



RED ESPAÑOLA DE SUPERCOMPUTACIÓN

HPC resources of the Spanish Supercomputing Network for the scientific community

Barcelona Supercomputing Center Centro Nacional de Supercomputación

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Spanish Supercomputing Network (RES)



Updated: September 2020



RED ESPAÑOLA DE SUPERCOMPUTACIÓN

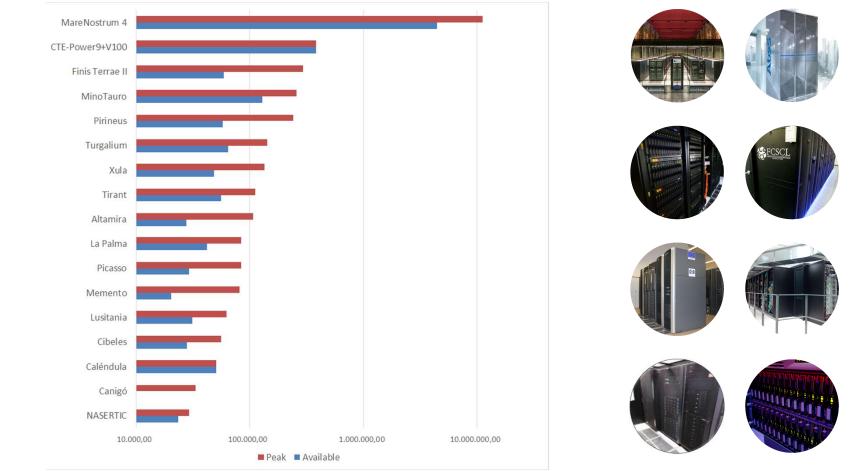
- Spanish national reference for HPC, providing HPC and data services to the international scientific community
- Networking of HPC users
- Education and training in HPC for new and expert users
- Internationalization: EU strategy and international projects
- Dissemination of HPC towards society and SME
 - Emerging Scientific Big Data Network





RES: HPC Services for Spain

RES is made up of **17 interconnected supercomputers**.



Access to internationalization Programs, projects, etc



Access to knowledge and expertise **Scientific seminars**



Access to training and skills development Open training courses and technical workshops





Supercomputing Centro Nacional de Supercomputación



RED ESPAÑOLA DE SUPERCOMPUTACIÓN



Access to Spanish supercomputing & data facilities Free allocation of computing hours to researchers and industry staff



Access to European supercomputing facilities **Mobility of researchers** and industry staff



Access to <u>networking</u> and awareness **Annual Users Conference, RES Newsletter**



Access to business innovation **Competence center DIH**, One-stop shop **EuroHPC**

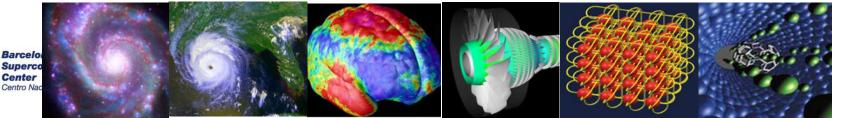




Scientific areas

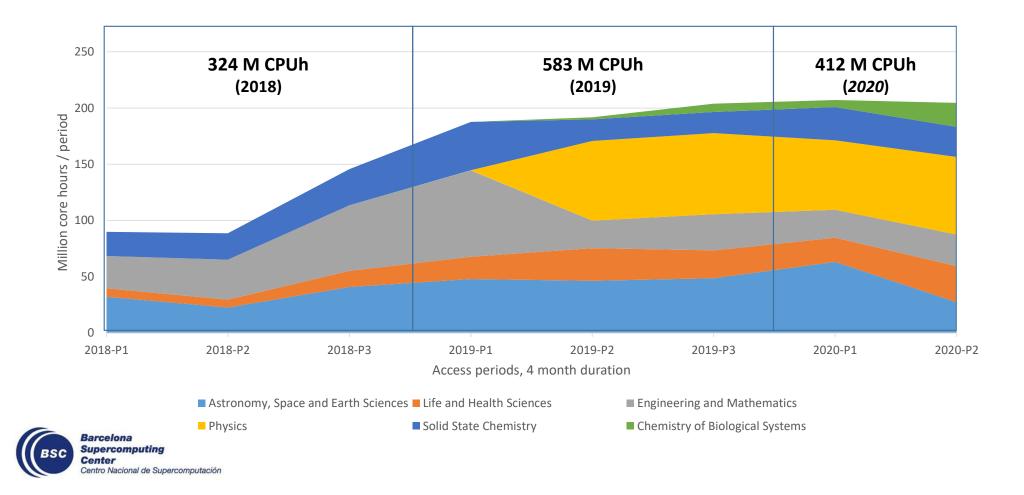
- Astronomy, Space and Earth Sciences (AECT)
- Physics (FI)
- Mathematics and Engineering (MI)
- Life and Health Sciences (BCV)
- Homogeneous Chemistry (QH)
- Heterogeneous Chemistry and Solids (QHS)







