

# Barcelona Supercomputing Center – Centro Nacional de Supercomputación

## Resolución Comité de Acceso, Asignación de Horas de Supercomputación para la Red Española de Supercomputación (RES) 2o período 2025

Barcelona, Junio 2025

## 1. Introducción

El Comité de Acceso del Barcelona Supercomputing Center – Centro Nacional de Supercomputación (BSC-CNS) es un órgano asesor del Director que informará sobre las peticiones de acceso recibidas de investigadores y grupos de investigación. El Comité propondrá al Director, en base a la calidad científica y técnica de las peticiones recibidas, una lista razonada y priorizada de las solicitudes. Corresponde al Director la decisión sobre los accesos autorizados.

El acceso es conjunto para los equipos de la Red Española de Supercomputación (RES), e incluye MareNostrum. La asignación entre los diferentes equipos se hace con motivos de necesidad y eficiencia de las actividades.

El protocolo de acceso aprobado por la Comisión Ejecutiva del BSC-CNS está publicado en la página de web del BSC, <http://www.bsc.es/RES>

## 2. Análisis

La RES ha asignado este período 768 millones de horas de CPU (140M de horas de nodo, 4.25M exaflop), que se obtienen sumando el acceso concedido en las diferentes arquitecturas, incluyendo con prioridad y sin prioridad. Esto incluye los sistemas instalados en Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS), Instituto Astrofísico de Canarias (IAC), Universidad de Cantabria (UC), Universidad de Málaga (UMA), Universidad de Valencia (UV), Universidad de Zaragoza (UZ), Fundación Pública Galega Centro Tecnológico de Supercomputación de Galicia (CESGA), Consorci de Serveis Universitaris de Catalunya (CSUC), CénitS-COMPUTAEX (CENITS), Fundación del Centro de Supercomputación de Castilla y León (SCAYLE), Universidad Autónoma de Madrid (UAM), Navarra de Servicios y Tecnologías (NASERTIC), y Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT). Algunos de los nodos en este periodo no han recibido ningún proyecto, al estar en fase de instalación de nuevas infraestructuras.

Todas las actividades han sido evaluadas por los paneles de expertos, clasificando las solicitudes según si eran excelentes, muy buenas y buenas. Adicionalmente, se han tomado en consideración los criterios de evaluación descritos en la sección [Comentarios sobre la evaluación](#). Con las actividades excelentes de mayor prioridad, se cubre el uso completo de las máquinas de la RES **para el próximo período de 5 meses**. Algunas actividades calificadas como excelentes no han podido recibir recursos por la gran cantidad de demanda recibida, y sólo han podido recibir horas sin prioridad.

A la mayoría de actividades que han obtenido recursos, se han asignado acceso a los equipos de la RES con utilización preferente. El resto de actividades que han obtenido recursos, es con utilización no preferente (es decir, utilizando el equipo cuando este no sea usado por las actividades preferentes, con lo que no se puede garantizar que puedan usar todo el acceso asignado). Las actividades no concedidas recibirán un e-mail indicando que no ha sido posible concederles acceso a las máquinas en esta convocatoria. Se anima a todos los solicitantes a presentar solicitud de acceso para la siguiente convocatoria, que iniciará la evaluación el próximo mes de Septiembre de 2025.

**Por primera vez, se ha distribuido también acceso a las tecnologías cuánticas de la RES en BSC-CNS, CESGA y SCAYLE, financiadas por el proyecto QuantumSpain.**

Para mejorar como se comparten los recursos asignados entre las diferentes actividades, y evitar así las concentraciones de uso de máquinas en determinados periodos de tiempos, se requiere la utilización proporcional de los recursos asignados. Así, si una actividad no utiliza la parte proporcional asignada en un periodo determinado, quedará reducida la asignación total de forma proporcional. Por ejemplo, si de una asignación de 400.000 horas en cuatro meses, no utiliza cerca de 100 mil horas el primer mes, su asignación para el periodo completo será reducida a 300.000. De la misma forma, se reducirá la prioridad de acceso a las actividades que sobrepasen su asignación proporcional en cada periodo de tiempo. Por ejemplo, si de una asignación de 400.000 horas en cuatro meses, se utiliza cerca de 200.000 horas el primer mes, se irá reduciendo la prioridad de los diferentes trabajos en el sistema para que la prioridad regularice el consumo. Así mismo, las horas no consumidas en el período no se pueden acumular para próximas convocatorias.

La utilización se medirá según "*elapsed time*", considerando la utilización por el número de procesadores y núcleos asignados. Por ejemplo, si se debe asignar el uso en exclusiva de un nodo (que tiene varios núcleos, dependiendo de la máquina) durante 1 hora, se considerará el uso de 48, 24, 16, 8, 4 o 2 horas, dependiendo de la máquina.

### 3. Comentarios sobre la evaluación

El Comité de Acceso del BSC-CNS ha seguido los siguientes criterios para la evaluación de las actividades:

#### 1. Reglas generales

- a. La relevancia del proyecto científico en que se enmarca la actividad propuesta (20 %)
- b. La justificación de la actividad propuesta y de los cálculos a realizar en la RES para la consecución del proyecto científico global (30 %)
- c. La calidad científica del grupo solicitante (10%)
- d. La experiencia y capacitación en el cálculo de alto rendimiento (10 %)
- e. La necesidad real de supercomputación para realizar el cálculo (20 %)

f. La adecuación técnica del proyecto a la arquitectura de los recursos de la RES (10 %)

2. Evaluación de los resultados presentados por las actividades de continuación

a. Publicaciones presentadas como resultado del acceso de actividades anteriores

b. Resultados técnicos obtenidos en los periodos anteriores

3. Utilización adecuada y completa de los recursos asignados en los periodos anteriores

4. Participación de grupos españoles en las actividades solicitadas

5. Actividad específica dentro de un proyecto de investigación. El acceso a los recursos de la RES corresponde a actividades específicas dentro de un proyecto de investigación, y no corresponden a agrupaciones de diferentes actividades de investigadores de comunidades virtuales.

6. Seguir adecuadamente las obligaciones adquiridas en la utilización de MareNostrum y los otros recursos de la RES

a. Envío a la RES de copia electrónica de las publicaciones científicas en las cuales el uso de los recursos de la RES ha resultado determinante.

b. Mencionar explícitamente en las publicaciones científicas la ayuda del RES en su proyecto mediante la frase "The author thankfully acknowledges RES resources provided by [centro] in [equipo] to [ID de actividad]"

c. Cumplimiento de las normas de utilización de los recursos de la RES y de las políticas de seguridad y confidencialidad determinados por la RES.

d. No hacer negocio con los resultados obtenidos en los recursos de la RES bajo el formato "Investigación Pública"

e. Proporcionar anualmente información y documentación, como vídeos, presentaciones, y cualquier otro material, para ser utilizado como material divulgativo de la RES.

7. Dada la alta competencia por recursos y la cantidad total disponible de estos, se recuerda a los proyectos que necesitan grandes volúmenes de recursos, que la infraestructura europea EuroHPC ([https://eurohpc-ju.europa.eu/participate/access-our-supercomputers\\_en](https://eurohpc-ju.europa.eu/participate/access-our-supercomputers_en)) ofrece proyectos de cómputo a partir de 30 millones de horas de CPU anuales, disponiendo de cinco convocatorias anuales para propuestas (Regular Access y Extreme Scale Access).

