20th & 21st September 2016, León (Spain)

10th RES Users' Conference

&

5th Annual HPC Advisory Council Spain Conferences

Book of Abstracts

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10th RES Users'Conference

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Programme

9:30 h	Registration and gathering			
10:00 h	Welcome to León by Ilmo. Sr. Antonio Silván Rodríguez, Alcalde de León Welcome by Excmo. Sr. Juan Carlos Suárez-Quiñones y Fernández, Consejero de Fomento y Medio Ambiente de la Junta de Castilla y León			
10:10 h	Welcome by MINECO Ilmo. Sr. Jose Ignacio Doncel, S.G. de Grandes Instalaciones Científico-Técnicas			
10:20 h	Red Española de Supercomputación: 10 years already Sergi Girona, BSC-CNS			
10:35 h	RedIris, la red que nos conecta Alberto Perez, Red.es			
10:50 h	Coffee break and poster exhibition			
11:20 h	How to access to RES and PRACE resources David Vicente, BSC-CNS			
11:45 h	Updates from RES User Committee Javier Junquera, Universidad de Cantabria			
12:10 h	How works the Scientific Steering Committee (SSC) of PRACE Ignacio Pagonabarraga, UB and member of PRACE SSC			
12:30 h	RESxPYME: Objetivos y estado del arte Javier Garcia Tobio, Director of CESGA			
12:50 h	Precision Medicine as a computational challenge Alfonso Valencia, CNIO			
13:30 h	Lunch			
	4 Parallel sessions dedicated to specific research areas with 6 speakers each one			
	Life and Health Sciences Chair: Mercedes Alfonso, UB Sala Quevedo	**Mathematics, Physics and Engineering** Chair: Ignacio Pagonabarraga, UB Sala Juni	**Astronomy, Space and Earth Sciences** Chair: Sascha Husa, UIB Sala Doncel	**Chemistry and Materials Science and Technology** Chair: Stefan T. Bromley, UB Auditorio Antiguo
14:30 h	Assembly of archaeal, salty and fat viruses: when a bit of grease helps. Nicola GA Abrescia, CIC bioGUNE Nicola GA Abrescia, CIC bioGUNE	Attosecond xuv-induced charge migration in biomolecules Fernando Martin, UAM	Simulations of dynamics of partially ionized solar atmosphere. Elena Khomenko, IAC	Structural, electronic and transport properties of distorted nanographenes by DFT methods. Blanca Biel, UGR

15:00 h	Is solvation/desolvation enough to unravel protein interactions? Examples on HIV-1 gp41-based miniprotein antibody eliciting and sGC ligand binding. Jordi Villà i Freixa, Universitat de Vic	GPU support in the SLEPc library for eigenvalue computations. Jose Roman, UPV	The tectonic evolution of the Western Mediterranean and the dynamic of double polarity subduction. Sergio Zlotnik, UPC	Atomistic modelling studies of electrode materials for rechargeable lithium and sodium batteries. Javier Carrasco, CIC energiGUNE
15:30 h	Allosteric inter-domain signalling controls SHIP2 phosphatase activity. Daniel Lietha, CNIO	Quench dynamics and counting statistics in interacting nanojunctions: quasi-particles trapping Rubén Seoane, UAM	Urban climate atlas and health impact: DECUMANUS Premium services. Roberto San José, UPM	Using supercomputers for fast advancing in heterogeneous photocatalysis technologies. Annapaola Migani, CIN2
16:00 h	Study of G protein-coupled receptors with molecular dynamics computer simulations. Leonardo Pardo, UAB	Thermal transport in disordered nanostructured materials. Riccardo Rurali, ICMAB	Impact of ocean resolution and initialisation in climate seasonal predictions. Eleftheria Exarchou, BSC-CNS	Computational design of advanced nanoalloy materials. Konstantin Neyman, ICREA-UB
16:30 h	Dynamic Undocking, a new tool for virtual ligand screening. Xavier Barrill, UB	Towards the modelling of combustion systems. Daniel Mira, BSC-CNS	The Marenostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe. Gustavo Yepes Alonso, UAM	The effect of strain and temperature on the mechanical properties of irradiated graphene. Maria Jose Cartula, Universidad de Alicante
17:00 h	Conformational modulation in a glycosyltransferase: evidence of mixed conformational selection and induced fit mechanisms by bias-exchange metadynamics. Javier Romero García, IQS-URL	Parallelization of Smoothed Particle Hydrodynamics for engineering applications with the heterogeneous architectures. Jose Manuel Domínguez Alonso, UVIG	Coalescence of Black Hole Binary systems. Sascha Husa, UIB	Computational Studies of Ice Nucleation. Carlos Vega, Universidad Complutense de Madrid
17:30 h	Conclusions, farewell and next RES Users Conference			
17:45 h	End of the conference			
18:30 h	Social event: Visit to León Cathedral			

The Spanish Supercomputing Network (RES) organizes the annual users' conference, aiming to highlight the scientific results obtained using RES resources. In addition, this event offers a discussion forum between RES users, the access committee and the users' committee (CURES). In this 10th edition, the plenary talks will also inform about how to request access to PRACE (Partnership for Advanced Computing in Europe), will provide information about RedIris, and will review the state of the project RESxPYME. The invited speaker Alfonso Valencia from CNIO will give the lecture entitled Precision Medicine as a Computational Challenge.