RES: HPC services provided





RES users have published +180 articles in scientific journals in 2020

https://www.res.es/es/investigacion/publicaciones

2020

Matemáticas, Física e Ingeniería On the onset of negative lift in a symmetric airfoil at very small angles of attack PHYSICS OF FLUIDS Aguilar-Cabello, J., P. Gutierrez-Castillo, L. Parras, C. del Pino, y E. Sanmiguel-Rojas

Química y Ciencia y Tecnología de los Materiales Neutral Organic Radical Formation by Chemisorption on Metal Surfaces JOURNAL OF PHYSICAL CHEMISTRY LETTERS Ajayakumar, M. R., C. Moreno, I. Alcon, F. Illas, C. Rovira, J. Veciana, S. T. Bromley, A. Mugarza, y M. Mas-Torrent

Astronomía, Espacio y Ciencias de la Tierra

The Three Hundred Project: Correcting for the hydrostatic-equilibrium mass bias in X-ray and SZ surveys ASTRONOMY & ASTROPHYSICS Ansarifard, S., E. Rasia, V. Biffi, S. Borgani, W. Cui, M. De Petris, K. Dolag, S. Ettori, S. M. S. Movahed, G. Murante, y G. Yepes

Astronomía, Espacio y Ciencias de la Tierra

Precipitation Features of the Maritime Continent in Parameterized and Explicit Convection Models JOURNAL OF CLIMATE Argueso, D., R. Romero, y V. Homar

Química y Ciencia y Tecnología de los Materiales

Three-dimensional effects on the aerodynamic performance of flapping wings in tandem configuration Journal of Fluids and Structures Arranz, G., O. Flores, y M. García-Villalba

Matemáticas, Física e Ingeniería A tutorial-driven introduction to the parallel finite element library FEMPAR v1.0.0 COMPUTER PHYSICS COMMUNICATIONS Badia, S., y A. F. Martin



Article

Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride

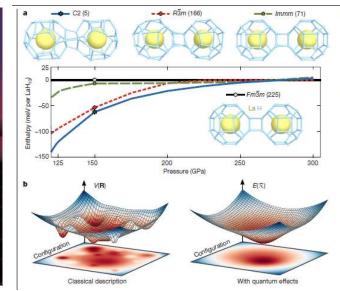
& José A. Flores-Livas4*

https://doi.org/10.1038/s41586-020-1955-z

Received: 24 July 2019

Accepted: 14 November 2019

nature



Ion Errea¹²³, Francesco Belli¹², Lorenzo Monacelli⁴, Antonio Sanna⁵, Takashi Koretsune⁶,

Terumasa Tadano⁷, Raffaello Bianco², Matteo Calandra⁸, Ryotaro Arita^{9,10}, Francesco Mauri^{4,11}

Fig. 1 Quantum effects stabilize the symmetric Fm3m phase of LaHin. a, Enthalpy as a function of pressure for different structures of LaH10, neglecting zero-point energy in the calculations. Here, pressure is calculated classically from $V(\mathbf{R})$, neglecting quantum effects on V(R). b, Left, a Born-Oppenheimer energy surface V(R), exemplifying the presence of many local minima belonging to distorted structures. R represents the positions of atoms treated classically as simple points. Right, the configurational energy surface $E(\mathcal{R})$, including quantum effects. R represents the quantum centroid positions, which determine the centre of the ionic wave functions-that is, the average atomic positions. By including quantum effects, all phases collapse to a single phase: the highly symmetric Fm3m,

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66 | Nature | Vol 578 | 6 February 2020