## 4. Consideraciones adicionales

### 4.1. Actividades industriales

Cualquier actividad industrial está sujeta a las mismas condiciones de calidad que las actividades de investigación pública. Todos los usuarios con actividades industriales, y con acceso a las máquinas de la RES deben pagar por el acceso a los recursos siempre que las actividades no sean incluyan en el concepto de Open R&D. El precio se calcula para cada una de las actividades que lo indiquen, teniendo en cuenta los recursos solicitados (humanos y técnicos) y el interés científico/económico de la actividad.

### 4.2. Política de uso de disco

En la actual resolución, se ha realizado asignación no sólo de tiempo de CPU, sino también de espacio de almacenamiento. Se ha tenido en cuenta el espacio solicitado, así como el espacio disponible y la eficiencia en la utilización de los recursos.

Para cada actividad, se ha asignado capacidad en dos espacios diferentes:

- Projects: para tener almacenados los resultados de las simulaciones que se necesitan durante todo el periodo de asignación
- Scratch: espacio necesario para realizar las simulaciones en cada momento. Se debe considerar que este es un espacio de disco que se debe liberar 7 días después de haber finalizado la simulación que lo ha producido

### 4.3. Paralelismo compulsivo

Para mejorar la eficiencia de los sistemas, es necesario que todas las actividades que han planteado simulación que requieren paralelismo compulsivo (muchas ejecuciones del mismo programa, con variación de los datos de entrada), utilicen la herramienta COMPSs (<https://www.bsc.es/research-and-development/software-and-apps/software-list/comp-superscalar>). El envío de trabajos secuenciales al sistema se limitará.

El equipo de soporte del BSC-CNS ofrecerá la ayuda necesaria para portar los códigos a esta tecnología. Se debe contactar con [support@bsc.es](mailto:support@bsc.es).

## 5. Listados y asignaciones

A continuación, se incluye la lista de las actividades que tendrán acceso a los diferentes nodos de la RES, con las asignaciones en miles de horas, y las capacidades en Gigabytes de los diferentes sistemas de ficheros. Las actividades asignadas se indican en miles de horas correspondientes a cada máquina (se ha considerado un rendimiento a la baja en cada máquina, de forma que el número de horas asignadas se corresponde en la mayoría de los casos con el correspondiente de las horas solicitadas). En el caso de nodos con mas de una máquina, se indica también la máquina específica asignada.

Lista de actividades aceptadas con acceso estándar.

| Líder                           | Título                                                                                                                                               | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|---------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Aaron Call Barreiro             | Extreme-data processing platforms to analyze the interaction of genomic variants and their association to common diseases                            | 800           |               | 200      | 200     | BSC/MN5-ACC  |
|                                 |                                                                                                                                                      | 4.000         |               | 200      | 200     | BSC/MN5-GPP  |
| Adeline de Villardi de Montlaur | Investigation on wall-modeled large-eddy simulations of sheared daytime atmospheric boundary layers over rough surfaces for wind-energy applications | 3.551,52      |               | 1.500    | 4.400   | BSC/MN5-GPP  |

| Líder                 | Título                                                                                                                                         | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Aitor Gonzalez-Agirre | Exploring techniques to efficiently transition from dense Large Language Models into Mixture-of-Experts architectures for enhanced performance | 4.211            |                  | 10.000   | 10.000  | BSC/MN5-ACC  |
| Aitor Gonzalez-Agirre | Iberian-Edu: Educational data detection and synthesis from large corpora for LLMs                                                              | 9.577            |                  | 10.000   | 10.000  | BSC/MN5-ACC  |
| Alba Cervera-Lierta   | Testing real quantum computer on healthcare challenges                                                                                         | 0,05             |                  | 4.000    | 4.000   | BSC/MN-ONA   |
|                       |                                                                                                                                                |                  | 10               | 4.000    | 4.000   | BSC/MN5-GPP  |
| Albert Civit Bertran  | 3D Non-linear non-adiabatic MHD simulations of 3D stellarators and tokamaks                                                                    | 972,16           |                  | 1.500    | 20.000  | BSC/MN5-GPP  |
| Albert Elias López    | 3D MHD dynamo in Hot Jupiters at different orbital distances                                                                                   | 3.041            |                  | 100      | 2.000   | BSC/MN5-GPP  |
| Albert Poater         | The role of entropy towards latent olefin metathesis catalysts                                                                                 | 1.935,36         |                  | 600      | 600     | CSUC/PIR3    |
| Albert Poater         | Tuning Rh/C?N? Reactivity in Hydroformylation through Boron and Phosphorus Doping                                                              | 1.364            |                  | 500      | 500     | BSC/MN5-GPP  |
| Albert Poater         | Electroreduction of CO2 on single-atom 2D materials                                                                                            | 1.092,27         |                  | 900      | 1.000   | BSC/MN5-GPP  |

| Líder                            | Título                                                                                               | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|----------------------------------|------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Albert Rimola                    | Amino Acid Formation on Space-Bound Silicates in Circumstellar and early-Earth Environments          | 2.000         |               | 500      | 1.000   | BSC/MN5-GPP  |
| Albert Rimola Gibert             | Non-diffusive Formation of iCOMs on Interstellar Water Ice Mantles: A Computational Approach         | 2.000         |               | 200      | 300     | BSC/MN5-GPP  |
| Alberto Fraile García            | Stability and structural properties of Aluminum oxides; Atomistic point of view.                     | 1.000         |               | 20       | 4       | CESGA/FT3    |
| Alberto Fraile García            | Ag-Pt nanoparticles; Structural properties as revealed by molecular dynamics simulations.            | 772           | 228           | 40       | 40      | CESGA/FT3    |
| Alejandra Renee Pillado Gonzalez | Calibration and validation of state-of-the-art neutron star black hole gravitational waveform models | 4.000         |               | 300      | 10.000  | BSC/MN5-GPP  |
| Alejandro Bermúdez               | Quantum characterisation for Error Correction and Mitigation                                         | 0,04          |               | 256      | 256     | BSC/MN-ONA   |
| Alejandro Bermúdez               | Quantum characterisation for Error Correction and Mitigation                                         |               | 10            | 256      | 256     | BSC/MN5-GPP  |
| Alejandro Molina Sánchez         | Spin waves in two-dimensional magnetic materials using ab initio methods                             | 2.000         |               | 4.000    | 8.000   | UZ           |

