

9th RES Users' Conference

23rd September, 2015

BOOK OF ABSTRACTS

Book of Abstracts
9th RES Users'Conference

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Acknowledgement

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About the RES

The Spanish Ministry of Science & Innovation (MICINN) created the Spanish Supercomputing Network (RES, Red Española de Supercomputación) in July 2006 as a response to the need of the Spanish scientific community for increased capacity and access to intensive calculation resources, considering the supercomputing resources as a decisive asset for the scientific and technological development of the country.

The RES consists of a distributed virtual infrastructure of supercomputers located in different sites, each of which contributes to the total processing power available to users of different R&D groups in Spain.

In addition to resources, the RES offers technical support to users as well as specific training. The goal of these actions is to improve the efficient usage of the resources and expand the use of supercomputing to a wider range of research areas.

Moreover, in order to maximize the scientific impact and inform of the return of investment, the RES gathers dissemination information of all the research activities developed in the RES framework. Besides, to promote the use of supercomputing and inform the society of the advantages that it offers, also organizes dissemination events aimed to specific scientific communities and to general public.

Additionally, technical trainings are arranged, taking into consideration that to offer the best service, the staff has to be perfectly trained and up-to-date with current applications, programming languages and other tools needed by the RES' users. These trainings also provide to the different RES teams –since there are eight different nodes – the opportunity to know each other, fostering further cooperation and joint efforts.

An last but not least, the RES Users' Committee (CURES) is an expert group that serves as a bridge among the users and the RES' management bodies to voice the users' concerns.

Programme

9th RES Users'Conference

(23 September 2015)

09.00h – Registration

10.00h – Welcome by José I. Doncel, MINECO

Session 1: Resources and services offered by the Spanish Supercomputing Network (RES)

Session chair: José I. Doncel, MINECO

10.10h – Supercomputing Resources in BSC, RES and PRACE, (Sergi Girona, BSC-CNS)

10.30h – RES Users Committee, (Montse González, BSC-CNS)

10.50h – KeyNote Talk: The XCHEM Project, (Fernando Martín, UAM)

11.20h – Performance Optimization and Productivity POP (Jesús Labarta, BSC-CNS)

11.40h – Poster exhibition and hosted coffee break

Poster: Development and consolidation of geo-spatial sustainability services for adaptation of environmental and climate change urban impacts (DECUMANUS)

Presenter: Juan L. Pérez, Technical University of Madrid (UPM).

Poster: European framework for online integrated air quality and meteorology modelling: aqmeii - air quality modelling evaluation international initiative

Presenter: Juan L. Pérez, Technical University of Madrid (UPM).

Poster: Computational exploration of the binding mode of the heme-dependent activator YC-1 into the active catalytic domain of soluble guanylate cyclase

Presenter: Luis Agulló, Universitat de Vic – Universitat Central de Catalunya.

Poster: Towards the modeling of turbulent lean premixed flames in industrial combustion systems.

Presenter: Daniel Mira, Barcelona Supercomputing Center - Centro Nacional de Supercomputación.

Programme

Session 2: The challenge of using PRACE supercomputers

Session chair: Jesús Labarta, BSC-CNS

12.00h – Supercomputation and realistic models of photocatalysts nanoparticles, (Francesc Illas, UB)

12.20h – Genomic variation associated to the metabolomics of autoimmune diseases, (Toni Julià, VHIR)

Session 3: Effects of Science on the society wellbeing

Session chair: Carme Rovira, Universitat de Barcelona

12.40h – Synthesize active molecules against drug-resistant mutants of influenza A virus, (Francisco Javier Luque, UB)

13.00h – The universe of neurotoxic proteins: A study of the conformational space of polyglutamine and β -amyloid, (Àngel Manuel Gómez Sicilia, Instituto Cajal in Madrid)

13.20h – Pause/hosted lunch break

Session 4: Increasing the knowledge on Earth and Cosmology Sciences

Session chair: TBD

14.30h – Impact of ocean resolution and initialisation in climate seasonal predictions, (Francisco Doblas Reyes, BSC)

14.50h – Microbial Oceanomics using Next-Generation Sequencing (454/Illumina), (Ramiro Logares, ICM)

15.10h – The Gaia Project, (Jordi Torra, UB)

Session 5: Industrial applications and fundamental research

Session chair: Anna Escoda, BSC-CNS.

15.30h – Random Field Ising Model in four spatial dimensions and beyond (Víctor Martín Mayor, UCM)

15.50h – Diffusion Monte Carlo simulation of quantum gases and solids, (Grigory E. Astrakharchik, UPC)

16.10h – Nucleation and anomalous properties of pure and salty water (Jose Luis F. Abascal, UCM)

16.30h – 3D Elastic Full Waveform Inversion: Toward Reflection Based Inversion, (Jean Korman, BSC)

16.50h – Conclusions, farewell and next RES Users Conference

17.00h – End of the conference

Keynote Speaker



Fernando Martín

Universidad Autónoma de Madrid

Fernando Martín graduated in Chemistry in 1984 and Physics in 1986 at the Universidad Autónoma de Madrid. He received his PhD degree at the same university in 1986. Then, he completed postdoctoral studies at the University of Bordeaux I (1988), the Université de Paris VI (1989-1990) and the University of Chicago (1995-1996). He is Full Professor at the Universidad Autónoma de Madrid since 2005. His research focuses on the theoretical modeling of photoexcitation and photoionization of atomic and molecular systems induced by synchrotron radiation and ultrashort laser pulses, as well as of complex molecular systems, isolated or deposited on surfaces. He has published over 350 articles and, since 2011, he is recipient of an Advanced Grant from the European Research Council. In 2000, he received the national research prize “Rey Juan Carlos I” and in 2010, the prize of the Spanish Royal Society of Chemistry in Chemical Physics. previous disciplines to build human-centric intelligent systems and improve the world with technology.