Centro Nacional de Supercomputación



Science, 26 June 2020

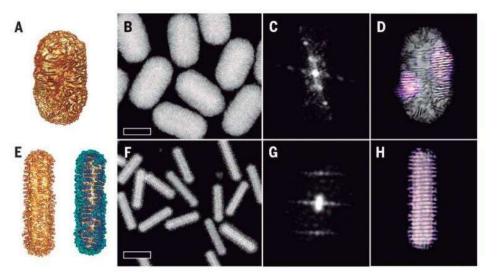
Micelle-directed chiral seeded growth on anisotropic gold nanocrystals

Guillermo González-Rubio^{1,*}, ⁽ⁱ) Jesús Mosquera^{1,*}, ⁽ⁱ) Vished Kumar¹, ⁽ⁱ) Adrián Pedrazo-Tardajos², ⁽ⁱ) Pablo Llombart^{3,4}, ⁽ⁱ) Diego M. Solís⁵, ⁽ⁱ) Ivan Lobato², ⁽ⁱ) Eva G. Noya⁴, ⁽ⁱ) Andrés Guerrero-Martínez³, ⁽ⁱ) José M. Taboada⁶, ⁽ⁱ) Fernando Obelleiro⁷, ⁽ⁱ) Luis G. MacDowell³, ⁽ⁱ) Sara Bals^{2,†}, ⁽ⁱ) Luis M. Liz-Marzán^{1,8,9,†}

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 ³ Departamento de Química Física, Universidad Complutense de Madrid, 28040 Madrid, Spain.
 ⁴ Instituto de Química Física Rocasolano, CSIC, E-28006 Madrid, Spain.
 ⁵ Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA.
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 ** These authors contributed equally to this work.

- Hide authors and affiliations

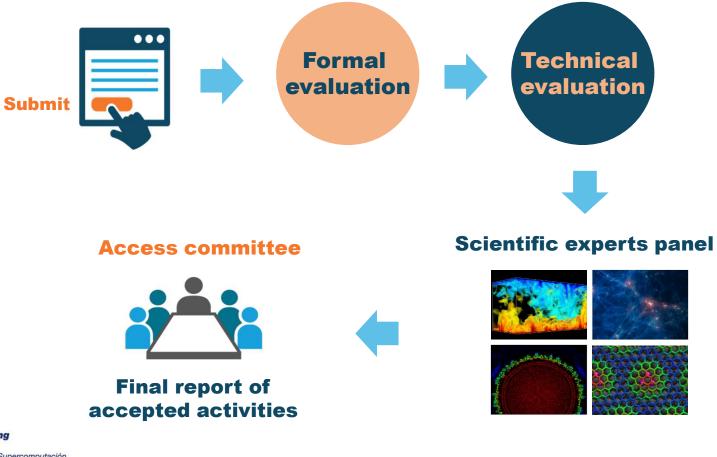
Science 26 Jun 2020: Vol. 368, Issue 6498, pp. 1472-1477



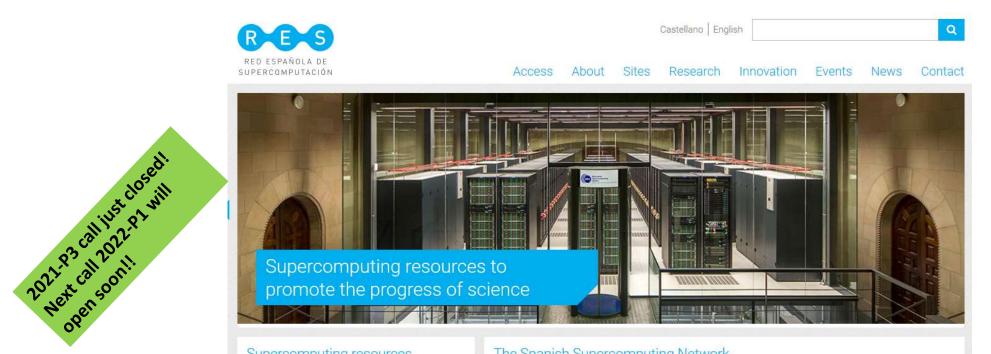




Application process: Proposal evaluation



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Supercomputing resources

Would you like to take advantage of RES resources? Click below to get more information about the application procedure.

