14th USERS CONFERENCE

16 - 17 September 2020

ONLINE CONFERENCE

@RES_HPC   #JURES20

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Welcome

Dear RES user,

We are facing one of the greatest threats to human population in this our generation. The virus SARS-CoV-2 and its corresponding disease COVID-19 has already changed the way we live, the way we interact with each other, how we teach, the way companies thrive every day, etc. We have adapted, as many others, to the new situation, and the RES access to our supercomputing resources and the support services have been maintained as before. We may say we have the privilege of being immersed already in the digital world. But we have to show our commitment to search a solution from the research and the HPC community.

The RES will allocate during 2020 more than 100 million CPU hours to research projects dealing with COVID-19. We all know that supercomputing, artificial intelligence, molecular modelling, *in silico* predictions, drug design, simulation of the infection propagation, molecular dynamic simulations, computational chemistry, etc, constitute very good tools to search for solutions. We will continue to offer support to the scientific community to pursue this common will.

Meanwhile, we will also celebrate our annual meeting. The Spanish Supercomputing Network (RES) annually organizes a user meeting to report on the latest developments in the RES and provide relevant information on access to RES resources and on the European ecosystem in HPC. Although this conference is normally a physical meeting space for all users, support technicians, the access committee and the user committee, we have to gather virtually in 2020. Besides great lectures by scientists from different disciplines and HPC technology experts, we will have a round table about the perception of HPC by businesses and society. We are also celebrating the second edition of the RES Award to the most Outstanding scientific paper.

Finally, we have to thank our kind sponsors Fujitsu, IBM and HPCNow! that will make it possible to feel closer by sharing a breakfast at home.

We hope to meet all of you in person for the 15th Users Conference to be held in Cáceres, September 2021.

Join us for this exciting new experience that brings HPC science directly to you!

Sergi Girona, *RES coordinator*

Program

Wednesday, September 16th

14:30   Registration

15:00   *Welcome*. José I Doncel, Ministerio Ciencia e Innovación

15:05   *Updates about the RES*. Sergi Girona, Barcelona Supercomputing Center (BSC-CNS)

15:15   Scientific Keynote: *Computation in Biomedicine: the COVID-19 case*. Alfonso Valencia, Life Science Department, Barcelona Supercomputing Center (BSC-CNS)

16:00   RES Outstading Paper Award 2019. *Metal–organic frameworks for electrocatalytic oxygen evolution reaction*. Manuel Ortuño, Institut Català d'Investigació Química (ICIQ)

16:20   *Update of the RES Users Committee* (CURES). Miguel-Angel Aloy, Universidad de Valencia

16:40   *Tailoring the electron-transfer properties of Azurin junctions via single-point mutations*. María Ortega, Scanning Probe Microscopy Theory and Nanomechanics Group, Universidad Autónoma de Madrid (UAM)

17:00   PAUSE BREAK

17:10   *Mesoscopic studies of phoretic phenomena in binary fluids*. Jurij Sablic, Statistics Physics Group, University of Barcelona (UB)

17:30   *Ab initio characterization of carbon nanotubes functionalized with antiferromagnetic molecules for applications in spintronics*. Simona Achilli, University of Milan, Catalan Institute of Nanoscience and Nanotechnology (ICN2)

17:50   *MareNostrum5 - the way to a EuroHPC pre-exascale supercomputer*. Javier Bartolomé, Barcelona Supercomputing Center (BSC-CNS)

18:05   *LUMI: the EuroHPC pre-exascale system of the North*. Pekka Manninen, Center for Science Computing (CSC) Finland

18:20   *The Leonardo EuroHPC pre-exascale system in the contest of the Bologna Tecnopolo project and vision*. Sanzio Bassini, Director Supercomputing Application Innovation, CINECA

SPONSORS SESSION

18:35   *Fujitsu a company committed to supercomputing*. Gonzalo Romeo, General Director Product Division Fujitsu Spain

18:40   *Advanced supercomputing services for science and engineering.* Pere Puigdomenech, Business Development Manager, HPCNow!