Talk “The XCHEM project: XUV/X-ray lasers for ultrafast electronic control in chemistry”

The development of attosecond laser pulses allows one to probe the inner working of atoms, molecules and surfaces on the timescale of the electronic response. In molecules, attosecond pump-probe

Resources and Services
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RESOURCES

spectroscopy enables investigations of the prompt charge redistribution and localization that accompany photo-excitation processes, where a molecule is lifted from the ground Born-Oppenheimer potential energy surface to one or more excited surfaces, and where subsequent photochemistry evolves on femto- and attosecond timescales. In this talk I will present a few numerical examples that mimic realistic molecular attosecond pump-probe experiments in which simple molecules are ionized with a single attosecond pulse (or a train of attosecond pulses) and are subsequently probed by one or several infrared or xuv few-cycle pulses. The evolution of the electronic and nuclear densities in the photo-excited molecule or remaining molecular ions is calculated with attosecond time-resolution and is visualized by varying the delay between the pump and probe pulses. The results of these theoretical calculations [1-7] allow us to explain several experimental observations as well as to guide future experimental efforts to uncover ultrafast electron and nuclear dynamics in molecules.

- [1] G. Sansone et al, Nature 465, 763 (2010).
- [2] S. E. Canton et al, Proc. Natl. Acad. Sci. 108, 7302 (2011)
- [3] A. González-Castrillo et al, Phys. Rev. Lett. 108, 063009 (2012)
- [4] A. Palacios et al, Proc. Natl. Acad. Sci. 111, 3973 (2014).
- [5] F. Calegari et al, Science 346, 336 (2014)
- [6] C. Ott et al, Nature 516, 374 (2014)
- [7] P. Ranitovic et al, Proc. Natl. Acad. Sci. 111, 912 (2014)

Talk presenters



Jesús Labarta

Barcelona Supercomputing Center

Jesus Labarta is full professor on Computer Architecture at the Technical University of Catalonia (UPC) since 1990. Since 1981 he has been lecturing on computer architecture, operating systems, computer networks and performance evaluation. His research interest

has been centered on parallel computing, covering areas from multiprocessor architecture, memory hierarchy, programming models, parallelizing compilers, operating systems, parallelization of numerical kernels, performance analysis and prediction tools.

Since 2005 he is responsible of the Computer Science Research Department within the Barcelona Supercomputing Center (BSC). He has been involved in research cooperation with many leading companies on HPC related topics. His major directions of current work relate to performance analysis tools, programming models and resource management. His team distributes the Open Source BSC tools (Paraver and Dimemas) and performs research on increasing the intelligence embedded in the performance analysis tools. He is involved in the development of the OmpSs programming model and its different implementations for SMP, GPUs and cluster platforms. He has been involved in Exascale activities such as IESP and EESI where he has been responsible of the Runtime and Programming model sections of the respective Roadmaps. He leads the programming models and

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resource management activities in the HPC subproject of the Human Brain Project.

Talk “Performance Optimization and Productivity POP”

The POP Center of Excellence led by BSC will start in October 2015. The project aims at providing expert assessment of the performance of applications to developers and users in both academia and industry.

The project is the only transversal CoE (across all areas of science and engineering) granted by the EC.

By using the tools developed at BSC and our deep understanding of machine operation we will identify the main performance problems exposed by applications and advise the developers on how to devote their restructuring efforts in the most productive direction.

This advice will be based on quantitative models estimating the potential gain achieved by different code transformations.

We will also provide specific guidance on how to use hybrid programming techniques (MPI+OpenMP) to achieve the objectives in the most effective and portable way.

The talk will present the project and encourage attendees to apply for its services.





Francesc Illas

Institut de Química Teòrica i
Computacional

Universitat de Barcelona (IQTCUB)

Francesc Illas (1954) carried out his chemistry degree studies and Ph. D Thesis at the Universitat de Barcelona where he became Full Professor of Physical Chemistry in 1992.

He spent several periods at different research centres (IBM Almaden Research Center and Los Alamos National Laboratory) and has been invited professor at Università della Calabria (Cosenza, Italy) and Université Pierre et Marie Curie (Paris, France). He received the Distinguished Professor Mention for the Research Promotion awarded by the Generalitat de Catalunya in 2001, the Bruker Physical Chemistry Research Award of the Spanish Royal Society of Chemistry in 2004 and was elected Fellow of the European Academy of Sciences in 2009, the same year he received the ICREA Academia Award. In 2012 he joined the Editorial Board of Surface Science and of Theoretical Chemistry Accounts. He published over 500 papers in international journals which received more than 13000 citations (h-index = 55). At present he serves as the Director of IQTCUB and of XRQTC.