Access our resources

If you are a RES user, access the intranet.

Barcelona Supercomputing Center

Centro Nacional de Supercomputación

The Spanish Supercomputing Network

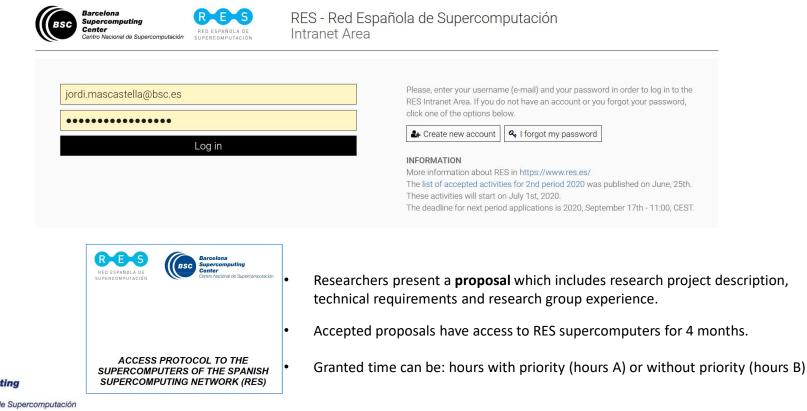
The Spanish Supercomputing Network (RES) is a distributed infrastructure involving the interconnexion of 12 supercomputers which work together to offer High Performance Computing resources to the scientific community. It is coordinated by the Barcelona Supercomputing Center (BSC).

The RES is a Unique Scientific and Technical Infrastructure (ICTS) distributed throughout Spain, which aims to support the development of top-quality cutting-edge research.

Read more

How to apply?

RES intranet: https://www.bsc.es/res-intranet

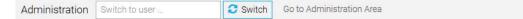






RES - Red Española de Supercomputación Intranet Area

Marketing Reviews Reviews Admin Resources Admin RES Users Committee External links 🗸 Jordi Mas 🗸



Original user: jordi.mascastella@bsc.es

Home > New Application

New Application

New activity application for period 2020-2 (2020, July 1st - 2020, October 31st)

Before applying ...

The deadline for next period applications is 12/05/2020 11:00:00, CEST.

Dear user,

Each application to the RES is expected to be destined to perform an activity (a term that can be understood as one experiment or several) and not for long term projects. The RES understands that one project can include more than one activity. Considering that, an applicant can submit more than one application for different activities framed in a same global project.

For activities whose computing needs require access to resources during more than a period to be properly developed, applicants can request access for up to two periods (a first period as new application and a second period as continuation activity). The request for a continuation will be evaluated and the applicants will have to report to the Access Committee the results obtained during the first period. For more information click here.

If you need help or any clarification, please contact us in applications@bsc.es.

Thanks for your cooperation, Spanish Supercomputing Network.

9 Before applying, read the Access Protocol to the equipment of the Barcelona Supercomputing Center and the Spanish Supercomputing Network (RES) document.



+ Create new application



RES - Red Española de Supercomputación Intranet Area

New Application

New activity application for period 2020-3 (2020, November 1st - 2021, February 28th)

1. COVID-19

A In accordance with the RD8/2020 of extraordinary urgent measures to face the economic and social impact of COVID-19, which establishes measures to support research on COVID-19 as a priority objective of the Government, promoting research on the disease for the development of effective drugs and vaccines that help contain the impact of future outbreaks, the RES Council propose to temporarily include in the access protocol he following criteria:

- for activities related to COVID-19. The researcher must mark it in the web application and it will be validated the corresponding scientific panel

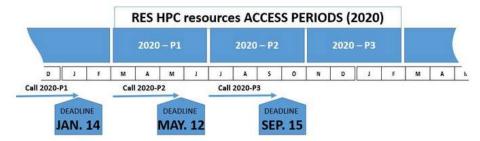
- for the call that ends on May 12, and which gives access from July to October 2020, both included
- for activities led or with confirmed participation of researchers located in Spain
- for activities that exceed a minimum quality threshold

they will have priority, up to 50% of the capacity of the RES in this period.

Is this activity related to COVID-19?