This book gathers the agenda of the conference and the abstracts of the parallel sessions talks. These parallel sessions are focused on four research areas (Life and Health Sciences; Mathematics, Physics and Engineering; Astronomy, Space and Earth Sciences; Chemistry and Materials Science and Technology), and count on the collaboration of recognized experts that will share their research results and their experience as RES users.

We hope that this publication is a valuable contribution to disseminate the applications of high performance computing technologies in research projects of many different areas.

The organizing committee

Acknowledgments

The RES gratefully acknowledges Fundación Centro de Supercomputación de Castilla y León (FCSCL) for their collaboration in organizing this conference.

1 Life and Health Sciences

Chair: Mercedes Alfonso, Universitat de Barcelona

1.1 Assembly of archaeal, salty and fat viruses: when a bit of grease helps

Nicola GA Abrescia, CIC bioGUNE/Ikerbasque

Archaeal viruses constitute the least explored niche within the virosphere. Structure-based approaches have revealed close relationships between viruses infecting organisms from different domains of life [1].
Some time ago using 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) at ~11 Å resolution [2]. We showed that the density of the two major capsid proteins (MCPs) recapitulates vertical single β-barrel proteins, that disulfide bridges stabilize the capsid and proposed that further proteins would aid the assembly of such large and complex viruses. However, the limited resolution frustrated a detailed structural analysis.
Recently, capitalizing on the immense advances in cryo-EM, we have been able to visualize HHIV-2 at 4.4 Å. This has also been possible thanks to the huge power of Picasso supercomputer at the University of Malaga within the RES. The near-atomic-resolution has allowed an unprecedented 3D snapshot of this large (800 Å edge-to-edge) archaeal virus with the model building de-novo of the two MCPs, spike complex proteins and ancillary proteins in the context of the internal membrane vesicle.
The unfolding picture provides the principles governing the assembly mechanism of vertical single β-barrel viruses.

[1] Abrescia NG, Bamford DH, Grimes JM, Stuart DI. (2012) Structure unifies the viral universe. Annu Rev Biochem. 81:795-822.
[2] Gil-Carton* D, Jaakkola* ST, Charro D, Peralta B, Castaño-Díez D, Oksanen HM, Bamford DH, Abrescia NG. (2015) Insight into the Assembly of Viruses with Vertical Single β-barrel Major Capsid Proteins. Structure 23:1866-77.

1.2 Is solvation/desolvation enough to unravel protein interactions? Examples on HIV-1 gp41-based miniprotein antibody eliciting and sGC ligand binding

Luis Agulló (1), Martin Floor (2) and Jordi Villà-Freixa (1)
(1) Computational Biochemistry and Biophysics lab, Research Group on Bioinformatics and Medical Statistics, Department of Systems Biology. Universitat de Vic – Central University of Catalonia.
(2) Departamento de Química Inorgánica y Analítica. Universidad de Chile

In this talk a discussion on the role of electrostatics in receptor-ligand interactions is explored through computer simulations of two systems of pharmacological interest.
In the first example, the interaction of soluble guanylate cyclase (sGC), the main target of nitric oxide (NO) that has been proven to have a significant role in coronary artery disease, pulmonary hypertension, erectile dysfunction, and myocardial infarction, to YC-1, a classic heme-dependent stimulator, is explored. In particular, we address its potential location on the catalytic domain, the unique that has been well characterized at the structural level, by an “in silico” approach. Homology models of the catalytic domain of sGC in “inactive” or “active” conformations were constructed using the structure of previously described crystals of the catalytic domains of “inactive” sGCs (2WZ1, 3ET6) and of “active” adenylate cyclase (1CJU). Extensive MD simulations and docking calculations to all frames of representative trajectories of “inactive” and “active” conformations, followed by calculation of absolute binding free energies with the linear interaction energy (LIE) method, revealed a potential high-affinity binding site on the “active” structure. The site, located between the pseudo-symmetric and the catalytic site just over the loop b2–b3, does not

overlap with the forskolin binding site on adenylate cyclases.
In the second example, we investigate the characteristics of the HIV-1 gp41 Membrane Proximal External Region (MPER) that provide its ability to be recognized by broadly neutralizing antibodies (bNAbs), which makes him a promising vaccine target. The results of the combined experimental and computational study support the notion that lipid modulation impacts immunogenicity of membrane-dependent antigens, providing helpful information for the generation of MPER-based carriers.

[1] Computational exploration of the binding mode of heme-dependent stimulators into the active catalytic domain of soluble guanylate cyclase. L. Agulló, I. Buch, H. Gutiérrez-de-Terán, D. Garcia-Dorado and J. Villà-Freixa, Proteins, 2016.
[2] Proteoliposomal formulations of an HIV-1 gp41-based miniprotein elicit a lipid-dependent immunodominant response overlapping the 2F5 binding motif Luis M Molinos-Albert, Eneritz Bilbao, Luis Agulló, Silvia Marfil, Elisabet García, Maria Luisa Rodríguez de la Concepción, Nuria Izquierdo-Useros, Cristina Vilaplana, F.-Xabier Contreras, Martin Floor, Pere J Cardona, Javier Martinez-Picado, Bonaventura Clotet, Jordi Villà-Freixa, Maier Lorizate, Jorge Carrillo, Julià Blanco, submitted.