| Líder                     | Título                                                                                                    | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|---------------------------|-----------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Alejandro Pozas Kerstjens | LOQAL: Localization of joint quantum measurements on spatially separated qubits                           | 0,03          |               | 256      | 256     | CESGA/FT-QMIO-QPU |
|                           |                                                                                                           | 0,03          |               | 256      | 256     | BSC/MN-ONA        |
|                           |                                                                                                           |               | 10            | 256      | 256     | CESGA/FT-QMIO-cpu |
|                           |                                                                                                           |               | 10            | 256      | 256     | BSC/MN5-GPP       |
| Alejandro Pozas Kerstjens | HACK-Q: row Hammer AttaCKs on Quantum computers                                                           | 0,03          |               | 256      | 256     | CESGA/FT-QMIO-QPU |
|                           |                                                                                                           |               | 10            | 256      | 256     | CESGA/FT-QMIO-cpu |
|                           |                                                                                                           | 0,03          |               | 256      | 256     | BSC/MN-ONA        |
| Aleksander Bach Lorentzen | Ab-initio simulation of time-dependent phenomena in THz driven scanning tunneling microscopes.            | 1.121,80      |               | 3.000    | 6.000   | CIEMAT/XULA       |
| Alex Vano-Vinuales        | Far-field infrastructure study for improving binary and strong field numerical relativity simulations     | 500           |               | 1.200    | 7.000   | BSC/MN5-ACC       |
|                           |                                                                                                           | 1.500         |               | 1.500    | 7.000   | BSC/MN5-GPP       |
| Alexis Molina             | PRISM: Federated Decoupled Pretraining of Protein Language Models Across Heterogeneous Biological Corpora | 3.000         |               | 15.000   | 4.000   | BSC/MN5-ACC       |
| Alexis Molina             | chaRNAbert2: Scaling RNA Language Models                                                                  | 1.500         |               | 15.000   | 25.000  | BSC/MN5-ACC       |

| Líder                  | Título                                                                                                                                                                | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Alfonso Valencia       | DARE co-design activity -- PhysiBoSS mini-apps benchmarking and full-organ virtual twin simulations                                                                   | 25            |               | 1        | 1       | BSC/MN5-ACC  |
|                        |                                                                                                                                                                       | 8.000         |               | 40.000   | 40.000  | BSC/MN5-GPP  |
| Alice-Agnes Gabriel    | CyberShake for ground-motion simulations and seismic-hazard assessment as a service installation of the Geo-Inquire project                                           |               | 400           | 1.000    | 1.500   | BSC/MN5-GPP  |
| Alicia Palacios        | Attosecond metrology exploiting new waveforms in intense HHG pulses and Free Electron Lasers                                                                          |               | 497           | 300      | 6.000   | BSC/MN5-GPP  |
|                        |                                                                                                                                                                       | 0,01          |               | 200      | 500     | BSC/MN-ONA   |
| Anders Kvellestad      | GAMBIT                                                                                                                                                                | 10.000        |               | 250      | 20.000  | BSC/MN5-GPP  |
| Andoni Zozaya Ursuegui | Verification that, over a field of characteristic 2, two random traceless 4×4 matrices generate an algebra isomorphic to the subalgebra of all traceless 3×3 matrices | 0,05          |               | 256      | 256     | BSC/MN-ONA   |
| Andres Pacheco Pages   | Monte Carlo Simulation for the ATLAS Experiment at the CERN LHC at the MareNostrum by IFAE/PIC Tier-1                                                                 | 7.150         |               | 9.000    | 9.000   | BSC/MN5-GPP  |
| Andreu Anglés-Castillo | Implementability of Quantum Imaginary Time Evolution                                                                                                                  | 0,01          |               | 256      | 256     | BSC/MN-ONA   |
| Andreu Anglés-Castillo | Implementability of Quantum Imaginary Time Evolution                                                                                                                  |               | 10            | 256      | 256     | BSC/MN5-GPP  |

| Líder                    | Título                                                                                                                               | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Ángel Morales Garcia     | Excited State Mechanisms in TiO2/MXene Composites: Ab Initio Quantum Dynamics                                                        | 1.083         |               | 500      | 500     | NASERTIC          |
| Anna Heffernan           | High Mass Ratio Compact Binaries                                                                                                     | 4.500         |               | 12.000   | 35.000  | BSC/MN5-GPP       |
| Antera Martel Quintana   | Bioinformatics for Genomic and Biochemistry Studies in cyanobacteria of Spain Bank of Algae (BEA)                                    | 518,40        |               | 5        | 20.000  | UMA               |
| Anthoni Alcaraz Torres   | Electronic properties and adsorption mechanisms of CH4, NO, H2, O3, CO2 and O2 over surfaces of CuSCN, CuNCN and ZnNCN.              | 500           |               | 1.000    | 1.000   | UZ                |
| Antoni Alou Román        | Optimal control of superconducting qubits with machine learning.                                                                     | 0,25          |               | 256      | 256     | BSC/MN-ONA        |
| Antoni Alou Román        | Optimal control of superconducting qubits with machine learning.                                                                     |               | 10            | 256      | 256     | BSC/MN5-GPP       |
| Antoni Ramos-Buades      | Highly accurate equal-mass eccentric precessing-spin binary black hole simulations                                                   | 4.000         |               | 15.200   | 15.200  | UMA               |
| Antonio Falcó Montesinos | An Algebraic Probability based framework for Quantum Computing with Applications in Numerical Analysis and Computational Mathematics | 0,01          |               | 256      | 256     | CESGA/FT-QMIO-QPU |

| Líder                    | Título                                                                                                                               | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|--------------------------|--------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Antonio Falcó Montesinos | An Algebraic Probability based framework for Quantum Computing with Applications in Numerical Analysis and Computational Mathematics |               | 10            | 256      | 256     | CESGA/FT-QMIO-cpu |
| Antonio Falcó Montesinos | An Algebraic Probability based framework for Quantum Computing with Applications in Numerical Analysis and Computational Mathematics | 0,01          |               | 256      | 256     | BSC/MN-ONA        |
| Antonio Falcó Montesinos | An Algebraic Probability based framework for Quantum Computing with Applications in Numerical Analysis and Computational Mathematics |               | 10            | 256      | 256     | BSC/MN5-GPP       |
| Antonio Picon            | Attosecond screening effects in monolayer MoS2                                                                                       | 3.500         |               | 2.000    | 2.000   | UMA               |
| Arghya Bhowmik           | Exploring the Cathode Space for Sodium-Ion Batteries Using Generative Models and GNNs                                                | 7.627         |               | 2.000    | 2.000   | BSC/MN5-GPP       |
| Arnau Riera              | Classical Simulation of Quantum Analog Computation                                                                                   | 7.000         |               | 5.000    | 5.000   | CIEMAT/TURGALIUM  |
| Arnau Rios Huguet        | Quantum computing for nuclear physics & convolutional machine learning applications                                                  | 3             |               | 256      | 256     | BSC/MN5-GPP       |
|                          |                                                                                                                                      | 0,01          |               | 256      | 256     | BSC/MN-ONA        |