Select an option

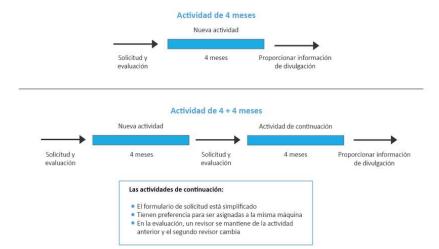




Las solicitudes recibidas son evaluadas cada 4 meses. El calendario anual de convocatorias es:

Periodo	Plazo para presentación de solicitudes	Fecha de inicio de las actividades
P1	Enero (confirmar fecha)	1 de marzo
P2	Mayo (confirmar fecha)	1 de julio
P3	Septiembre (confirmar fecha)	1 de noviembre

La duración de las actividades está limitada a un periodo de 4 meses. Las actividades que requieran acceso a los recursos durante más tiempo pueden solicitar una **actividad de continuación**, con la obligación de informar sobre los resultados intermedios al Comité de Acceso.



When to apply?





RES @RES_HPC · 24 nov.

NEW!! The first call for RES Data Projects is now open! This call will be accepting proposals requiring to store, share, publish and connect large data sets with computing and data services for exploitation services. More info: res.es/en/access-to-r... #ICTSNews #data #HPC

ARCHIVAL RESOURCES

Which resources are available?

Researchers can request to store, share, publish, or connect large data sets with data and/or computing services on all the RES's nodes. The data storage services and the services necessary for their exploitation constitute a data project for the RES, and for which the RES offers infrastructure and support.

Who can request access to the RES?

Scientific groups with the need to store large volumes of data associated with their exploitation services can respond to the call.

How can resources be requested?

Data storage is granted through competitive access calls. The first call for data projects will open once the terms of the call are approved by the Council and will remain open for a minimum period of 2 months. Successive calls will be opened each year in November.

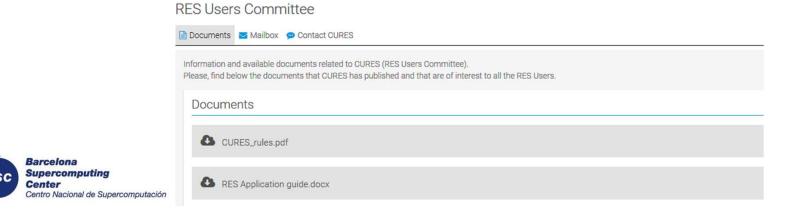
To participate in the RES calls, each data project must present its own data management plan (DMP) according to the template published in the call, which will be subject to peer evaluation for its approval. An internal access committee will carry out the evaluation made up of technicians, managers, and scientists to evaluate each project presented. The information required for the DMP can be consulted in this document RES Application Guide for archival resources. The terms of the first call for the RES data project can be found in the document "Call for Data Projects."

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RES resources are awarded according to criteria of excellence and impact of the research activity and are free for all research groups. For more information, see the RES Frequently Asked Questions (FAQ) for applicants and users.

RES Users' Committee

- CURES aims to provide advice and feedback to RES coordinators:
 - Promotes optimal use of high performance computing facilities
 - Shares information about users' experiences
 - Voices user concerns
- You can **contact CURES** through RES intranet:



Users satisfaction survey 2017-18



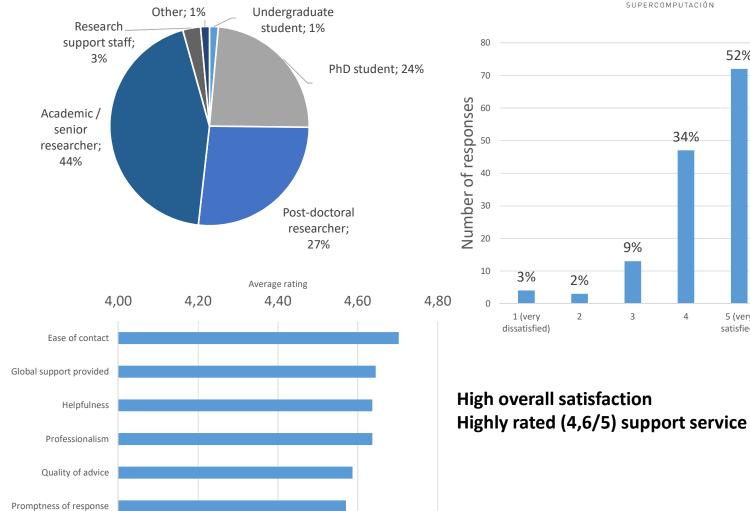
34%

4

52%

5 (very

satisfied)







RES events: networking & training opportunities (Around 1.000 attendees reached)

GR 22

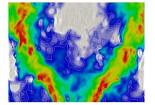


RES Users' Conference

Networking, scientific & technical lectures, poster sessions, users' committee meeting, training workshops, social activities, etc.