1.3 Allosteric inter-domain signalling controls SHIP2 phosphatase activity

Daniel Lietha, Cell Signalling and Adhesion Group, Spanish National Cancer Research Centre (CNIO), Madrid

SH2-containing inositol phosphatases (SHIPs) dephosphorylate the 5-phosphate of phosphatidylinositol 3,4,5-trisphosphate (PIP3) and therefore play an important role in the regulation of the PI3K/Akt pathway. Despite the importance of SHIP enzymes in physiology and disease, such as diabetes and cancer, little is known on a structural and mechanistic level, how enzyme activity is regulated. Using a combination of experimental (X-ray crystallography, biochemistry and mutagenesis) and computational methods (molecular dynamics simulations and modeling of substrate complexes) we provide detailed mechanistic insight on the functioning and regulation of SHIP2. Structural studies show that the SHIP2 phosphatase domain is rigidly associated to its C2 domain, which despite no homology resembles the architecture in PTEN, the only other enzyme degrading PIP3. Although located distant to the active site, the C2 domain greatly enhances catalytic turnover. Employing molecular dynamics and mutagenesis we identify distinct allosteric signaling pathways emanating from hydrophobic or polar C2 interactions, differentially affecting PIP3 or the soluble inositol-1,3,4,5-tetrakisphosphate substrate. Together, this study reveals details of multilayered C2 mediated regulatory effects on SHIP2, indicating new possibilities for therapeutic interventions.

1.4 Study of G protein-coupled receptors with molecular dynamics computer simulations

Leonardo Pardo, Laboratori de Medicina Computacional, Unitat de Bioestadística, Facultat de Medicina, Universitat Autònoma de Barcelona.

We will show, in this presentation, how to combine structural bioinformatics, molecular dynamics and data-mining of structure and sequence databases with experimental results from site-directed mutagenesis, functional assays and biophysical techniques to study the structure and mechanism of activation of G protein-coupled receptors (GPCRs), and how this knowledge is translated into predictive tools for the selection and design of molecules with a therapeutic potential.
We have selected the GPCR family of proteins because is one of the most prevailing protein families in the human genome. GPCRs are receptors for sensory signals of external origin such as odors, pheromones, or tastes; and for endogenous signals such as neurotransmitters, (neuro)peptides, hormones, and others. These proteins are key in cell physiology, and their malfunction is commonly translated into pathological outcomes. Thus, GPCRs constitute one of the most attractive drug targets.
GPCRs have been classically described as monomeric receptors that form a ternary complex: ligand-receptor-G protein. Nevertheless, it is now accepted that different GPCRs may interact to form heteromers that are novel signaling units. Thus, we will also show how GPCR (hetero)oligomerization influences the physiological role of receptors, and their use as therapeutic targets.

1.5 Dynamic Undocking, a new tool for virtual ligand screening

Xavier Barrill, Departament de Fisicoquímica, Facultat de Farmàcia, Universitat de Barcelona; Institut de Biomedicina de la Universitat de Barcelona (IBUB); Catalan Institution for Research and Advanced Studies (ICREA).

Structure-based methods for drug design aim to predict the thermodynamic stability of protein-ligand complexes, but we show that structural stability is equally important. This property can be assessed with inexpensive dynamic undocking calculations, which are an excellent complement to existing methods (e.g. molecular docking). The efficacy of the approach is demonstrated on a virtual fragment screening application.

1.6 Conformational modulation in a glycosyltransferase: evidence of mixed conformational selection and induced fit mechanisms by bias-exchange metadynamics

Javier Romero García (1) and Xevi Biarnés (1)
(1) Laboratory of Biochemistry, Institut Químic de Sarrià, Universitat Ramon Llull, Barcelona, Spain.

Glycosyltransferases, the enzymes responsible for the biosynthesis of a wide variety of glyco-conjugates exhibit great flexibility. Many structures of this family of enzymes reveal a loop, close to the active site, in two different conformations: i) open in the unliganded protein and ii) closed in the complexed form. These changes have traditionally been regarded as being induced by the binding of substrates. Recent X-Ray structures of a Mycobacterium tuberculosis glycosyltransferase reveals the co-existence of both conformations of the loop in the unligand protein1, whereas only the active form is detected in the Michaelis complex2. This poses a new scenario in which the conformational selection mechanism acquires more relevance. By means of molecular dynamics and metadynamics we have studied the thermodynamics of this loop in the presence and absence of ligands. In the unliganded protein, both open and closed states of the loop are in equilibrium, although highly displaced towards the open conformation. The binding of substrates to the protein shifts this equilibrium towards the closed conformation of the loop, in line with an induced fit mechanism. But both open and closed states are still accessible in the presence of ligands. Measurements of substrate binding affinities to different states of the protein loop reveal a preference for the closed conformation. The two latter facts are in line with a conformational selection scenario. Furthermore, different ligand conformations have been detected inside the active center, with different binding affinities to the protein. All together suggests a complex substrate binding process in this glycosyltransferase where a combination of the canonical conformational selection and induced fit mechanisms can be used to explain the conformational changes detected at both protein and ligands level.