Talk “Supercomputation and realistic models of photocatalysts nanoparticles”

Under UV irradiation, titanium dioxide (TiO₂) anatase-like nanoparticles decompose water into hydrogen and oxygen. This photocatalytic reaction is of huge technological relevance since it provides a simple, clean and almost endless fuel. The problem is, however, that only a fraction of sunlight arrives to the Earth surface in the form of UV

radiation, this precludes the direct use of this material and claims for suitable modifications in the resulting electronic structure so that the same chemical reaction could be triggered by sunlight in the visible range. To this end it is necessary to understand the properties of this material and, hence, be able to produce suitable modifications. Most of the effort has been focused on the electronic structure of bulk TiO₂ anatase and derived materials or on extended surfaces. In the present work we go one step further by considering more realistic models. To this end, (TiO₂)_n nanoparticles of increasing size (n= 10, 84, 165, 286, 455) have been constructed, their atomic structure optimized by means of density functional theory within the PBE Exchange-correlations functional and the electronic structure refined by the PBE0 functional. The calculations have been carried out using the highly parallel FHI-AIMS code running on the marenstrum supercomputer with up to 4096 cores. Results provide useful information about the dependence of electronic structure with particle size and open the way study for the study of chemically modified nanoparticles with possible photocatalytic activity towards water splitting in the visible.

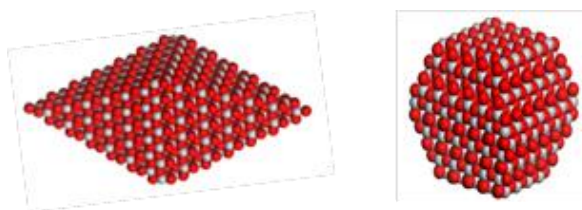


Fig. Bipyramid anatase TiO₂ nanoparticles exhibiting (101) facets (left), Truncated bipyramid anatase TiO₂ NP exhibiting (101) and (001) facets (right). Key: O – red, Ti – grey.



Toni Julià

Rheumatology Research Group, Vall d'Hebron

Antonio Julià (PhD) is the head of Bioinformatics at the Rheumatology Research Group from the Vall d'Hebron Hospital Research Institute, Barcelona, Spain. He has a PhD in Biochemistry and Molecular Biology from the Autonomous University of Barcelona. His primary research interests are the development of new bioinformatic tools for the analysis of genomic data and the transference of “omic” data into the clinical setting. He has published several Genome-Wide Association Studies (GWAS) in common autoimmune diseases, using Caucasian populations of Southern European ancestry. His current research involves the identification of the genomic variation associated with key phenotypic features in chronic inflammatory diseases including treatment response, disease activity and molecular endophenotypes like the transcriptome or the metabolome.

Talk “Genomic variation associated to the metabolomics of autoimmune diseases”

High throughput technologies have enabled the characterization of human variation at its most fundamental levels. One of the actual challenges in biomedicine is the combination the information from different molecular sources to reveal new aspects of human normal physiology and human disease. However, one of the main bottlenecks in the analysis biomedical high throughput data is the need for powerful computational resources that are be able to cope with the large amount of data and complexity of the analysis methods. In this project, we have used the PRACE supercomputing infrastructure to integrate whole-

genome genetic data from patients with autoimmune diseases and healthy controls together with metabolite profiles obtained from biofluids from these same individuals. Autoimmune diseases are a group of highly prevalent diseases characterized by immune responses to self antigens, leading to chronic and highly debilitating inflammatory processes. Autoimmune diseases have a major socioeconomic impact and significantly reduce the quality of life of many individuals. Using the unique supercomputational resources provided by PRACE, we are being able to characterize the genetic variation that influences the levels of metabolites in body fluids and, importantly, how these patterns are modified by the presence of a specific disease or group of diseases.

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Francisco Javier Luque **Barcelona Supercomputing Center**

F. Javier Luque (1962) obtained his degree in Chemistry from the Universitat Autònoma de Barcelona in 1985 and his PhD in Chemistry from the same university in 1989. His scientific career involved post-doctoral periods at the Swiss Federal Institute of Technology (1992), University of Pisa (1995) and University of Nancy (1998), where he was invited professor in 1999. In 1991 he was appointed assistant professor at the University of Barcelona, where he was full professor in 2003. In 2002 he was awarded with the Catalan Distinction for the Promotion of University Research for Young Scientists. He is leading the Computational Biology and Drug Design group in the Institute of Biomedicine (University of Barcelona).

Talk “Modelling drug binding to the M2 proton channel using enhanced sampling methods”

The M2 protein is a 97-residue long protein that, once assembled as an homotetramer in the virion surface, serves as a pH-gated proton channel that allows the acidification of the viral interior. Since such process is essential for the release of genetic material to the intracellular media, the M2 channel plays a critical role in the life cycle of the influenza A virus. The FDA approved drugs amantadine (Amt) and rimantadine effectively inhibit the wild type form of the channel. However, widespread of Amt resistance mutations found in flu circulating strains (including pandemic 2009 H1N1 swine flu and the highly lethal H5N1 chicken flu) impelled the CDC to advise against its use as flu treatment, dramatically decreasing the available therapeutical options. How mutations affect the energetic and structural determinants

of drug binding to the M2 channel is a key question to address the design of new compounds targeting Amt-resistant flu strains. In order to better understand such process, a set of unrestrained Molecular Dynamics simulations have been combined with enhanced sampling techniques to gain insight into the binding and unbinding of M2 channel blockers. Specifically, the results have disclosed the existence of distinct binding modes in the interior of the channel and allowed us to characterize the energetics of the Amt binding pathway. These findings provide valuable guidelines for the development of new inhibitors against influenza.