18:45   *IBM POWER10: IBM's new processor for the Cognitive era*. Albert Valls, CTA - Systems Architect IBM

18:50   Closing

Thursday, September 17th

9:30   Registration

10:00   Technical keynote: *Reduced Order Modelling: From HPC to edge applications*. Riccardo Rossi, Kratos Multiphysics, International Centre for Numerical Methods in Engineering (CIMNE)

10:40   *Highest resolution 3D solar magneto-convection simulations up to the chromospheric heights*. Elena Khomenko, Solar Physics group, Instituto de Astrofísica de Canarias (IAC)

11:00   *Staircase conductivity of polyoxovanadates adsorbed on Au(111)*. Coen de Graaf, Universitat Rovira i Virgili (URV)

11:20   *Macroscopic simulations of the microscopic quantum dynamics of laser-matter interaction to structure ultrafast light pulses*. Carlos Hernández-García, University of Salamanca

11:40   *Machine learning and deep learning services in the European Open Science Cloud*. Álvaro López García, Instituto de Física de Cantabria (IFCA – CSIC)

12:00   SHORT BREAK

12:10   *DeepHealth, an example of HPC-AI convergence in benefit of more efficient new biomedical applications*. Mónica Caballero, Everis

12:30   *HeAT - a distributed and GPU-accelerated tensor framework*. Markus Götz, Steinbuch Centre for Computing (SCC), Karlsruhe Institute of Technology (KIT)

12:50   Round table: *HPC towards business and society*. Moderator: Jordi Mas, RES

- Juan José Palacio Burgos, Autonomous University of Madrid (UAM)
- Silvia Simón, University of Girona (UdG)
- Nuria Lopez, Institu Cataà d'Investigació Química (ICIQ)

14:00   *Closing*. Sergi Girona, RES, BSC

15:00   *Technical session* (for RES nodes staff only). Coordinator: Jorge Rodríguez, BSC

- *Monitorización con Influx y Grafana en CénitS-CPD*. J. Calle, F. Lemus y L. I. Jiménez, CENITS
- *HPC Containers*. Óscar Hernández, Support BSC
- *Technological updates at BSC 2020*. Sergi Moré, Sysadmin BSC

Abstracts

The abstracts appear in alphabetical order of the last name of the speaker.

Ab initio characterization of carbon nanotubes functionalized with antiferromagnetic molecules for applications in spintronics

S. Achilli[1,*], Z. Zanolli[1,**], P. Ordejon[1]

[1] Catalan Institute of Nanoscience and Nanotechnology – ICN2
[*] Current affiliation: University of Milan
[**] Current affiliation: Utrecht University

We will report on our recent study on electronic and magnetic properties of carbon nanotubes functionalized with [M4L2(OAc)4] molecules (H2L = 2,6-bis-(1-(2-hydroxyphenyl)iminoethyl)pyridine, HOAc = acetic acid, and M = Mn^{II} or Co^{II}) that display a quasi-tetrahedral core of magnetic ions, antiferromagnetically coupled. Through ab initio calculations we explored different spin configurations to determine the strength of the magnetic coupling in the molecules.

Moreover we analyzed the role of the Hubbard U correction in Density Functional Theory calculations and of the Spin Orbit coupling for both Co_4 and Mn_4 core. Exploiting our recent implementation in the SIESTA code we studied also the behavior in an externally applied magnetic field. Thanks to this complete characterization we are able to show the similarities and differences between the two molecules and discuss how they are expected to perform when grafted to carbon nanotubes for spintronics applications.