Acknowledgements: This work was supported by grant GLYCOZYMES (BIO2013-49022) from MICINN, Spain. Computational Resources were provided by the Red Española de Supercomputación (RES).

[1] Urresti S., et al. (2012) Mechanistic insights into the retaining glucosyl-3-phosphoglycerate synthase from mycobacteria. J. Biol. Chem. 287:24649-24661.
[2] Albesa-Jové D., et al. (2015). A native ternary complex trapped in a crystal reveals the catalytic mechanism of a retaining glycosyltransferase. Angew. Chem. Int. Ed. Engl. 54:9898-9902.

2 Mathematics, Physics and Engineering

Chair: Ignacio Pagonabarraga, Universitat de Barcelona

2.1 Attosecond xuv-induced charge migration in biomolecules

Fernando Martin, Universidad Autónoma de Madrid (UAM)

Sudden ionization of a molecule by an attosecond pulse is followed by charge redistribution on a time scale from a few-femtoseconds down to hundreds attoseconds, which is usually followed by fragmentation of the remaining molecular cation. This dynamics is the consequence of the coherent superposition of electronic continua associated with the ionization thresholds reached by the broadband attosecond pulse. Thus, a correct theoretical description of the time evolution of the ensuing wave packet requires the knowledge of the actual ionization amplitudes associated with all open ionization channels, as well as of the ensuing nuclear dynamics, a real challenge for large and medium-size molecules. In this talk, I will present the results of the first calculations of this kind, which have allowed us to interpret ultrafast electron dynamics observed in attosecond pump-probe experiments performed on N2 and the amino acid phenylalanine.

[Trabattoni et al, Phys. Rev. X 2015, 5, 041053; Calegari et al, Science 2014, 346, 336]

2.2 GPU support in the SLEPc library for eigenvalue computations

Jose Roman, Universitat Politècnica de València (UPV)

SLEPc is an MPI-based library for the solution of large-scale eigenvalue problems in scientific computing applications. It provides a number of solvers to compute a few eigenvalues and eigenvectors of large matrices, which are typically sparse. We are recently adding GPU support so that the computation can make use of GPU's available in clusters such as minotauro. We present results in the several situations, in particular an application where the matrix is sparse and symmetric and exterior eigenvalues are required, and another application where matrices are non-symmetric block-tridiagonal and required eigenvalues are interior to the spectrum.

2.3 Quench dynamics and counting statistics in interacting nanojunctions: quasi-particles trapping

Rubén Seoane, Departamento de Física Teórica de la Materia Condensada, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid.

The shot noise and the higher order cumulants contain valuable information about interactions and quantum correlations between electrons. While these studies have traditionally been restricted to the stationary case, the recent technological advances in the direction of the single electron detection have attracted an increasing interest in the time resolved full counting statistics. The objective of the presentation is to give a brief overview of the role of interactions and electronic correlations in the relaxation of a single electronic level abruptly coupled to metallic electrodes.

Firstly, I will present our work devoted to the study of the molecular junctions, which are modelized as an electronic level locally coupled to a vibrational mode. By using the recently developed expressions for the time resolved full counting statistics, we have access to the transport properties such as the current cumulants and the single electron probabilities in the transient regime. In the cumulants, the effect of interactions leads to long transient dynamics showing features of the electron-phonon coupling, while preserving an universal scaling law at short times.

Finally, I will introduce our recent work focused on the study of nanostructures coupled to superconducting electrodes. The possibility for using this kind of devices as an implementation for superconducting qubits,

has biased several theoretical and experimental works in the recent years. In the time dependent regime and due to the correlations between electrons, the system is unable to relax and it remains into an excited state due to the quasiparticle trapping in the system. I will devote last part of the talk to the characterization of the final state.

2.4. Thermal transport in disordered nanostructured materials

Riccardo Rurali, Institut de Ciències de Materials de Barcelona (ICMAB-CSIC)

Solid state physics often deals with periodic systems. There, the most important properties of a material can be described theoretically with simulations that involve a few atoms, i.e. those belonging to the primitive cell. Describing at the atomistic level any kind of perturbation of the ideal, ordered crystal is a challenge, because it requires much larger computational cells. Disorder, in particular, is the ultimate frontier in material simulation for what the size of the system required is concerned. In this talk I will describe two of such cases: (a) thermal transport in porous Si and porous Si nanowires and (b) thermal transport in isotope engineered Si nanowires. Both these case are pragmatic examples of efficient thermoelectric materials by design.

2.5. Towards the modelling of combustion systems

Daniel Mira, Dpt. Computer Applications in Science and Engineering, Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS)

The design of modern combustion systems needs to address new challenges in aspects related to reduction of pollutant emissions, increment in flexibility of operation and avoid thermo-acoustic instabilities. To achieve these goals, numerical simulations are becoming increasingly important during the design process as they provide detailed insights into the physical processes of these multiphysics and multiscale systems. However, the interaction of turbulence, chemical reactions and thermodynamics needs to be accurately reproduced. Due to the different time and length scales existing in the combustion process, an integration of detailed chemistry in reacting flow simulations is still a challenge.