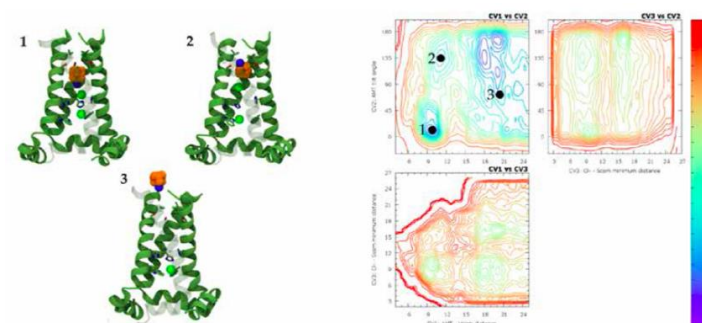


Fig. Free energy surface determined from multiple-walker metadynamics simulations for the binding of amantadine to the M2 proton channel.



Àngel Gómez-Sicilia

Instituto Cajal-CSIC

Àngel graduated in Physics in the University of Barcelona, and mastered in Biophysics with minor in bioinformatics and computation in the same university. After a final master project on modelling tumor growth, he moved to Madrid to complete his PhD in neurotoxic proteins studied both from an experimental and a theoretical point of view.

Talk “The universe of neurotoxic proteins: A study of the conformational space of polyglutamine and β -amyloid”

Polyglutamine and β -amyloid are proteins implicated in neurodegenerative diseases, currently incurable. These proteins do not acquire a fold but are rapidly fluctuating. In this work, using Bias Exchange Molecular Dynamics, we explore the conformational space of these disease-inducing proteins including their wild-type form as well as some mutants and conclude that the toxicity of the species correlates with the residence time of the conformations adopted by the proteins. Furthermore, some conformers are hard to process by the cellular degradation machinery due to their high mechanical stability or the presence of knots in their topology, which may damage or hinder the functioning of the unfolding machinery.



Francisco Doblas Reyes **Barcelona Supercomputing Center**

Francisco started working on climate variability at the Universidad Complutense de Madrid (Spain) in 1992, where he did my PhD that I defended in 1996. He then worked as a postdoc in Météo-France (Toulouse, France), at the Instituto Nacional de Técnica Aeroespacial (Torrejón, Spain) and as a researcher for ten years at the European Centre for Medium-Range Weather Forecasts (Reading, UK). He is the director of the Department of Earth Sciences of the Barcelona Supercomputing Center (BSC-CNS), where he led the largest FP7 project in climate prediction. He is author of more than 100 peer-reviewed papers, member of several international scientific committees of the World Meteorological Organization, PI of seven national and international projects, and supervisor of three PhD students. His research interests start from the fact that global climate is highly variable, which implies that there is much more to understand than just anthropogenic climate change. Climate prediction aims at predicting the variations of regional climate at different time scales, ranging from one month to several years beyond the start of the forecast. He uses an Earth system model based on discretized differential equations to explore the limits of the forecast quality over different parts of the globe, in particular over Africa, South America and Southern Europe, and statistical techniques to adapt the resulting climate information to specific user needs. Improving the application of this climate information to different socio-economic sectors, with a special focus on energy and disaster risk management, is the final target and one of his main motivations.

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Talk “Impact of resolution and initialisation in climate seasonal predictions”

Climate predictions in the seasonal-to-decadal range have a strong dependence on the initial conditions. It is thus possible to increase their skill by using an improved initialization approach that takes full advantage of all available observations and is, at the same time, able to mitigate the impact of the forecast drift due to intrinsic model deficiencies. The full-field and the anomaly initialization approaches are attracting the interest of most climate centres worldwide. In this presentation a fair comparison between these initialization methods using a state-of-the-art Earth system model is illustrated. The conditions leading to one approach outperforming the other are highlighted and help designing the more appropriate procedure to be applied depending on the model and observational constraint, as well as on the time horizon of interest. But apart from an adequate initialization, the forecast quality of seasonal predictions is affected by the climate model systematic error. Substantial efforts are being made to investigate the impact of the increase in the ocean and atmosphere resolution of the EC-Earth3 climate forecast system on the quality of global climate predictions. The results obtained contribute to the activities planned in the FP7 projects SPECS and PREFACE.