| Líder                   | Título                                                                                                              | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-------------------------|---------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Arturo Montejo<br>Ráez  | Training small language models for text retrieval in High Energy Physics                                            | 1,40             |                  | 20       | 500     | NASERTIC     |
| Aurelio Gallardo        | Computational characterization of the on-surface metalation of Carbaporphyrinoid-based quantum molecular polymers.  | 298              |                  | 500      | 300     | UC           |
| Beñat Gurrutxaga-Lerma  | Machine Learning Interatomic Potentials for High Entropy Alloys                                                     | 80               |                  | 1.000    | 1.500   | BSC/MN5-ACC  |
| Beñat Gurrutxaga-Lerma  | Machine Learning Interatomic Potentials for High Entropy Alloys                                                     | 8.848            |                  | 10.000   | 15.000  | BSC/MN5-GPP  |
| Bo Chen                 | Helium Compression Chamber: an in silico tool to investigate benzene nanothread formation mechanisms under pressure | 2.300            |                  | 1.000    | 400     | BSC/MN5-GPP  |
| Borja Aizpurua          | Quantum nanoLLM                                                                                                     |                  | 224              | 600      | 200     | BSC/MN5-GPP  |
|                         |                                                                                                                     | 0,20             |                  | 256      | 256     | BSC/MN-ONA   |
| Bruno Julia             | Quantum Computing for Quantum Many-body physics                                                                     | 0,02             |                  | 60       | 20      | BSC/MN-ONA   |
| Carlos Hernández-García | High harmonic topological spectroscopy at the attosecond timescale                                                  | 150              |                  | 500      |         | BSC/MN5-ACC  |
| Carlos Hernández-García | High harmonic topological spectroscopy at the attosecond timescale                                                  | 1.000            |                  | 500      |         | BSC/MN5-GPP  |

| Líder                  | Título                                                                                                                                           | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Carlos Palenzuela      | Properties of the ejecta in binary neutron star mergers with realistic initial magnetic fields and neutrino radiation transport                  | 500              |                  | 40.000   | 50.000  | BSC/MN5-ACC  |
|                        |                                                                                                                                                  | 9.500            |                  | 80.000   | 120.000 | BSC/MN5-GPP  |
| Carme Rovira           | Modelling protein glycosylation mechanisms                                                                                                       | 464              |                  | 150.000  | 150.000 | BSC/MN5-ACC  |
|                        |                                                                                                                                                  | 7.056            |                  | 150.000  | 150.000 | BSC/MN5-GPP  |
| Carme Rovira           | Modeling the degradation of macroalgae polysaccharides by marine bacteria                                                                        | 504              |                  | 150.000  | 150.000 | BSC/MN5-ACC  |
|                        |                                                                                                                                                  | 7.701            |                  | 150.000  | 150.000 | BSC/MN5-GPP  |
| Carmen Domene          | Role of Membrane Adaptation and Chemical Modifications in the Neutralization Process of MPER HIV-1 Antibodies                                    | 190              |                  | 2.000    | 10.000  | BSC/MN5-ACC  |
| Carmen Sousa           | Ground and Excited state Reactivity for the Water Splitting Reaction in Surface Terminated MXenes                                                | 726              |                  | 1.000    | 1.200   | BSC/MN5-GPP  |
| Celia Pérez Souto      | High-res UTLS simulations to disentangle role and feedbacks on atmospheric structure and composition                                             | 3.024            |                  | 120.000  | 200     | CESGA/FT3    |
| César González Pascual | First-Principles Investigation of Gas Adsorption on Fe <sub>3</sub> O <sub>4</sub> Surfaces for Magnetic Nanoparticle-Based Sensing Applications | 200              |                  | 1.000    | 1.000   | UC           |

| Líder                    | Título                                                                                                                                            | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Claudio Cazorla          | Giant Photocaloric Effects in Low-Dimensional Materials for Solid-State Cooling                                                                   | 3.737            | 560              | 300      | 1.000   | UAM          |
| Coen de Graaf            | Non-orthogonal configuration interaction for self-assembled stacks of perylenediimide molecules                                                   | 967              |                  | 2.000    | 2.000   | BSC/MN5-ACC  |
| Consuelo Guardiola       | Advanced Monte Carlo simulations for the validation of experimental dosimetry in FLASH radiotherapy                                               | 2.000            |                  | 300      | 1.000   | UV           |
| Cristina Díaz Blanco     | Electronic transport in molecular devices built with 2-dimensional electrodes II                                                                  | 3.700            |                  | 1.000    | 1.300   | BSC/MN5-GPP  |
| Cristina España i Bonet  | Development of a Speech-To-Text Translation model based on an end-to-end Speech LLM focused on Iberian Languages                                  | 640              |                  | 5.000    | 5.000   | BSC/MN5-ACC  |
| Cristina España i Bonet  | Languages of Spain (LoS): Development of a Robust ASR Model for the Languages Spoken in Spain Under the Umbrella of the Project ILENIA (NEL-AINA) | 1.200            |                  | 5.000    | 5.000   | BSC/MN5-ACC  |
| Daniel García Figueroa   | Probing New Physics with Gravitational Waves                                                                                                      | 4.460            |                  | 30       | 30      | BSC/MN5-GPP  |
| Daniel Hernangómez Pérez | Efficient modelling of many-body electronic and optical properties of van der Waals heterobilayers                                                | 268              |                  | 32.000   | 32.000  | BSC/MN5-ACC  |

| Líder                    | Título                                                                                                                                        | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina  |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|---------------|
| Daniel Hernangómez Pérez | Efficient modelling of many-body electronic and optical properties of van der Waals heterobilayers                                            | 2.698,90         |                  | 32.000   | 32.000  | BSC/MN5-GPP   |
| Daniel Mira Martinez     | Modelling aerodynamic effect of aircraft wings using body forces and their subsequent effect on dispersion of pollutants from aircraft engine | 6.547,20         |                  | 5.000    | 5.000   | BSC/MN5-GPP   |
| Daniel Muñoz-Santiburcio | Understanding the phase behavior of nanoconfined water with an ab initio hydrostatic pressurizer                                              | 896              |                  | 10.000   | 10.000  | BSC/MN5-GPP   |
| Daniel Muñoz-Santiburcio | Computing the IR spectra of water and the solvated proton and hydroxide from ab initio simulations                                            | 2.055            |                  | 10.000   | 10.000  | UMA           |
| David Dalmau Ginesta     | AI-Guided Design of Selective and Efficient Biocatalysts for Sustainable Chemistry                                                            | 210              |                  | 200      | 500     | CESGA/FT3     |
|                          |                                                                                                                                               | 215              |                  | 500      | 500     | CESGA/FT3-GPU |
| David De Sancho          | Grammar of biomolecular phase separation from model peptides                                                                                  | 240              |                  | 10.000   | 10.000  | BSC/MN5-ACC   |
| David Keitel             | Gravitational-wave lensing candidate follow-ups and improved detection methods                                                                | 1.000            |                  | 2.000    | 5.000   | UMA           |