The talk will cover some fundamental aspects of the challenges associated to the modelling of power and propulsion systems, with emphasis on high-fidelity numerical simulations using High-Performance Computing. Different strategies to describe turbulence/chemistry interactions and approaches to develop multiscale combustion applications will be presented. As turbulent combustion is a fundamental part of the engine performance, further research is needed to develop turbulent combustion models that can be reliable and used with confidence to predict the combustion performance and the pollutant formation of practical energy systems.

2.6 Parallelization of Smoothed Particle Hydrodynamics for engineering applications with the heterogeneous architectures

Jose Manuel Domínguez Alonso, EPHYSLAB Environmental Physics Laboratory, Universidad de Vigo

Smoothed Particle Hydrodynamics (SPH) method is a powerful technique used to simulate complex free-surface flows. However, one of the main drawbacks of the method is its high computational cost and the large number of particles needed in 3D simulations. High Performance Computing (HPC) becomes essential to accelerate SPH codes and perform large simulations. In this study, parallelization using MPI and GPUs (Graphics Processing Units) is applied for executions on heterogeneous clusters of CPUs and GPUs.

3 Astronomy, Space and Earth Sciences

Chair: Sascha Husa, Universitat de les Illes Balears

3.1 Simulations of dynamics of partially ionized solar atmosphere

Elena Khomenko, Instituto de Astrofísica de Canarias (IAC)

Supercomputing has arisen as a new method of research in astrophysics in our attempt to remedy the impossibility to perform experiments on our objects of research. Among the recent successful examples in the field of numerical astrophysics, one can list the realism achieved in simulations of solar convection and magneto-convection, which has allowed to resolve the long standing problems of spectral line shapes and abundance determination derived from them; models of local dynamo; simulations of magnetic field emergence from the interior to the solar surface; numerical models of eruptive phenomena and reconnection; wave propagation and energy transport in solar magnetic structures, and so on. Spatial resolution of the simulations often exceeds that achieved in observations making them a valuable tool for predicting new phenomena to be searched for in observations. The major breakthrough to be achieved in the coming years will consist in taking into account the physical consequences of the very low degree of ionization of the solar atmospheric plasma on its dynamics, and on the energy propagation and release. Such modeling requires multiple scales to be resolved simultaneously, from the smallest ones imposed but the micro-physics of partially ionized plasma, to the largest ones imposed by the size of typical solar structures. This constitutes a perfect challenge for a supercomputing experiment. In this contribution I will review recent results of the numerical modeling of solar process and will describe our recent effort to develop models incorporating plasma partial ionization into numerical codes.

3.2. The tectonic evolution of the Western Mediterranean and the dynamic of double polarity subduction

Sergio Zlotnik, Universitat Politécnica de Catalunya (UPC-Barcelona Tech)

The evolution of the Western Mediterranean is highly debated by geologists and geophysicists. Even though most scientists agree in considering slab roll-back to be the driving mechanism of the tectonic evolution of this area, there is still no consensus about the initial setup and its time evolution. A recent model suggests a lateral change in subduction polarity of the oceanic domain to explain the formation and evolution of the Betic-Rif orogenic system and the associated Alboran back-arc basin. The aim of this study is to analyze the dynamic evolution of a double-polarity subduction process and its consequences in order to test the physical feasibility of this interaction and provide geometries and evolutions comparable to those proposed for the Western Mediterranean. The physical model representing plate tectonics and its evolution through time in the Million year scale and the numerical scheme used to solve it will be presented. A multiphase flow model with complex non-linear visco-plastic rheologies is used to simulate the long-term thermo-mechanical system of plate tectonics. We study the influence of the boundary conditions in the model evolution, and the slab deformation produced by the proximity between both plates. Moreover the case of asymmetric friction on the lateral sides of slabs is also considered. Simulations of single subduction models are used as a reference, to compare results and understand the influence of the second plate.

3.3 Urban climate atlas and health impact: DECUMANUS Premium services

Roberto San José, Universidad Politécnica de Madrid (UPM)

This work is part of the European project DECUMANUS. We have identified the highlight areas with elevated exposure to global climate from different point of views: comfort, health and energy; this information can be used to prepare plans and implement adaptations to reduce effects of climate change on the citizen and building energy demand. We have studied direct effects of the two future (2030, 2050 and 2100) climate projections, IPCC RCP 4.5 (stabilization emission scenario) and RCP 8.5 (little effort to reduce emissions), respect to present (2011), over three European cities: Madrid, Milan and London with very high spatial resolution: 50 meters. Climatic variables and air pollution concentrations are dynamically downscaled from 1o to 50m using a computational dynamical downscaling modelling system. The outputs of the Community Earth System Model (CESM) and its coupling with Weather Research and Forecasting and Chemical (WRF/Chem) model (25 km, 5km and 1km spatial resolutions) provides present and future climate scenarios. The output from the WRF/Chem model at 1 km resolution is used to drive a micro-scale computational fluid dynamics model, MICROSYS (50 m). The methodology to estimate percentages of climate/pollution-related deaths and hospital admissions due to global climate are based on epidemiologic analysis of weather/air pollution and health data to
characterize and quantify mortality/morbidity associations. Building energy simulations are implemented with the EnergyPlus model using buildings prototypes which are based on ASHRAE 90.1 Prototype Building Modeling Specifications but they have been customized to Europe. Also urban comfort (wind, thermal) indicators from a pedestrian point of view are calculated. We propose to use the Dutch wind nuisance standard (NEN 8100) which applies a discomfort threshold for the hourly mean modeled wind speed. The physiological equivalent temperature (PET) is calculated every grid cell as index of the urban thermal comfort. We have run 40 annual simulations of the WRF-Chem model and MICROSYS model with 5 km and 1 km and 50 meters of spatial resolution respectively. Several independent simulations, using Greasy software provided by the Barcelona Supercomputer Center (BSC), were grouped to allow get the deadlines of the project. We have consumed 1716000 CPU hours during two access periods.