Víctor Martín Mayor **Universidad Complutense de Madrid**

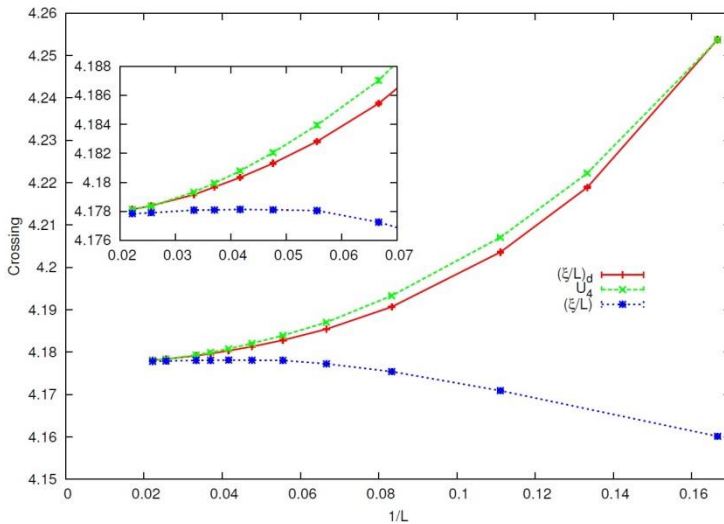
The random-field Ising model (RFIM) is of paramount importance in the field of disordered systems. A plethora of problems, ranging from hysteresis in magnetic systems to random pinning of polymers and fluids in porous media, can be studied via the RFIM. As such, the RFIM is under intense research for more than 30 years now. Yet, surprisingly, some of its most fundamental questions remain unanswered. Our group, using powerful algorithms and statistical analysis tools from the pools of Statistical Physics and Computer Science provided clear answers for the three-dimensional model. Nevertheless, a complete picture of the RFIM's critical behavior requires the understanding of the role of the spatial dimensionality. The goal of the present proposal is to fill this gap by studying the model at four dimensions and beyond.

Talk “Random Field Ising Model in four spatial dimensions and beyond”

Víctor completed his PhD in the Universidad Complutense de Madrid, in 1998. His postdoctoral work has been carried out in the Universities of Roma La Sapienza (1999-2002), and Universidad Complutense (where he was recruited thanks to the Ramon y Cajal program, and where he became faculty in 2007). He has been Principal Investigator in national research grants since 2003.

His research interests have been always related to the field of statistical mechanics, with an emphasis in glassy and disordered systems. Computers are major tools in this field. In fact, the RES is an invaluable asset for his research. Besides he has designed new simulation

algorithms and he has been involved in the design of computer specific for simulation in Physics (the Janus family of computers, see <http://bifi.es/en/infrastructures/scientific-equipment/janus>).



Several determinations of the critical point of the RFIM in four spatial dimensions, for a Gaussian distribution of disorder, as a function of the inverse system size. Although the different estimates are mutually incompatible, they approach to each other when the system size grows. This phenomenon is named "corrections to scaling". Accounting for it is absolutely crucial to reach valid conclusions from simulation data.



Jose Luis F. Abascal **Universitat Politècnica de Catalunya**

Jose Luis F. Abascal is a Catedrático de Universidad (Full Professor) at the Universidad Complutense de Madrid (UCM). He made his PhD at UCM and, except for a year spent in Paris, has been affiliated with UCM ever since. He has also been visiting fellow of a number of foreign research centers with stages lasting two months or

more at the Universities of Kent at Canterbury (UK), Pierre et Marie Curie (Paris VI, France,) UC Berkeley (USA), UC San Diego (USA), Maria Skłodowska (Lublin, Poland) and UNAM (Cuernavaca, Mexico).

He developed his PhD on Perturbation theories of the liquid state in 1981. After that he became interested in the investigation of the liquid state using molecular simulation, both Monte Carlo and Molecular Dynamics. He has studied a broad range of systems from simple liquids to electrolyte and polyelectrolyte solutions including DNA with implicit solvent. Most of its recent work has been devoted to water and ionic solutions with explicit solvent.

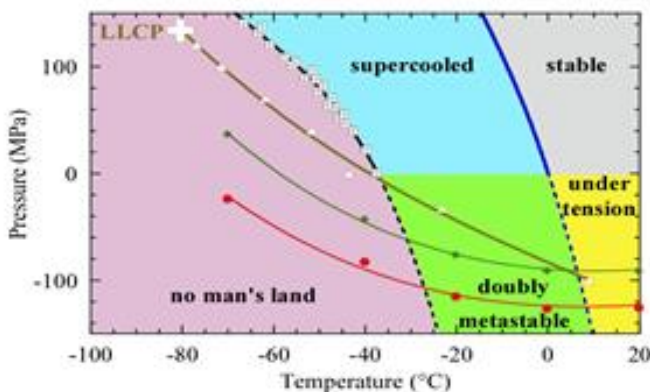
Citation metrics: h-index =30, 1 article with more than 600 citations and 8 with more than 100 citations.

Talk “Nucleation and anomalous properties of pure and salty water”

Water is the most familiar liquid and, arguably, the most complex. Water properties are sensibly different to those of other liquids. These anomalies are greatly enhanced in the supercooled and in the negative pressure regions. Competing explanations of this behaviour have been

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proposed. We have performed molecular dynamics simulations trying to shed light on this issue. In particular, we have calculated the loci of several water anomalies using a successful water model. The results suggest the possibility to rule out some of the proposed scenarios for water anomalies, and put further constraints on the remaining ones. Closely related is the study of the nucleation process that transforms the metastable liquid into its stable phase (ice or vapour). Our simulations of the homogeneous nucleation have yielded the nucleation rate and the size of the critical cluster as a function of the difference between the temperature of the metastable liquid and the freezing temperature. Our calculations predict that water freezing at the most relevant temperatures in Earth must necessarily be heterogeneous. Finally, the effect of adding salt to water has been analyzed.