RES RED ESPAÑOLA DE SUPERCOMPUTACIÓN **14th USERS CONFERENCE** 16 - 17 September 2020







Scientific seminars supported





Technical training sessions organized





RES events: networking opportunities

The agenda includes:

- Information about RES and the European HPC ecosystem
- Plenary sessions
- Parallel scientific & technical sessions
- RES Award Best scientific paper



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REGISTRATION STILL OPEN!! AT: https://www.res.es/es/eventos/15th-users-conference

15th USERS CONFERENCE 🖋



Users meeting - 16 SEP 2021 - ONLINE

The 15th USERS CONFERENCE brings together supercomputing users to share knowledge and experience in the use of HPC.

The Spanish Supercomputing Network (RES) organises the **Annual RES Users Conference** to inform about RES news and to provide information of interest about access to its resources and about the European HPC ecosystem. This event is a meeting place for all users, support technicians, the access committee and the users committee. The duration of the conference will be 2 days, starting on Thursday 16 September, with plenary sessions and technical and scientific conferences by leading supercomputing specialists. The second day, Friday 17th September, will continue with sessions

focused on scientific and technical topics within the HPC world and will end with an awards ceremony for the most relevant contribution in the HPC area.

PROGRAM & ABSTRACTS BOOK, you can download the document here.

3rd EDITION OF <u>RES AWARDS (call closed!)</u>: Once again, the RES Award for the best scientific article using RES resources will be announced. More information on the call can be found at the following link. Users can submit their proposal while resgistering for the conference.

To receive news about the 15th USERS CONFERENCE, subscribe to our newsletter. You can also check our Twitter profile: @RES_HPC

Sponsors







RES events: networking opportunities

Scientific seminars

The RES promotes and sponsors scientific meetings which address supercomputing technology applications in specific scientific areas.



Upcoming events

www.res.es/en/events



New Trends in Computational Chemistry – 2021 Scientific seminar - 09 SEP 2021 -The emergence of data sciences in atomistic modelling



Fusion HPC Workshop Comparison Compariso

2nd Fusion HPC Workshop Scientific seminar - 02 DEC 2021 - Barcelona / Online The 2nd Fusion HPC Workshop covers all computer applications using High Performance Supercomputing (HPC) in the field of fusion research.



These workshops are organized by the RES nodes and aim at providing the knowledge and skills needed to use and manage the supercomputing facilities.

- Check the agenda in RES website: <u>https://www.res.es/en/events?event_type=technical_training</u>
- **PATC courses in BSC** (PRACE Advanced Training Center): <u>https://www.bsc.es/education/training/patc-courses</u>





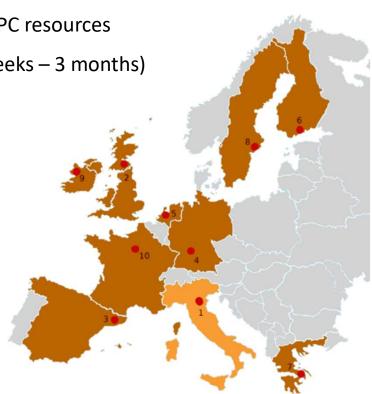
Funded by the EC: 2017 - 2021



- ✓ Mobility grants for researchers using HPC resources
- ✓ Short stays to visit scientific hosts (3 weeks 3 months)
- ✓ Funds for travel and living allowance
- ✓ Access to European HPC facilities











HPCEuropa3 @HPCEuropa3 · 14 may.
New call open! Apply by 9/9/21.
Programme ends 30/4/22
◆ Use world-class #HPC systems
◆ Collaborate with host researcher in your field
◆ Get HPC technical support
◆ Plus travel & living expenses