3.4 Impact of ocean resolution and initialisation in climate seasonal predictions

Eleftheria Exarchou, Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS)

In the RES activity entitled “Impact of Ocean Resolution and initialisation in climate seasonal predictions” we have investigated the impact of the increase in the horizontal ocean resolution and of different strategies used to initialise the ocean and land-surface components of a climate model, in particular the EC-Earth3 system, on the quality of seasonal-to-interannual global climate predictions. Two sets of seasonal retrospective predictions were performed in Marenostrum3, with a total cost of 1950 kh of CPU time. The first set comprised simulations performed at both standard resolution and high resolution, while the second set comprised simulations where the ocean was initialized with two different ocean reanalyses products, namely ORAS4 and GLORYS2v1. This set of simulations offered a unique framework to systematically examine the impact of model resolution and ocean initialization on forecast quality. The evaluation of the model biases showed that the use of ORAS4 as oceanic initial conditions and the increase of the model resolution led to an improved representation of the overall mean state of the forecast. In the aspect of the forecast skill in predicting the sea surface temperatures, using ORAS4 led to an improvement compared to GLORYS2v1. The high resolution led to an improvement in the SST prediction skill in the tropical Pacific and in the Indian Ocean, and in the prediction of the North Atlantic Oscillation. These results highlight the importance of both assessing the initialization techniques and the impact of the model resolution as an integral part of the ongoing effort to increase forecast quality.

3.5 The Marenostrum Numerical Cosmology Project: Grand Challenge simulations of structure formation in the Universe

Gustavo Yepes Alonso, Universidad Autónoma de Madrid (UAM)

Computer simulations are 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 Cosmology. The only way to do experiments and test hypotheses of theoretical cosmological 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. In 2005, when the first MareNostrum supercomputer was installed at the Barcelona Supercomputer Center, we set up the MareNostrum Numerical Cosmology Project. The aim of this project 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 (our Local Universe and the Local Group of galaxies we live in). During the past 11 years of running simulations in MareNostrum, we have been able to produce an extensive database of virtual cosmic objects that are made publicly available to the astronomical community.

3.6 Coalescence of Black Hole Binary systems

Sascha Husa, Universitat de les Illes Balears (UIB)

This project is part of a long-term program to study the orbital dynamics of black hole binaries in general relativity, with special emphasis on simulating the gravitational wave signals emitted during the inspiral and coalescence of black holes due to radiation reaction. Like black holes, gravitational waves are predictions of Einstein's general relativity, generated as massive compact bodies dynamically distort the surrounding spacetime.

The Einstein equations were solved as a system of coupled nonlinear partial differential equations with high order finite difference methods and mesh refinement techniques for a range of initial configurations, and analytical models for the 7-dimensional space of non-eccentric coalescing black hole binaries were calibrated to the numerical simulations. These models were used by the LIGO-Virgo collaboration to identify the sources of the first detections of gravitational waves by the LIGO detectors, and determine their masses, spins, and location and orientation in the sky. In this talk I will outline the challenges involved in the numerical solution of the Einstein equations, describe the simulations performed, how waveform models are distilled from the simulations and summarise how these models are used to obtain observational results from gravitational wave detections.

4 Chemistry and Materials Science and Technology

Chair: Stefan T. Bromley, Universitat de Barcelona

4.1 Structural, electronic and transport properties of distorted nanographenes by DFT methods

Blanca Biel, Universidad de Granada (UGR)

The work we present is framed within the ERC NANOGRAPHOUT project. The scientific aim of NANOGRAPHOUT is to embed non-hexagonal rings into an otherwise planar graphene lattice as a new tool for the preparation of unprecedented materials for organic electronics. The project thus requires precise control over the introduction of defects into nanographenes to probe their physical properties and utilize them for useful applications. The experimental team follows a bottom-up approach based on building up the target molecules from molecular building blocks, and the size and number of defects are chemically controlled. The comprehensive study of the optical and electronic properties will afford consistent structure/property relationships allowing the controlled design of new devices based on graphene materials. A comprehensive study clarifying the influence of defects in the properties of nanographenes represents the commencement of a fundamentally new approach for the construction of materials based on the inclusion of imperfect nanographenes.