Pressure-temperature phase diagram of water. The melting line of ice Ih is shown at positive pressure by a solid blue curve. Beyond this line liquid water is in a metastable state. The solid black curve show the experimental supercooling limit. The plot shows that the region of large anomalies can not be reached at positive pressures but it is accessible at negative pressures

[Pallares et al., PNAS 111, 7936 (2014)]



2010 he works at BSC.

Jean Korman **Barcelona Supercomputing Center**

Jean studied Mechanics in Strasbourg and after that he studied in Les Mans an engineering degree majoring in vibration and acoustics specialization. He also studied a MSC Acoustic Engineering, ETSII and finally pursued in Madrid his PhD in Physics. Since

Talk “3D Elastic Full Waveform Inversion: Toward Reflection Based Inversion”

Full Waveform Inversion (FWI) is one of the most challenging procedures to obtain quantitative information of the subsurface. On land seismic surveys, obtaining information from the recorded seismograms requires a full elastic approach. This shortcoming has been reduced as high-performance computing makes 3D elastic FWI more affordable. However, there is still a key issue for overcoming its computational burden and mitigate the requirement of having long-offset data. Here we introduce a Dynamic Offset Control, that is a data selection method for adapting the longer receiver offset to the current inverted frequency. We exemplify our approach through 2D and 3D synthetics, and afterwards, the algorithm was used to invert a real line from a 3D high resolution seismic reflection dataset acquired to image a shallow subsurface. This high resolution dataset images a 500x500 m block located in the Zancara river basin (Spain). The study area is characterized by a relatively heterogeneous geology revealed by the borehole data available and features topographic variations on the order of a few meters. As it is a very shallow target, free-surface effects and

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topography are critical issues which the code needs to handle appropriately. The obtained 3D velocity models were contrasted with other geophysical data available.

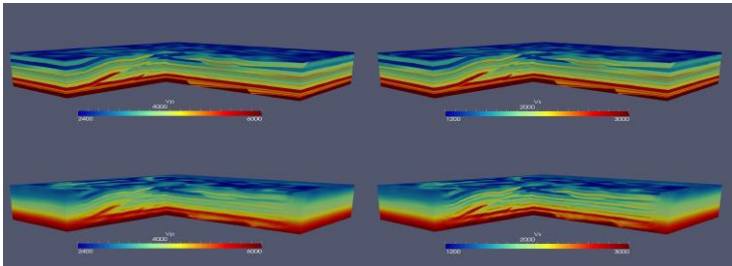


Fig. Comparison between target and inverted model after 40 iterations.

Poster presenters



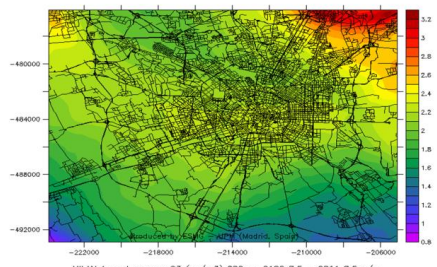
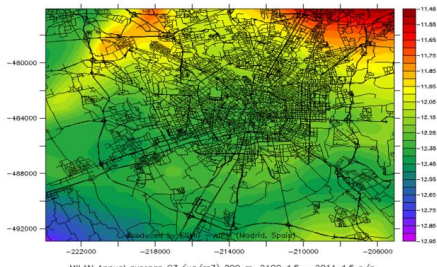
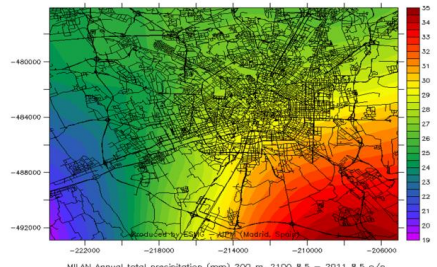
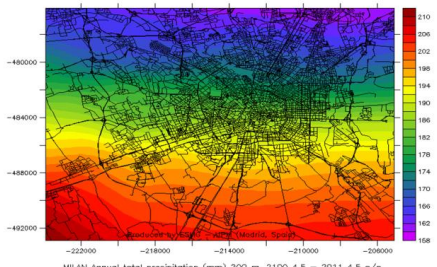
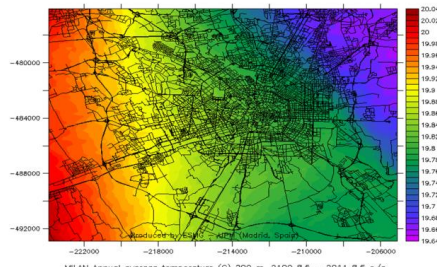
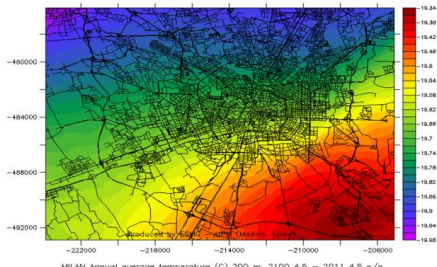
Juan Luis Pérez

Universidad Politécnica de Madrid

Juan Luis Pérez graduated in Computer Sciences at Computer Science School of the Technical University of Madrid in 2000, and in 2005 he defended a PhD thesis related to operational modelling of the MM5-CMAQ system over the internet. He has been an associate professor since 2005 and permanent professor since 2011. He is involved in some international and national research projects about atmospheric simulations and has published many papers in journals and conference proceedings.

