galicia (CESGA), Santiago de Compostela (Spain).
[3]Mercator-Océan, Toulouse (France).

In the framework of CMEMS (Copernicus Marine Environment Monitoring System), the IBI-MFC (Monitoring & Forecasting Center) produces, in the Finisterrae 2 (FT2) machine from the Centro de Supercomputación de Galicia (CESGA), daily model forecasts and best estimates for the IBI (Iberia-Biscay-Ireland) sea region. This operational service provides physics, biogeochemistry and wave products in the mentioned area by launching simulations with the NEMO, PISCES and WAM models, respectively, and by processing the input and output data needed in such tasks.

The NEMO model simulates the marine baroclinic circulation in the IBI area at an eddy-resolving horizontal resolution of 1/36º and 50 vertical levels, which results in a matrix of more than 108 points. On the other hand, the PISCES biogeochemical model is coupled with the NEMO physics model and shares its same 3D grid. Finally, the WAM model resolves the IBI wave conditions at a 0.1º resolution on a 2D grid.

These three operational suites demand a very important number of computational resources due to the huge amount of iterations to be performed in each matrix point within the simulations, as well as to the need of delivering the products to the users at a scheduled time.

Regarding the physics and biogeochemistry forecasts, the IBI domain is divided in 1500 subdomains, of which 990 cover sea areas that must be numerically resolved by means of FT2 cores. Considering the additional cores employed for the I/O management of NEMO and PISCES models, 1032 cores distributed in 43 nodes are thus dedicated to the physics and biogeochemistry operational chains. As for the wave forecast, 6 nodes from FT2 are fully dedicated accounting for a total of 144 cores.

These computing configurations ensure efficient modelling performances and a prompt products delivery to the ever-growing users of CMEMS IBI operational oceanographic outputs.

- ***AECT 5: Climate simulations and services on HPC, Cloud and Grid infrastructures***

Antonio S. Cofiño
Department of Applied Mathematics and Computational Sciences, Universidad de Cantabria, Spain

Cloud, Grid and High Performance Computing have changed the accessibility and availability of computing resources for Earth Science research communities, specially for Climate community. These paradigms are modifying the way how climate applications are being executed.

By using these technologies the number, variety and complexity of experiments and resources are increasing substantially. But, although computational capacity is increasing, traditional applications and tools used by the community are not good enough to manage this large volume and variety of experiments and computing resources.

In this contribution, we evaluate the challenges to run climate simulations and services on Grid, Cloud and HPC infrastructures and how to tackle them. Grid and Cloud infrastructures will be evaluated, as well as HPC resources and institutional clusters. To solve those challenges, solutions using WRF4G and DRM4G frameworks will be shown. Both provide a good framework to manage big volume and variety of computing resources for climate experiments.

This work has been supported by the Spanish National R&D Plan under projects WRF4G (CGL2011-28864), INSIGNIA (CGL2016-79210-R) and MULTI-SDM (CGL2015-66583-R) ; the IS-ENES2 project from the 7FP of the European Commission (grant agreement no. 312979); the European Regional Development Fund—ERDF and the Programa de Personal Investigador en Formación Predoctoral from Universidad de Cantabria and Government of Cantabria.

Poster presentations

Chemistry and Materials Sciences and Technology

1. ***Selective conversion of biomass by Mo-based compounds***
Marcos Rellán-Piñeiro and Núria López (Institut Català d'Investigació Química, ICIQ)

Life and Health Sciences

2. ***Study of cluster phases in attractive micro-swimmer suspensions***
Francisco Alarcón Oseguera (Universidad Complutense de Madrid), Eloy Navarro Argemí (Universitat de Barcelona), Ignacio Pagonabarraga (Universitat de Barcelona) and Chantal Valeriani (Universidad Complutense de Madrid).

3. ***Study of cyclic peptide nanotubes in a membrane environment via Molecular Dynamics simulations***
M. Calvelo (CIQUS, University of Santiago de Compostela, Spain), J. R. Granja (CIQUS, University of Santiago de Compostela, Spain), R. Garcia-Fandiño (CIQUP-Facultade de Ciencias, Universidade do Porto, Portugal)

4. ***Microbial community analysis in wastewater N-removal technologies by 16S rRNA gene metagenomics***
N. Fernandez-Gonzalez, A. Pedrouso, A. Val del Río, N. Morales, J.R. Vázquez-Padín, J.L. Campos, R. Méndez and A. Mosquera-Corral (Universidade de Santiago de Compostela)

5. ***Binding of Amantadine to the M2 proton channel: Molecular basis of the inhibition mechanism***
Carolina Estarellas, Jordi Juarez-Jimenez, Elnaz Adelavood, Adrian Roitberg, F. Javier Luque (University of Barcelona)

6. ***Exploring the action mechanism of aniline-based inhibitors of influenza A Hemagglutinin***
Tiziana Ginex, F. Javier Luque (University of Barcelona)

Mathematics, Physics and Engineering

7. ***GPU-based Stochastic Problem Solving and Scalability in Superconductivity***
Juan Rodríguez-García, Manuel Rodríguez-Pascual, José A. Moríñigo, Rafael Mayo-García (CIEMAT)

8. ***Introduction of obstacles in bidimensional Vicsek model***
Raúl Martínez, Francisco Alarcón, Jorge Ramírez, Chantal Valeriani (Universidad Complutense de Madrid)

9. ***Dynamic task migration in HPC for Exascale challenge***
M. Rodríguez-Pascual, José A. Moríñigo, R. Mayo-García (CIEMAT)

Astronomy, Space and Earth Sciences

10. ***Off-line lagrangian particle tracking: Efficient implementation of a Vertical Dispersion algorithm***
Ignacio Vidal-Franco (University of A Coruña - A Coruña Oceanographic Centre)

The abstracts of poster presentations are available in:
www.res.es/users-conference-2017/posters

#RESusers17

www.res.es/users-conference-2017