Within this context, simulation methods provide a valuable tool to predict the electronic and optical properties of the nanographenes, as well as their relative stability, and can hence facilitate and speed up the experimental work. To this aim, we performed ab initio calculations of the building molecular blocks and the target molecules to be synthesized experimentally, analyzing their structural and electronic properties and contrasting them to the experimental results.

In addition, to gain further insight on the transport and optical properties of the nanographenes and help the experimental team to concentrate their efforts on those target molecules with the preferred physical properties, we carried out DFT-NEGFs and Bethe-Salpeter calculations for selected nanographenes.

In this talk I will introduce the experimental work and will then present the theoretical methodology and the main results obtained since the project was launched in September 2015 [1].

[1] [Marquez2016] Versatile Synthesis and Enlargement of Functionalized Distorted Heptagon-Containing Nanographenes, I.R. Márquez et al. (submitted).

4.2 Atomistic modelling studies of electrode materials for rechargeable lithium and sodium batteries

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Energy storage technology has already proven to offer great opportunities for technological progress. A clear example of this is the indispensable role of the Li-ion rechargeable battery, making possible the revolution of portable electronics. But far away from previous achievements, energy storage technology possesses a significant potential to offer a number of new economic and environmental benefits by means of replacing systems powered by fossil fuels (such as electric vehicles) and balancing the fluctuating generation of renewable power sources to facilitate their penetration in the electrical grid.

In the quest to find new sustainable electrode materials for batteries, quantum chemistry computation is an exciting starting point. Computational predictions of the performance of energy materials are now sufficiently mature to be applied successfully in many cases. In particular, density functional theory is helping in the experimental discovery of new materials or extracting important insights from known compounds. Here we discuss a selection of our most exciting examples of recent work in this area using the RES supercomputing facilities.

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

4.3 Using supercomputers for fast advancing in heterogeneous photocatalysis technologies

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Heterogeneous photocatalysis is a very active area of research because of its potential for applications in synthesis, energy and environmental technologies. [1] In heterogeneous photocatalysis, the activity of an organic molecule adsorbed on the solid catalyst's surface is promoted by the creation of an excited state through light irradiation. This process corresponds to a photo-redox reaction: the initially inert organic adsorbate is transformed in a highly reactive intermediate upon oxidation or reduction through interaction with the hole-electron pair of the electronic excitation. Evidently the efficiency of this process is controlled by the interfacial level alignment of the organic adsorbate's frontier levels with the band structure of the solid catalyst's surface.

In recent years the O-H bond photocatalytic dissociation for H2O or CH3OH on rutile TiO2(110) interfaces has been subject of extensive examination by surface science techniques in ultra-high vacuum conditions. [2,3] This process is important as it represents the first step in the molecular oxygen evolution reaction, which is one of the two reactions in water splitting, and methanol to formaldehyde photo-oxidation. The molecular-level interpretation of these experiments require theoretical approaches that go beyond ground state density functional theory, such as the quasi particle GW and Bethe Salpeter equation (BSE) methods. These methods allow for an accurate description of electronic and optical properties by including the treatment of many body effects. The scalable implementation of these methods in popular electronic structure codes and advances in supercomputing has enabled expert users to carry out calculations employing these sophisticated methods for large, complex systems.

This contribution is dedicated to recent work [4] done using the implementation of the quasi particle GW and BSE methods in the VASP code and Magerit@CeSViMa supercomputer to study the O-H bond photocatalytic dissociation mechanism for the H2O and CH3OH on TiO2(110) interfaces. I will show that these calculations are critical to obtain a detailed understanding of the nexus between the interfacial level alignment, optical properties and the resulting chemistry. The O-H bond dissociation is found to undergo an interfacial proton-coupled electron transfer mechanism. Altogether, this understanding could help expedite developments in heterogeneous photocatalysis technologies.

[1] Friend, C.M. Perspectives on Heterogeneous Photochemistry. Chemical record (New York, N.Y.). 2014, 14, 944-951.

[2] Zhou, C. et al. Site-specific photocatalytic splitting of methanol on TiO2(110). Chem. Sci. 2010, 1, 575–580.

[3] Tan, S. et al. Observation of Photocatalytic Dissociation of Water on Terminal Ti Sites of TiO2(110)-1 × 1 Surface. J. Am. Chem. Soc. 2012, 134, 9978–9985.

[4] Migani, A. & Blancafort, L. Interfacial Proton-Coupled Electron Transfer Mechanism in the Photocatalytic Oxidation of Methanol to Formaldehyde on TiO2(110), submitted.

4.4 Computational design of advanced nanoalloy materials

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Metal nanoparticles (NPs) are key components of many functional materials, in particular, heterogeneous catalysts. Yet, monometallic NPs are often insufficiently versatile, which limits their use. Conversely, mixed-metal NPs (nanoalloys) are so diverse that their properties can be tailored for a given application much easier. However, the complexity of nanoalloys makes the understanding of their structureproperty relations a great problem. Importantly, it is very laborious to experimentally determine the atomically resolved composition (chemical ordering) in nanoalloys, which is mandatory to rationalize their catalytic activity. We proposed an innovative method to predict chemical ordering in nanoalloys using density functional calculations.[1] This innovative method is applicable to various combinations of transition metals with each other and with s,p-elements.[1-5] It allows one to reliably predict the thermodynamically stable atomically resolved 3-dimensional structures of nanoalloys, which can be then manufactured. We shall outline the method and present examples of its application to various nanoalloys based on Pd [1], Pt [2-4] and Ni [5].