| Líder                                     | Título                                                                                                                                                    | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| David Torrents Arenales                   | Large scale integrative analysis of genetic, clinical and environmental factor interactions involved in the risk and prevention of 3,872 complex diseases | 2.961,22         |                  | 5.000    | 5.000   | BSC/MN5-GPP  |
| Dorde Dangic                              | Search for ambient pressure hydride perovskite superconductors                                                                                            | 2.000            |                  | 5.000    | 5.000   | UC           |
| Dr Weiguang Cui                           | The300th Project: SIDM and the new Crocodile simulation runs                                                                                              | 9.520            |                  | 100.000  | 100.000 | BSC/MN5-GPP  |
| Dr. Carlos Martí-Gastaldo                 | Tailoring titanium organic frameworks for carbon capture applications                                                                                     | 3.801,60         |                  | 1.300    | 2.000   | BSC/MN5-GPP  |
| Dr. Fabiola Cavaliere(SEAT BU specialist) | Q-ARCO (Quantum Advanced Real-time Car-body Optimization)                                                                                                 | 0,10             |                  | 256      | 256     | BSC/MN-ONA   |
|                                           |                                                                                                                                                           |                  | 10               | 256      | 256     | BSC/MN5-GPP  |
| Dr. Vladimir Lapin                        | Tuning and Validation of EC-Earth4 for CMIP7                                                                                                              | 6.160            |                  | 2.000    | 10.000  | BSC/MN5-GPP  |
| Edgardo Saucedo                           | Massive screening of ionic diffusion in solid-state electrolytes: from first-principles simulations to machine learning models                            | 4.000            |                  | 300      | 700     | UV           |
| Edilberto Sánchez                         | Global particle-in-cell simulations of turbulence in stellarators: zonal flows and electromagnetic effects                                                | 7.893            |                  | 30.000   | 25.000  | BSC/MN5-GPP  |

| Líder                        | Título                                                                                                                                                | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Eduardo Javier Pérez Sánchez | High-fidelity detailed chemistry simulations and Large-Eddy simulations for H2/air flames with strong preferential and differential diffusion effects | 5.200         |               | 20.000   | 20.000  | BSC/MN5-GPP  |
| Eleanor Hamilton             | Assessing the efficacy of current gravitational wave analyses to analyse precessing binary-black-hole remnants                                        | 1.215         |               | 2.000    | 5.000   | UMA          |
| Elena Akhmatskaya            | Multiscale Modelling of Composite Polymer Electrolytes Incorporating High Entropy Oxides: the Impact of Strong Dielectric Fillers                     | 580           |               | 300      | 500     | BSC/MN5-ACC  |
| Elena Bascones               | Low Temperature Electronic Properties of Twisted Bilayer Graphene                                                                                     | 3.820         |               | 50       | 50      | BSC/MN5-GPP  |
| Elena Lloret Pastor          | Quantum Mechanics for Natural Language Processing                                                                                                     | 0,02          |               | 500      | 500     | BSC/MN-ONA   |
| Elisa Jimenez Izal           | Small Pt units diffusion on epitaxial graphene grown on Ir(111)                                                                                       | 7.884,80      |               | 1.500    | 2.500   | BSC/MN5-GPP  |
| Eliseo Ruiz                  | Spin Crossover Systems under Electric Fields                                                                                                          | 1.080         |               | 120      | 4       | BSC/MN5-GPP  |
| Esteban Ferrer               | WhaleNoise: Simulation of offshore wind turbines and aeroacoustic impact                                                                              | 9.800         |               | 5.000    | 1.000   | BSC/MN5-GPP  |

| Líder                                | Título                                                                                                      | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina  |
|--------------------------------------|-------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|---------------|
| Estefanía<br>Fernández<br>Villanueva | CO2 hydrogenation to methanol over Cu- and Ga- doped MgO catalysts: Insight into the roles of Cu+ and Ga3+. | 973,35           |                  | 500      | 1.000   | BSC/MN5-GPP   |
| Estefania German<br>Gorosito         | Infrared spectra of *niobium-fullerene complexes to elucidate structural configurations                     | 900              |                  | 2.000    | 1.000   | CSUC/PIR3     |
| Eusebio Valero<br>Sánchez            | TRANSDIFFUSE: Discovering Flow control in TRANsonic difFUsing paSsagEs                                      | 4.320            |                  | 70.000   | 50.000  | BSC/MN5-ACC   |
| Eusebio Valero<br>Sánchez            | TRANSDIFFUSE: Discovering Flow control in TRANsonic difFUsing paSsagEs                                      | 560              |                  | 70.000   | 50.000  | BSC/MN5-GPP   |
| Eva Durán<br>Camacho                 | Exploring the multi-scale interplay of Milky Way dynamics and star formation                                | 250              |                  | 7.000    | 15.000  | UV            |
| Evangelia<br>Ntormousi               | Magnetic Fields at the Epoch of Reionization: Modeling the origins of galactic magnetization                | 8.110,08         |                  | 2.000    | 500     | BSC/MN5-GPP   |
| F. Javier Luque                      | Conformational study of the essential Ndh reductase from M. tuberculosis attached to a model membrane       | 806              |                  | 6.000    | 2.000   | CSUC/PIR3-GPU |
| Fabio Del Sordo                      | Global High-Resolution simulations of stellar dynamos under the effect of star-planet interaction           | 4.665            |                  | 2.000    | 20.000  | BSC/MN5-GPP   |

| Líder                              | Título                                                                                                                                                                                | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina     |
|------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|------------------|
| Federico Calle-Vallejo             | Comprehensive assessment of Ir and Ru oxides as OER electrocatalysts: from extended surfaces to nanoparticles.                                                                        | 732,67           |                  | 900      |         | CIEMAT/TURGALIUM |
| Federico Nicolas Pedron Casabianca | Machine Learned Atom-Centered Basis Sets for Electronic Structure                                                                                                                     | 200              |                  | 25.000   | 50.000  | BSC/MN5-ACC      |
|                                    |                                                                                                                                                                                       | 1.500            |                  | 25.000   | 50.000  | BSC/MN5-GPP      |
| Federico Schianchi                 | Effects of magnetic fields and neutrino transport in simulations of binary neutron star mergers with short lived remnant: magnetic field amplification and secular ejecta mechanisms. | 3.600            |                  | 40.000   | 40.000  | BSC/MN5-GPP      |
| Felipe J. Blas                     | Molecular Insights into Hydrate Nucleation and Phase Equilibria: Toward Sustainable Energy and Climate Solutions                                                                      | 9.900            |                  | 6.000    | 6.000   | UV               |
| Fernando Iglesias-Suarez           | Development and Implementation of Climate Emulator for Destination Earth (DestinE)                                                                                                    | 2.000            |                  | 128.000  | 128.000 | BSC/MN5-ACC      |
| Fernando Martín                    | Attosecond electron dynamics in molecules induced by broadband light pulses                                                                                                           | 9.910            |                  | 1.000    | 200.000 | BSC/MN5-GPP      |
| Fernando Martín García             | Optoelectronics of organic donor-acceptor molecules on NaCl substrates                                                                                                                | 4.550            |                  | 5.000    | 9.000   | BSC/MN5-GPP      |
| Ferran Feixas                      | Unraveling the dynamic conformational ensemble of nitrogenase upon electron transfer                                                                                                  | 220              |                  | 5.000    | 5.000   | CESGA/FT3-GPU    |