MareNostrum5 - the way to a EuroHPC pre-exascale supercomputer

Javier Bartolomé

Barcelona Supercomputing Center

The Kingdom of Spain, the Republic of Portugal, the Republic of Croatia and the Republic of Turkey proposed to join forces with the EuroHPC Joint Undertaking (JU) to procure, host and operate a precursor to exascale supercomputer called MareNostrum5, which will be installed at the Barcelona Supercomputing Center – Centro Nacional de Supercomputación. The consortium seeks to help building European HPC ecosystem, and developing knowledge and expertise in these countries with the BSC-CNS leadership. This presentation will describe which components MareNostrum5 will be composed of, acting as one of the future EuroHPC pre-exascale supercomputers. Compute partitions, technologies used, storage subsystem and datacenter requirements are the main topics that will be explained.

DeepHealth, an example of HPC-AI convergence in benefit of more efficient new biomedical applications

Mónica Caballero

R+D Project Manager, Everis

DeepHealth is a H2020 EU Project, coordinated by everis, that relies on unifying the traditionally separated high-performance computing and big data/deep learning analytics environments. Its main objective is to put HPC power at the service of biomedical applications with Deep Learning and Computer Vision needs to support new and more efficient ways of diagnosis, monitoring and treatment of diseases. The presentation will show how DeepHealth addresses the convergence of Deep Learning with HPC, how it exploits these technologies for the benefit of biomedical applications; and how it facilitates its easy adoption by the industry for the health sector and beyond it. Main expected outcomes will be also introduced: the DeepHealth Toolkit and libraries, the HPC infrastructure support for an efficient execution of the libraries; the integration of the libraries into different (industrial) platforms and their joint use in 14 different use cases.

Staircase conductivity of polyoxovanadates adsorbed on Au(111)

Almudena Notario-Estevez[1], Xavier López[1], Coen de Graaf[1, 2]

[1]*Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Tarragona*
[2]*ICREA, Barcelona*

The molecular conductivity of V6O19 on Au(111) is studied to clarify the stepwise increase of the current with increasing voltage. It was hypothesized that the V6O19 is reduced upon increasing voltage, causing a sudden increase of the molecular conductivity. We have computationally established a relation between oxidation state and conductivity in line with experiment. Next, we studied a much larger system with 18 V atoms. This polyoxovanadate (POV) has many more oxidation states accesible at not too high potential. It was therefore proposed as a candidate with better stepwise behaviour. However, we have not found any indication for significantly different conduction in the resting state and the double reduced or oxidized forms due to the large number of unpaired electrons in the resting state. Larger conduction-potential staircases should exist in POV systems that can be reduced multiple times, but has no unpaired electrons in its resting state.

HeAT - a distributed and GPU-accelerated tensor framework

Markus Götz

Steinbuch Centre for Computing (SCC), Karlsruhe Institute of Technology (KIT)

HeAT is an array-based numerical framework for large-scale processing in the Python programming language. Its goal is to bridge the gap between data analytics and machine learning libraries with a strong focus on on single-node performance, and traditional high-performance computing (HPC). For this, HeAT provides highly optimized algorithms and data structures for tensor computations using CPUs, GPUs and distributed cluster systems on top of MPI. The Python-first, NumPy-like interface integrates seamlessly with the existing data science ecosystem and makes it as effortless to write scalable data science applications. HeAT provides both, low-level array-based computations, as well as various higher-level algorithms, including among others neural networks, dimensionality reductions and clusterers. Compared with applications written in similar frameworks, such as Dask, HeAT achieves speedups of up to two orders of magnitude.

Macroscopic simulations of the microscopic quantum dynamics of laser-matter interaction to structure ultrafast light pulses

Carlos Hernández-García

Grupo de Investigación en Aplicaciones del Láser y Fotónica (ALF-USAL)
Dpto. Física Aplicada, Universidad de Salamanca, Spain

Ultrashort pulses of coherent structured light are opening excellent opportunities to control the primary electronic response of matter at unprecedented temporal and spatial scales. During the last decade we have developed theoretical tools to simulate the intense laser-matter interaction processes that provide such light sources. In order to do that, one needs to fulfill sub-attosecond (10^{-18} sec.)/sub-nanometer (10^{-9} m.) resolution at the quantum scale and picosecond (10^{-12} sec.)/milimeter (10^{-6} m.) resolution at the macroscopic scale. Our micro+macroscopic methods, in combination with high-performance computing strategies, have allowed us to tackle this challenge. Our simulation results helped us not only to understand, but to propose new experiments that have been successfully realized by our collaborators. In particular, we have recently predicted the generation of new forms of structured laser light at the attosecond timescale with novel properties as the self-torque.