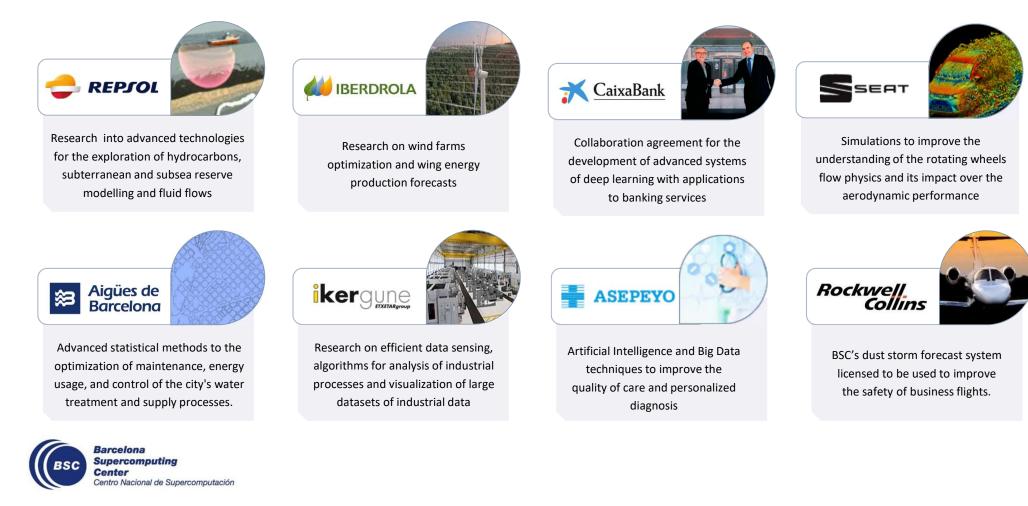
@BSC_CNS @Cineca1969 @CSCfi @EPCCed @grnet_gr @HLRS_HPC @ichec @SURF_onderzoek

Read more

1.1

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Collaborations with Industry



RES as National HPC Competence Centre





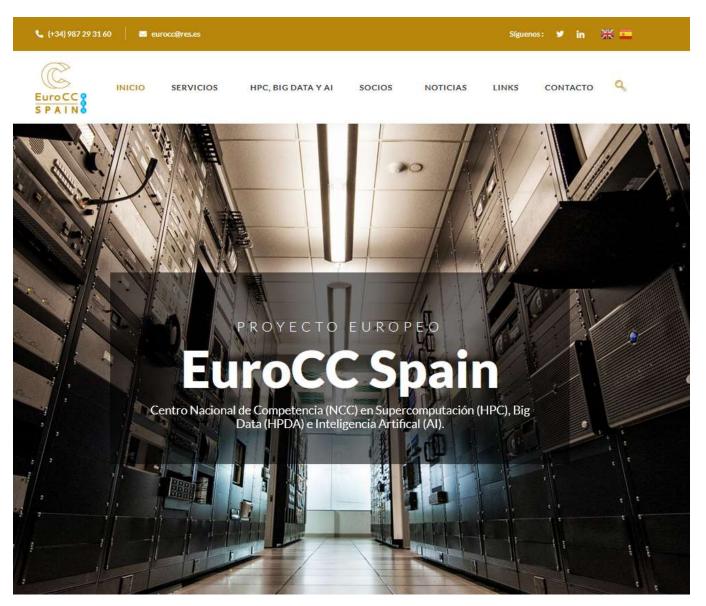












https://eurocc-spain.res.es/





OBJECTIVES:

Make companies aware of the National Center for Supercomputing Competencies , as well as national strengths in highperformance computing (HPC), supercomputing, as well as High Performance Data Analysis (HPDA) and Artificial Intelligence capabilities. (AI) to increase the usability of these technologies in national companies.

SCHEDULE

- 10:00-10:05 Welcome. SCAYLE, Castilla y León Supercomputing. 10:05-10:15 Presentation of the National Center for Supercomputing Competencies. BSC-CNS, National Supercomputing Center.
- Round table . The map of competences in HPC, IA, Big Data in Spain. 10: 15-10: 35 -BIFI, Institute of Biocomputation and Complex Systems. Mr. Alfredo Ferrer Marco, Technical and research staff hired . -COMPUTAEX-CénitS, Extremadura Computing and Advanced Technologies Foundation. D. Javier Corral



Centro Nacional de Supercomputación

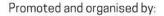
Innovation Journey 2021



Innovation Journey is a workshop series that aims to promote collaboration between research personnel in need of entrepreneurship management skills; and industry and SME professionals searching for new ventures in the field of High-Performance Computing, Big Data and Al.