| Líder                             | Título                                                                                                           | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina  |
|-----------------------------------|------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|---------------|
| Ferran Feixas                     | Time-resolved mechanism of the photopharmacological allosteric regulation of metabotropic glutamate receptor 5   | 230,40        |               | 5.000    | 5.000   | CESGA/FT3-GPU |
| Francesc Coll I Cerezo            | Genomic and evolutionary analyses to study mutational adaptation of Enterococcus faecium                         | 234           |               | 6.144    | 6.144   | UMA           |
| Francesc Viñes Solana             | Homo and Hetero Transition Metal Dimers Embedded on Nitrogen-Doped Grazynes for CO2 Reduction                    | 2.050         |               | 800      | 1.000   | BSC/MN5-GPP   |
| Francesc Viñes Solana             | CO2RR on Copper Nanoislands: Stability and Reactivity of Cun Clusters                                            | 3.360         |               | 800      | 900     | BSC/MN5-GPP   |
| Francesc Viñes Solana             | C2H4 Hydrogenation on Molybdenum Carbides Nanoparticles Supported on the Au (111) Surface                        | 1.129         |               | 1.000    | 1.200   | BSC/MN5-GPP   |
| Francesc Xavier Trias Miquel      | A rational length scale for Large-Eddy Simulation of turbulent flows                                             | 7.400         |               | 256      | 61.440  | BSC/MN5-GPP   |
| Francisco (Xisco) Jimenez Forteza | Exploring the rich phenomenology of the binary black hole ringdown                                               |               | 500           | 12.000   | 75.000  | BSC/MN5-GPP   |
| Francisco Javier Salvador Rubio   | Using an Adaptive Mesh Refinement code for the DNS study of the atomization process of a pressure-swirl atomizer | 2.000         |               | 38.000   | 40.000  | BSC/MN5-GPP   |

| Líder                | Título                                                                                                                                   | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Gabriele De Chiara   | Quantum denoising diffusion models                                                                                                       | 0,05          |               | 256      | 256     | BSC/MN-ONA        |
|                      |                                                                                                                                          |               | 10            | 256      | 256     | BSC/MN5-GPP       |
| Gara Villalba        | Inverse modelling of biogenic and anthropogenic greenhouse gas emissions as a tool to support urban climate change mitigation strategies | 774           |               | 15.000   | 15.000  | UMA               |
| Germán RODRIGO       | Quantum algorithms for collider physics                                                                                                  | 0,04          |               | 1        | 1       | BSC/MN5-GPP       |
| Germán RODRIGO       | Quantum algorithms for collider physics                                                                                                  | 0,02          |               | 1        | 1       | BSC/MN-ONA        |
| Giancarlo Castellano | Enhancer disruption: the new generation of epigenetic targeted therapy in Ewing sarcoma.                                                 | 18            |               | 10.000   | 10.000  | UC                |
| Giannicola Scarpa    | Fingerprinting of quantum processors                                                                                                     | 0,01          |               | 20       | 20      | CESGA/FT-QMIO-QPU |
|                      |                                                                                                                                          |               | 10            | 20       | 20      | CESGA/FT-QMIO-cpu |
|                      |                                                                                                                                          | 0,01          |               | 20       | 20      | BSC/MN-ONA        |
|                      |                                                                                                                                          |               | 10            | 20       | 20      | BSC/MN5-GPP       |
| Giovanni Arico       | Constraining cosmology and astrophysics with emulators of the large-scale structure of the universe                                      | 6.000         |               | 64.000   | 64.000  | BSC/MN5-GPP       |

| Líder                            | Título                                                                                                                                          | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|----------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Giuliano Iorio                   | Shedding light on a Galactic mystery: state-of-the-art stellar evolution simulations to investigate the formation of metal-rich RR Lyrae stars. | 500              |                  | 8.000    | 2.000   | CSUC/PIR3    |
| Giuseppe Battaglia               | A computational study on the MRC1-mUNO interaction and the calculation of the binding free-energy                                               | 1.200            |                  | 1.500    | 1.500   | UAM          |
| Giuseppe Battaglia               | A computational study of the LRP8 receptors and its interaction with synthetic and natural ligands and its implication in BBB function          | 2.000            |                  | 2.500    | 2.500   | UAM          |
| GONZALEZ BALLESTER, MIGUEL ANGEL | Quantum generative diffusion models for medical imaging.                                                                                        | 0,05             |                  | 4.000    | 4.000   | BSC/MN-ONA   |
|                                  |                                                                                                                                                 |                  | 10               | 4.000    | 4.000   | BSC/MN5-GPP  |
| Gonzalo Rubio                    | High-Fidelity GPU-Accelerated Simulations for Turbulence Modeling and AI-Enhanced Aerodynamic Design                                            | 4.968            |                  | 60.000   | 80.000  | BSC/MN5-ACC  |
|                                  |                                                                                                                                                 | 560              |                  | 80.000   | 60.000  | BSC/MN5-GPP  |
| Guillaume Monteil                | Data assimilation of Sentinel 5 NO2 observations (CAMEO project)                                                                                | 8.000            |                  | 70.000   | 120.000 | BSC/MN5-GPP  |
| Hervé Petetin                    | Building the eMONARCH emission-sensitive AI-based emulator of the MONARCH air quality model                                                     | 4.500            |                  | 60.000   | 200.000 | BSC/MN5-GPP  |

| Líder                           | Título                                                                                                                                | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina      |
|---------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|-------------------|
| Horacio Andres<br>Vargas Guzman | Positioning small RNAs onto Functionalized<br>Surfaces of Manifold Polarities for High-<br>Resolution 3D Structural Ensembles Imaging | 115              |                  | 4.000    | 4.000   | CESGA/FT3         |
|                                 |                                                                                                                                       | 576              |                  | 15.000   | 12.000  | CESGA/FT3-GPU     |
| Hugo Cristian<br>Ojeda          | Quantum-Enhanced Protein Folding for<br>Sustainable Insect-Based Nutrition                                                            | 0,01             |                  | 200      | 200     | CESGA/FT-QMIO-QPU |
|                                 |                                                                                                                                       |                  | 10               | 200      | 200     | CESGA/FT-QMIO-cpu |
| Ignacio<br>Pagonabarraga        | Controlling emergent collective morphologies in<br>complex active systems and active materials                                        |                  | 100              | 10.000   | 10.000  | BSC/MN5-ACC       |
|                                 |                                                                                                                                       | 9.900            |                  | 200.000  | 200.000 | BSC/MN5-GPP       |
| Ignacio Soto Molina             | Nationwide High-Resolution Environmental<br>Noise Modeling in Spain                                                                   | 1.728            |                  | 500.000  | 500.000 | BSC/MN5-GPP       |
| Iker León Ona                   | Computational Investigation of Cereblon-<br>Binding Drugs: Mechanistic Studies of<br>Racemization and Protein-Ligand Interactions     | 300              |                  | 500      | 150     | BSC/MN5-ACC       |
| Iker León Ona                   | Computational Investigation of Cereblon-<br>Binding Drugs: Mechanistic Studies of<br>Racemization and Protein-Ligand Interactions     | 100              |                  | 500      | 150     | BSC/MN5-GPP       |
| Iñaki Comas                     | Large-scale genomic analyses to unveil<br>complex phenotypes associated to<br>Mycobacterium tuberculosis genotypes                    | 180              |                  | 150.000  | 150.000 | CESGA/FT3         |