Poster “Development and consolidation of geo-spatial sustainability services for adaptation of environmental and climate change urban impacts (DECUMANUS)”

This work describes the results of a modelling system for climate change impact assessments on urban climate and air quality. The system takes the outputs from a global climate model, which are injected into a dynamical regional climate model (WRF-Chem) with the nested capability activated, with 25 km spatial resolution. In addition, the system uses a diagnostic meteorological model (CALMET) to produce urban detailed information (with 200 m spatial resolution) using this downscaling procedure. At the city level, a simplified chemical-transport model (based on CMAQ and using linear chemistry) is used to map the spatial distribution of the pollutants. The system is applied to five European cities: Madrid, Antwerp, Milan, Helsinki and London



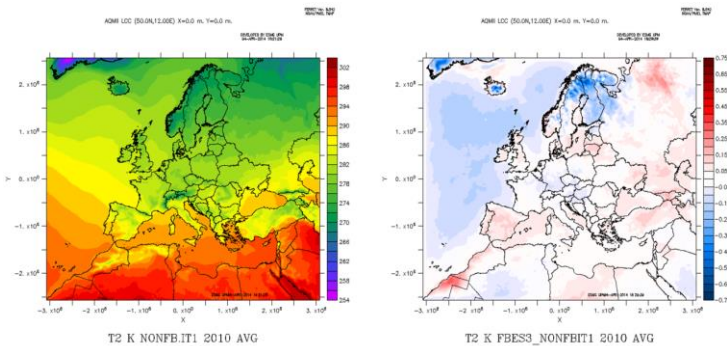
Milan differences (percentage %) between 2100 and 2011 spatial distribution (200 meters of resolution) of one-year average air temperature (top), total precipitation (middle) and ozone (bottom) with RCP 4.5 (left) and RCP 8.5 (right).
 Downscaling simulations using CALMET-CMAQL from the European WRF-Chem

(Kensington-Chelsea area). The modelling system was used to simulate the climate and air quality for present year (2011) and future years (2030, 2050 and 2100) using 2011 emissions as control run, because we want to investigate the effects on the global climate on the actual (2011) cities. Effects on temperature, precipitation, and ozone are also considered. We compare the climate and air concentrations in future years 2030, 2050 and 2100 with the control year (2011). Comparison of simulations for present situation (using NNRP reanalysis 2011 data sets) shows acceptable agreement with measurements which give us strong confidence on the results for the RCP IPCC climate future simulations for 4.5 and 8.5 scenarios. This work is part of FP-7 EU DECUMANUS project. The aim of this project is the development and consolidation of a set of sustainable decision support services that allow city managers to deploy geo-spatial products in the development and implementation of their energy efficiency and climate change strategies, in meeting the diverse challenges of sustainable urban planning and development.

Poster “European framework for online integrated air quality and meteorology modelling: aqmeii - air quality modelling evaluation international initiative”

To investigate the impact of the aerosol effects on meteorological variables and pollutant concentrations two simulations with the WRF-Chem model have been performed over Europe for year 2010. We have performed a baseline simulation without any feedback effects and a second simulation including the direct as well as the indirect aerosol effect. Although low aerosol particle concentrations are detected, the inclusion of the feedback effects results in an increase of solar radiation at the surface over cloudy areas (North-West, including the Atlantic) and decrease over more sunny locations (South-East). Aerosol effects

produce an increase of the water vapor and decrease the planet boundary layer height over the whole domain except in the Sahara area, where the maximum particle concentrations are detected. Significant ozone concentrations are found over the Mediterranean area. Simulated feedback effects between aerosol concentrations and meteorological variables and on pollutant distributions strongly depend on the aerosol concentrations and the clouds. WRF-Chem variables are evaluated using available hourly observations in terms of performance statistics.



2010 mean two meter temperature for the base case (left) without feedback and simulated changes (feedback-non feedback, right) due to effects of aerosols. Simulation with WRF-Chem 23 km. of spatial resolution.

Standardized observations from the ENSEMBLE system web-interface were used. The research was developed under the second phase of Air Quality Model Evaluation International Initiative (AQMEII). WRF-Chem demonstrates its capability in capturing temporal and spatial variations of the major meteorological variables and pollutants, except the wind speed over complex terrain. The wind speed bias may affect the accuracy in the chemical predictions (NO₂, SO₂). The analysis of the

correlations between simulated data sets and observational data sets indicates that the simulation with aerosol effects performs slightly better. These results indicate potential importance of the aerosol feedback effects and an urgent need to further improve the representations in current atmospheric models to reduce uncertainties at all scales.