Highest resolution 3D solar magneto-convection simulations up to the chromospheric heights

Elena Khomenko

Solar Physics group, IAC, Spain

This contribution summarizes the recent results from our research project based on Mare Nostrum supercomputing resources. The aim of our project is to investigate one of the most puzzling and persisting problems in Solar Physics - heating mechanisms of the solar chromosphere. We include a novel methodology that takes into account non-ideal effects derived from the very low ionisation degree of solar plasma. We perform high-resolution 3D simulations of self-consistent magnetic field generation by non-ideal battery effect acting in outer solar convection zone, its subsequent amplification through the local dynamo action, current redistribution through the Hall effect, and current dissipation and energy release due to the action of ambipolar effect. These simulations are highly demanding because non-ideal effects saturate at very small spatial scales, but at the same time, large domains and long time series are needed to cover solar dynamical phenomena. In this contribution, we will discuss the most recent results from our highest resolution simulations.

Machine learning and deep learning services in the European Open Science Cloud.

Álvaro López García

IFCA - CSIC

The DEEP-HybridDataCloud project offers a development framework for all users, including non-experts, enabling the transparent training, sharing and serving of Artificial Intelligence, Machine Learning and Deep Learning models both locally or on hybrid cloud systems in the context of the European Open Science Cloud. The DEEP solution is based on Docker containers packaging already all the tools needed to deploy and run the models in a transparent way for the users.

In this session we will present the current service offer, allowing scientsits to share and publish models ready to be used (through the DEEP marketplace); to develop, build and train models (through the DEEP training facility); and to deploy them as services (through the DEEP as a Service).

LUMI: the EuroHPC pre-exascale system of the North

Pekka Manninen

Development Manager, CSC, Finland

The EuroHPC initiative is a joint effort by the European Commission and 31 countries to establish a world-class ecosystem in supercomputing to Europe (read more at https://eurohpc-ju.europa.eu/). One of its first concrete efforts is to install the first three "precursor to exascale" supercomputers. Finland, together with 9 other countries from the Nordics and central Europe, will collaboratively host one of these systems in Kajaani, Finland. This system, LUMI, will be the one of the most powerful and advanced computing systems on the planet at the time of its installation. The vast consortium of countries with an established tradition in scientific computing and strong national computing centers will be a key asset for the successful infrastructure. In this talk we will discuss the LUMI infrastructure and its great value and potential for the research community.

Tailoring the electron-transfer properties of Azurin junctions via single-point mutations

María Ortega[1], J. G. Vilhena[2], Carlos Romero-Muñiz[3,1], Ismael Díez- Pérez[4], Juan Carlos Cuevas[1,5], Linda A. Zotti[6,1, 5] and Rubén Pérez[1,5]

[1]*Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain*
[2]*Department of Physics, University of Basel, Basel, Switzerland*
[3]*Department of Physical, Chemical and Natural Systems, Universidad Pablo de Olavide, Seville, Spain*
[4]*Department of Chemistry, Faculty of Natural & Mathematical Sciences, King's College London, UK*
[5]*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain*
[6]*Departamento de Física Aplicada I, Escuela Politécnica Superior, Universidad de Sevilla, Seville, Spain*

Protein-based electronics is an emerging field which has attracted considerable attention over the past decade. Here, we combine ab-initio calculations with atomistic molecular dynamics simulations to analyze the formation and electronic structure of a metal-protein-metal junction based on the blue-copper azurin from pseudomonas aeruginosa. Moreover, we inspect the effect of single amino-acid mutations on protein structural stability and electronic structure. The results obtained confirm that neither the interaction with the electrodes nor the introduction of mutations affects the azurin electronic structure. More importantly, our results reveal that the introduction of mutations quench protein vibrations resulting in its overall stiffening. Given the role of the protein vibrations on both its dehydration process and reorganization energy, we suggest that this mutation-induced stiffening effect could influence the electron-transfer properties of these protein junctions.