| Líder                 | Título                                                                                                       | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina  |
|-----------------------|--------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|---------------|
| Iñaki Comas           | Large-scale genomic analyses to unveil complex phenotypes associated to Mycobacterium tuberculosis genotypes |                  | 25               | 30.720   | 30.720  | CESGA/FT3-GPU |
| Iñaki Tuñón           | Simulating ATP Hydrolysis with Machine Learning Potentials                                                   | 240              |                  | 16.000   | 16.000  | BSC/MN5-ACC   |
| Iñaki Tuñón           | Simulating ATP Hydrolysis with Machine Learning Potentials                                                   | 4.500            |                  | 16.000   | 16.000  | BSC/MN5-GPP   |
| Inés Corral           | Photochemical and photophysical profile of the artificial Hachimoji nucleobase Z                             | 1.932            |                  | 900      | 1.500   | BSC/MN5-GPP   |
| Inés Corral           | Decoding Advanced Photophysical Properties of Nanographenes Through Computational Modeling                   | 5.315            |                  | 500      | 2.000   | CENITS        |
| Isaac Salazar Ciudad  | What can development tell us about the mode and tempo of evolution?                                          | 2.120            |                  | 2.000    | 1.000   | UMA           |
| Ivano E. Castelli     | Understanding self-healing in halide perovskite photovoltaic materials through defect dynamics               | 2.000            |                  | 4.000    | 2.000   | NASERTIC      |
| Ivano Eligio Castelli | Probing Ultrafast Dynamics in Battery Cathodes with Automated Workflows                                      | 2.100            |                  | 3.000    | 3.000   | BSC/MN5-GPP   |
| Javier Carrasco       | Reconstructive Solid-State Phase Transitions: Integrating Graph Theory and Computational Chemistry Methods   | 765              |                  | 950      | 750     | BSC/MN5-GPP   |

| Líder                      | Título                                                                                              | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina      |
|----------------------------|-----------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|-------------------|
| Javier Cerrillo<br>Moreno  | Modeling NV Center Clusters with Qutrit-Based Quantum Simulation                                    | 0,03             |                  | 50       | 50      | BSC/MN-ONA        |
|                            |                                                                                                     |                  | 10               | 50       | 50      | BSC/MN5-GPP       |
| Javier Gonzalez-<br>Martin | MEGAFILD: Non-linear hybrid simulations of MHD-induced fast-ion transport in 3D tokamaks            | 11.745           |                  | 20.000   | 10.000  | BSC/MN5-GPP       |
| Javier Gonzalez-<br>Martin | MEGAMHD: Non-linear hybrid simulations of Alfvén Eigenmodes and Edge Localized Modes in 3D tokamaks | 8.239            |                  | 20.000   | 10.000  | BSC/MN5-GPP       |
| Javier Jimenez<br>Sendin   | Large-scale motion in wall-bounded shear flows: Waleffe flow                                        | 18.000           |                  | 10.000   | 10.000  | BSC/MN5-GPP       |
| Javier Prieto<br>Tejedor   | Novel quantum algorithm for optimization with application to the TSP problem                        | 0,01             |                  | 256      | 256     | CESGA/FT-QMIO-QPU |
|                            |                                                                                                     |                  | 10               | 256      | 256     | CESGA/FT-QMIO-cpu |
|                            |                                                                                                     | 0,01             |                  | 256      | 256     | BSC/MN-ONA        |
|                            |                                                                                                     |                  | 10               | 256      | 256     | BSC/MN5-GPP       |
| Javier Principe            | Simulation and design of magnetohydrodynamics flow devices                                          | 200              |                  | 24       | 512     | BSC/MN5-GPP       |
| Jeremias Likerman          | Assessment of geothermal potential in volcanic regions through thermomechanical numerical modeling  | 1.781            |                  | 2.400    | 4.800   | BSC/MN5-GPP       |

| Líder                     | Título                                                                                                                                                                                                                                | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Jesús Balsinde            | Lipidomics in metabolic diseases                                                                                                                                                                                                      | 2             |               | 1.000    | 3.000   | UMA          |
| Joan Calafell Sandiumenge | Dataset Generation for Turbulent Flow Reconstruction in External Aerodynamics Using Sparse Sensor Data                                                                                                                                | 2.280         |               | 12.000   | 12.000  | BSC/MN5-ACC  |
| Joan Torras Costa         | EU Computational study of the aggregation propensity of the peptides/peptidomimetics scaffolds for regenerative medicine                                                                                                              | 333           |               | 10.240   | 2.040   | BSC/MN5-ACC  |
|                           |                                                                                                                                                                                                                                       | 6.666         |               | 10.240   | 2.048   | BSC/MN5-GPP  |
| Jordi Abante Llenas       | Leveraging artificial intelligence to discover genetic modifiers in Huntington's disease                                                                                                                                              | 60            |               | 1.000    | 100     | BSC/MN5-ACC  |
|                           |                                                                                                                                                                                                                                       | 40            |               | 1.000    | 100     | BSC/MN5-GPP  |
| Jordi Martí Rabassa       | Simulation and modelling of biosystems with applications to medicine: the effect of guanosine pentaphosphate/tetraphosphate on the metabolism of Helicobacter pylori and in silico drug design for blocking its antibiotic resistance | 4.500         |               | 200      | 100     | BSC/MN5-ACC  |
| Jordi Martí Rabassa       | Exploring the structural diversity of MYC proto-oncogenes and in silico design of new anticancer drugs                                                                                                                                |               | 100           | 1.500    | 500     | BSC/MN5-ACC  |
| Jordi Vallverdú           | Modeling Artificial Sleep in Hippocampal Circuits: A Neurophilosophical and Computational Neuroscience Approach                                                                                                                       |               | 100           | 200      | 200     | BSC/MN5-ACC  |

| Líder                    | Título                                                                                                       | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|--------------------------|--------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Jordi Ventosa Molina     | Unsteady dynamics of tip leakage flow and corner separation at off design conditions in compressor cascades  | 610           |               | 1.024    | 30.000  | BSC/MN5-ACC  |
|                          |                                                                                                              | 58,24         |               | 1.024    | 45.000  | BSC/MN5-GPP  |
| Jorge Ferrer             | Processing of IMPaCT Whole Genome Sequences                                                                  | 7.300         |               | 31.000   | 145.000 | BSC/MN5-GPP  |
| Jorge Laranjeira         | Unraveling 1D furan nanothread superconductivity                                                             | 430           |               | 1.000    | 500     | NASERTIC     |
| Jorge Macías Sánchez     | Tsunami Hazard Assessment for Puerto Rico. A first study of variable friction coefficient with Tsunami-HySEA | 180           |               | 800      | 100     | BSC/MN5-ACC  |
| JORGE R. ESPINOSA        | Fast-scan of protein post-translational modifications in biocondensate material properties and ageing        | 2.717         |               | 1.000    | 1.000   | BSC/MN5-GPP  |
| Jose Angel Silva Guillen | Correlated phases and superconductivity in rhombohedral graphene                                             | 1.108         |               | 3.000    | 20.000  | CIEMAT/XULA  |
| Jose Angel Silva Guillén | Transition metal chalcogenides: A DFT study of their different polytypes and charge density waves.           | 6.600         |               | 2.000    | 20.000  | BSC/MN5-GPP  |
| José Antonio Font Roda   | Numerical relativity simulations of highly eccentric binary black hole systems with high mass ratios         | 5.645         |               | 200      | 7.000   | BSC/MN5-GPP  |