Our new method is capable of generating databases of structures and energies of nanoalloys spanning the Periodic Table. Simplicity and reliability of this approach open a way to provide researchers with unique opportunities to efficiently perform simulations of various kinds of nanoalloys with thousands of atoms. Applications of the method will radically accelerate the discovery of tailor-made nanoalloy materials and deepen the understanding of chemical bonding in nanoalloys.

* In collaboration with Gábor Kovács and Sergey Kozlov.

[1] S.M. Kozlov, G. Kovács, R. Ferrando, K.M. Neyman. How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. Chem. Sci. 6 (2015) 3868

[2] G. Kovács, S.M. Kozlov, I. Matolínová, M. Vorokhta, V. Matolín, K.M. Neyman. Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. Phys. Chem. Chem. Phys. 17 (2015) 28298

[3] M. Vorokhta, I. Khalakhan, M. Václavů, G. Kovács, S.M. Kozlov, P. Kúš, T. Skála, N. Tsud, J. Lavková, V. Potin, I. Matolínová, K.M. Neyman, V. Matolín. Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. Appl. Surf. Sci. 365 (2016) 245

[4] A. Neitzel, G. Kovács, Y. Lykhach, S.M. Kozlov, N. Tsud, T. Skála, M. Vorokhta, V. Matolín, K.M. Neyman, J. Libuda. Atomic ordering and Sn segregation in Pt-Sn nanoalloys supported on CeO2 thin films, Top. Catal. (2016), in press

[5] A. Wolfbeisser, G. Kovács, S.M. Kozlov, K. Föttinger, J. Bernardi, B. Klötzer, K.M. Neyman, G. Rupprechter. Surface composition changes of CuNi-ZrO2 catalysts during methane decomposition. Catal. Today (2016), doi: 10.1016/j.cattod.2016.04.022

4.5 The effect of strain and temperature on the mechanical properties of irradiated graphene

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Free standing graphene presents out-of-plane displacements, ripples, whose magnitude depends on temperature. In this molecular dynamics study we show how these ripples can also be modified by the application of a tensile or a compressive strain and how defect production under irradiation is affected by the initial strain. We present simulations of 140 eV Ar+ irradiation of a graphene membrane under applied strains between -0.25% (compressive) and 0.25% (tensile) and two different temperatures, 10K and 300K. These simulations reveal that the roughness of the graphene membrane is heavily modified by the irradiation, removing the randomness of the ripple distribution existing before irradiation. Nanoindentation simulations of the irradiated and unirradiated membrane under different strains provides information about the mechanical properties of this material. The two-dimensional Young modulus, E2D, is extracted from these simulations and showing a strong dependence with defect production and ripple distribution. These results could provide a path to minimize defect.

4.6 Computational Studies of Ice Nucleation

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When water is cooled below the melting point it becomes mestastable and it should freeze. However freezing from the supercooled liquid is an activated process and it is required to surmount a free energy barrier before this process occurs (like many chemical reactions that while spontaneous from a thermodynamic point of view do not occur on a reasonable time scale as they may have a high activation energy). For this reason it is necessary to wait some time before freezing occurs. Understanding the freezing of water in the absence of impurities is relevant to understand the formation of ice in the small droplets of supercooled water appearing in the upper atmosphere. Since ice is reflecting the sun light in a different way that liquid water the formation of ice in in the atmosphere has an impact on the world climate.

In this work we shall present simulation results (using Molecular Dynamic simulations and the program GROMACS) and the water potential models developed in our group (TIP4P/2005 and TIP4P/ICE) aimed to understand the ice nucleation from a molecular perspective. By using the resources of RES we study the formation of ice in supercooled water for large systems containing up to 200000 molecules of water.

The size of the critical cluster for the homogeneous freezing of water can be evaluated. For temperatures between -15 and -35 degrees below freezing the sizeo f the critical clusters varies from 8000 molecules to 600.[1] The interfacial ice-water free energy can be estimated by using the expression of Classical Nucleation Theory for the size of the critical cluster (we obtained values in good agreement with experimental reported results).[2] These calculations will allow to determine by the first time the homogeneous nucleation rate for the formation of ice from the melting point up to a supercooling of -70 degrees.[3] We shall also discuss the connection between the formation of ice and the possible existence of a second critical point in supercooled water.[4]

[1] E. Sanz and C. Vega and J. R. Espinosa and R. Caballero-Bernal and J.L.F. Abascal and C.Valeriani J. Am. Chem. Soc. 135 15008 (2013)
[2] J. R. Espinosa, C. Vega and E. Sanz J. Phys. Chem. C 120 8068 (2016)
[3] A. Zaragoza, M. M. Conde, J. R. Espinosa , C. Valeriani, C. Vega and E. Sanz J.Chem.Phys., 143, 134504 (2015)
[4] J. R. Espinosa, E. Sanz, C. Valeriani, and C. Vega J.Chem.Phys. 141 18C529 (2014)

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