Metal–Organic frameworks for electrocatalytic oxygen evolution reaction

Manuel A. Ortuño

Postdoctoral reseacher, ICIQ, Spain

In a world with increasing energy needs, we face the challenge of developing sustainable and efficient energy sources to reduce our dependence on non-renewable fossil fuels. Electrocatalysis appears as a promising solution to store renewable energy of discontinuous sources into clean fuels derived from simple molecules, such as water or carbon dioxide. In that regard, the tunable porosity and chemical versatility of metal–organic frameworks can merge the advantages of homogeneous and heterogeneous catalysis. Herein, we compute the oxygen evolution reaction with periodic density functional theory to elucidate the active sites of these porous materials at the atomic level of detail.

Reduced Order Modelling: From HPC to edge applications

Riccardo Rossi

CIMNE

The maturity of numerical methods, combined with the availability of high computational power makes nowadays possible the simulation of highly complex engineering problem. A current challenge is to make available such capabilities for the construction of Digital Twins, able to accompany engineered products through their entire life span. Achieving this goal implies fitting complex models into compute constrained edge devices. "Reduced Order Modelling" opens up the possibility of using HPC power for the training of "simplified" models, which can fit in such constrained environments. This implies combining HPC simulation with the use of data mining techniques for the extraction of relevant patterns in training data. Contrarily to "classical" ML, such models may provide probably good, and "understandable" results thus providing an excellent alternative to black box approaches.

Mesoscopic studies of phoretic phenomena in binary fluids

Jurij Sablić[1, 2] and Ignacio Pagonabarraga[1, 3, 4]

[1]Departament de Física de la Matèria Condensada, Universitat de Barcelona, Spain
[2]Laboratory for Molecular Modeling, Theory Department, National Institute of Chemistry, Ljubljana, Slovenia
[3]CECAM, Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lasuanne (EPFL), Batochime, Lausanne, Switzerland
[4]Universitat de Barcelona Institute of Complex Systems (UBICS), Universitat de Barcelona, Spain

We study the diffusophoretic and diffusoosmotic behavior of binary fluid mixtures on mesoscopic scale. To this end we use the Lattice Boltzmann method, incorporated in the code Ludwig. The flow in the simulated systems is driven by an externally imposed chemical potential gradient. We investigate how the fluid's interaction with the wall affects the flow as well as how the flow behaves in the presence of the porous media (i.e. SCC, BCC, FCC crystals). In the latter case, the majority of computational domain consists of solid nodes and not of the fluid ones, which leads to the load balancing problems of simulated systems. We further investigate these by carrying out a set of strong and weak scaling tests, which reveal the discrepancy of the speedups in the presence of porous media in the system. All the simulations of phoretic phenomena in binary fluid mixtures are conducted on the MareNostrum supercomputer, which is a valuable infrastructure in these kind of studies.

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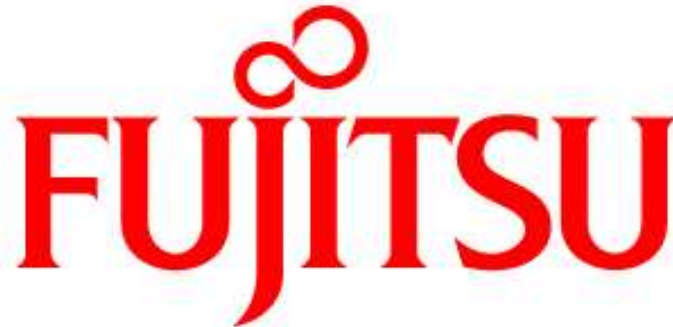
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