The goal is to accompany researchers as they make their first contact with the private sector and to foster the use of HPC technologies in industry and SME initiatives.

The seven-session program will offer business training through interactive workshops and an approach to the implementation of practical solutions in the market, as well as mentoring and guidance by entrepreneurs, which will be established through a rigorous curriculum.







This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 951732. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Germany, Bulgaria, Austria, Croatia, Cyprus, the Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, the United Kingdom, France, the Netherlands, Belgium, Luxembourg, Slovakia, Norway, Switzerland, Turkey, Republic of North Macedonia, Iceland, Montenegro



EUROCC SPAIN RES & THE BSC-CNS PRESENT: INNOVATION JOURNEY Find your inner entrepreneur

OCT 1ST - NOV 12TH 2021

ARE YOU A RESEARCHER WITH A LOT OF POTENTIAL?

We are sure you are.

In fact, you are probably aware of that too. And you might have started thinking: what if all my potential could be further developed in the **private sector?**



LEARNING BY DOING A methodology that works

The Innovation Journey is a **success** story: 3 companies emerged after participating in the last edition*. This year, you will also be able to **collaborate** with **companies** that will bring their expertise to assist you on your way to the private sector.

**10/10 participants in last edition, assured they would recommend the programme to their colleagues

YOU HAVE THE SCIENTIFIC POTENTIAL Let yourself discover your inner entrepreneur

The Innovation Journey will take place during **7 full-day sessions** in seven consecutive weeks. It will combine a **theoretical** and **practical** "learning by doing" methodology, which will approach **actual enterprises and businesses**.

It will take off on October 1st.

Follow us for info updates!

*** RES @RES_HPC - 28 ene.

DO NOT MISS! The 11th call for applications is OPEN until 20th February 2020. @HPCEuropa3 @BSC_CNS access to Europe's biggest Supercomputers #HPC + mobility program (travel grants, etc.)



RES @RES_HPC · 7 feb. 000

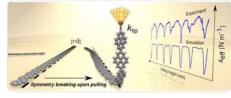
El 12-13 de febrero nos encontrarás en #Transfiere2020 #ICTSNews y empieza ya tu camino hacia la innovación en colaboración con una infraestructura científica y técnica singular (ICTS)



RES Newsletter 🖋

RES @RES_HPC · 20 feb. 000 #HPC boosts research production in 2020. The first 10 papers of this year using @RES_HPC resources: res.es/es/investigaci... (9)Pawlak et al. measured

the force-induced changes at the single-monomer level in polymers bending and twisting around carbon-carbon single bonds #ICTSNews



tl Retwitteaste



CénitS - COMPUTAEX @cenits · 21 feb. Cenits - COMPUTARA BECHIG - CTICA. El nuevo Supercomputador de Extremadura, #LUSITANIAIII, ya se encuentra en funcionamiento. CénitS alcanza así una capacidad de cálculo de 93 TFlops más 120 TFlops de computación gráfica, sobre red Infiniband de hasta 100 Gbps, y un total de 3.696 cores y 40.960 cuda cores.







NEWSLETTER December 2019



Newsletter Diciembre 2019

Entrevista a Alfonso Tarancón, I Premio RES RES Newsletter entrevista a Alfonso Tarancón. Lee la entrevista en el

Alfonso Tarancón (UNIZAR, BIFI) es galardonado con

La Red Española de Supercomputación (RES) concedió, el pasado 18 de septiembre, el I PREMIO RES 2019 a la trayectoria científica en el ámbito de la supercomputación al catedrático de la Universidad de Zaragoza

Alfonso Tarancón, quien recibió el galardón de manos del Subdirector General de Grandes Instalaciones Científicas y Técnicas. José Ignacio

enlace.

Esta última edición del año recoge las noticias ocurridas recientemente, las convocatorias previstas, así como plantea los proyectos y eventos de futuro para el año 2020. News

el I PREMIO RES



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THANK YOU!