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Luis Agulló obtained his PhD in Chemistry in 1992 (University Autónoma de Madrid, 1992), worked at the University Autònoma de Barcelona and the Vall d’hebron Research Institute and recently moved to the Systems

Biology Department of the University of Vic. He has been working mainly on the field of cell biology, specifically in the area of signal transduction. During the last years he is applying different computational techniques as homology modeling, molecular dynamics and ligand docking to this area of research.

Poster “Computational exploration of the binding mode of the heme-dependent activator YC-1 into the active catalytic domain of soluble guanylate cyclase”

Soluble guanylate cyclase (sGC), the main target of nitric oxide (NO), has been proven to have a significant role in coronary artery disease, pulmonary hypertension, erectile dysfunction and myocardial infarction. Several drugs that increase the activity of this enzyme are now in clinical phase of development: some of them are heme-dependent and

might interact with the catalytic domain and others are heme-independent and supposedly bind to the sensory domain. The absence of reliable structural information is one of the factors that have precluded knowledge of the precise site of interaction of these molecules and of the mechanism of activation of the enzyme.

Homology models of the catalytic domain of sGC in 'inactive' or 'active' conformation were constructed using, for the β -chain, the structure of recently published crystal of a nonphysiological homodimer of β subunits of human guanylate cyclase (2WZ1), for the α -chain, a similar domain of the green algae *Chlamydomonas reinhardtii* (3ET6) and, for monomer arrangement, the sGC 'inactive' structure (3ET6) or the 'active' catalytic domain of adenylate cyclase (1CJU). Molecular dynamics simulations of about 1 μ s each were run on all relevant models (NAMD/ACEMD, Amber99SB).

Docking of YC-1, a classic heme-dependent activator, to all frames of this trajectory and absolute binding free energies with the linear interaction energy method (LIE) for selected poses revealed one potential binding site located between pseudo-symmetric and catalytic sites just over the loop β 2- β 3. This site would be compatible with the binding of a second GTP or an inhibitory ATP to the pseudo-symmetric site.



Daniel Mira

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Daniel Mira is doctor in Mechanical Engineering in the area of Computational Fluid Dynamics and Combustion by Lancaster University, UK. He was involved in a nationally funded project in the UK focused on Modelling turbulent mixing and combustion of hydrogen enriched fuels using

large-eddy simulation. He was awarded with the EPSRC Doctoral Prize from Lancaster University in 2013 for the scientific contribution of the research conducted during the PhD. He gained a postdoctoral Marie Curie fellowship at Barcelona Supercomputing Centre (BSC) on the COPA-GT project (Coupled Parallel Simulations of Gas Turbines) working on fluid-structure interaction, turbulent reacting flows and heat transfer. He has been visiting researcher at CERFACS (France) and the University of Twente (The Netherlands) and his expertise is on advanced models for multiphysics applications in the context of High Performance Computing. He is currently supervising a PhD thesis on multicomponent interactions in gas turbines and another PhD thesis on turbulent combustion modelling.

Poster “Towards the modeling of turbulent lean premixed flames in industrial combustion systems”

The design of modern combustion systems needs to address several challenges in aspects related to reduction of pollutant emissions using lean mixtures, increment in flexibility of operation and avoiding thermo-acoustic instabilities. To achieve these goals, numerical methods are becoming increasingly important during the design process as they

provide detailed insights into the physical processes at relatively low cost.

Tabulated chemistry allows including detailed finite rate chemical kinetics into the flow solver to take into account chemistry effects without accounting for transport equations for all the species involved in the combustion process. Therefore, the stiffness of the problem is reduced and permits to obtain accurate predictions of radicals and products for different combustion regimes.

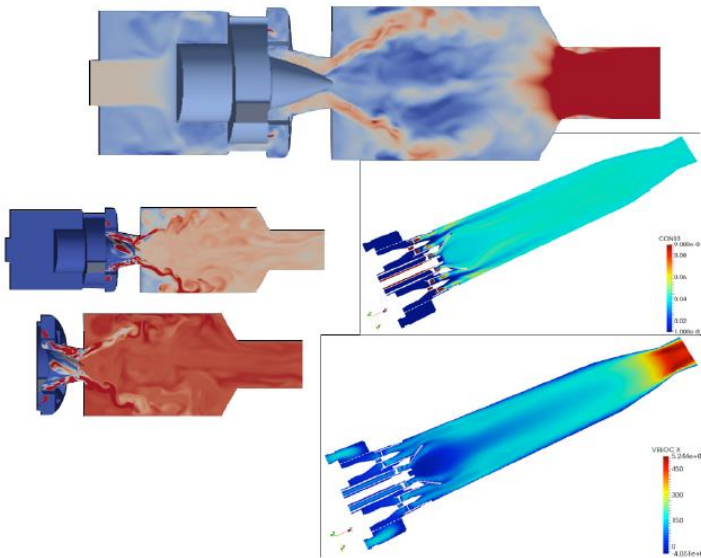


Fig. Sample results of the reacting flow field of the PRECCINSTA burner using LES (left) and RANS results of the reacting field of the can combustor SGT5-8000H (right).

The proposed project aims to use high-fidelity numerical simulations to predict flame stability mechanisms and pollutants formation in real combustors. This work takes place in the context of an academic and scientific framework, but with a strong industrial purpose and aims to enhance the accuracy, flexibility, user decision and applicability of numerical tools for industrial design.

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