| Líder                                        | Título                                                                                                                           | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina  |
|----------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|---------------|
| Jose Guilherme Vilhena<br>Albuquerque D'Orey | Breakdown of Ballistic Heat Transport Single-Molecule Junctions                                                                  | 270           |               | 6.000    | 6.000   | CESGA/FT3-GPU |
|                                              |                                                                                                                                  | 835           |               | 6.000    | 6.000   | UMA           |
| José Ignacio ROJAS GREGORIO                  | WOW-CONTROL - WP2: parametric analysis of passive flow control with Gurney flaps with 2D CFD; DTU 10MW and MuWind (continuation) |               | 3.064,80      | 2.048    | 4.096   | BSC/MN5-GPP   |
| José Javier Honrubia Checa                   | Proton generation and transport for fast ignition of inertial fusion targets                                                     | 1.536         |               | 10       | 100     | BSC/MN5-GPP   |
| Jose Javier Plata Ramos                      | Thermoelectric performance of solids solutions                                                                                   | 950           |               | 2.000    | 2.000   | CENITS        |
| Jose Javier Ruiz Pernia                      | Biological Motors: from the Chemical to the Motion Side. Application for Dengue NS3 Helicase.                                    | 780           |               | 16.000   | 16.000  | BSC/MN5-ACC   |
|                                              |                                                                                                                                  | 3.970         |               | 16.000   | 18.000  | BSC/MN5-GPP   |
| JOSE LUIS SANCHEZ GOMEZ                      | Weather forecast for scheduling operations in sectors heavily impacted by adverse conditions II. (FScheduler II)                 | 1.576,96      |               | 900      | 3.000   | BSC/MN5-GPP   |
| Jose Luis Tamarit Mur                        | Graph equivariant diffusion models: from de novo drug discovery to crystal material generation                                   | 50            |               | 300      | 700     | CESGA/FT3-GPU |

| Líder                        | Título                                                                                                                                       | Con<br>prioridad | Sin<br>prioridad | Projects  | Scratch | Site/Máquina |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|-----------|---------|--------------|
| José Manuel<br>García Regaña | Turbulence Simulations Database for<br>Stellarators: Electrostatic Regime in TJ-II and<br>W7-X                                               | 8.150            |                  | 25.000    | 50.000  | BSC/MN5-GPP  |
| Jose Manuel Ruiz<br>Franco   | Understanding Soft Matter Mechanics: From<br>Polymer Networks to Granular Systems                                                            | 270              |                  | 10.000    | 2.000   | CESGA/FT3    |
|                              |                                                                                                                                              | 270              |                  | 10.000    | 2.500   | SCAYLE       |
| Jose Maria del<br>Peso       | ATLAS (LHC) simulation of detector response<br>to proton-proton collisions (UAM_m7y2025)                                                     | 2.500            |                  | 1.500     | 4.000   | BSC/MN5-GPP  |
| José María García<br>Oliver  | Effect of chemical timescale definition on<br>Partially-Stirred Reactor Large Eddy<br>Simulations of hydrogen-enriched gas turbine<br>burner | 6.000            |                  | 15.000    | 15.000  | BSC/MN5-GPP  |
| Josep Flix Molina            | MC Simulation for the CMS Experiment at the<br>CERN LHC                                                                                      | 11.800           |                  | 2.000.000 | 10.000  | BSC/MN5-GPP  |
| Juan Aragó                   | Understanding and engineering enzymes for<br>plastic degradation from multiscale simulations                                                 | 65               |                  | 16.000    | 16.000  | BSC/MN5-ACC  |
| Juan Aragó                   | Understanding and engineering enzymes for<br>plastic degradation from multiscale simulations                                                 | 4.440            |                  | 16.000    | 16.000  | BSC/MN5-GPP  |
| Juan José<br>Palacios Burgos | Excitons in two-dimensional magnetic materials                                                                                               | 1.500            |                  | 20        | 500     | UV           |

| Líder                        | Título                                                                                                                                                                                    | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina         |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|----------------------|
| Juan M. Murillo              | Smart Quantum Scheduler Optimization for Efficient Circuits Execution                                                                                                                     | 1                |                  | 256      | 256     | CESGA/FT-QMIO-cpu    |
|                              |                                                                                                                                                                                           | 0,01             |                  | 256      | 256     | CESGA/FT-QMIO-QPU    |
|                              |                                                                                                                                                                                           | 1                |                  | 256      | 256     | CESGA/FT-QMIO-QULACS |
|                              |                                                                                                                                                                                           | 0,01             |                  | 256      | 256     | BSC/MN-ONA           |
| Juan Manuel<br>Andrés Bort   | Mechanistic Insights into Reactive Oxygen Species Formation on Molybdate and Wolframate Nanostructures: Surface Engineering and Catalytic Pathways                                        | 2.500            |                  | 4.000    |         | UMA                  |
| Juan Manuel<br>Andrés Bort   | Enhancing the sensing performance of inorganic semiconductor by formation of nanoheterojunctions and femtosecond laser irradiation: a combined experimental and theoretical investigation | 1.200            |                  | 4.000    |         | UMA                  |
| Juan Manuel Cruz<br>Martínez | Quantum Accelerated Monte Carlo Integration                                                                                                                                               | 0,01             |                  | 256      | 256     | BSC/MN-ONA           |
| Juan Manuel Cruz<br>Martínez | Quantum Accelerated Monte Carlo Integration                                                                                                                                               |                  | 10               | 256      | 256     | BSC/MN5-GPP          |
| Juan Maria García<br>Lastra  | Illuminating multi-scale charge-transport processes in feldspar starting from first principles                                                                                            | 2.000            |                  | 1.200    | 1.200   | UC                   |

| Líder                   | Título                                                                                                                                            | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Laura Rodríguez Soriano | Evaluation of a Noise-Aware Routing Method on a Superconducting Quantum Processor                                                                 | 0,01          |               | 256      | 256     | CESGA/FT-QMIO-QPU |
| Laura Sáez-Ortuño       | Pilot test of quantum algorithms for market segmentation and consumer behavior prediction                                                         | 0,20          |               | 256      | 256     | BSC/MN-ONA        |
| Lluís Blancafort        | Machine-learning approach to the chemistry of eumelanin components - generation of a training set for DHI trimers                                 | 480           |               | 200      | 100     | CSUC/PIR3         |
| Lluís Blancafort        | Collisional excitation of ZnTPP photosensitizer by protons                                                                                        | 180           |               | 50       | 50      | CSUC/PIR3         |
| Lluís Brotons           | Pipeline implementation of modeling and predicting the distribution, population trends, and changes in distribution of bird species across Europe | 120           |               | 1.000    | 200     | BSC/MN5-GPP       |
| Lorena Ruiz Pérez       | MD Simulations of A $\beta$ 42 Self Assembly and Peptide Mediated Inhibition                                                                      | 1.200         |               | 1.500    | 1.500   | UAM               |
| Lucia Romero Perez      | Optimization of Purkinje system for electromechanical simulations                                                                                 | 5.100         |               | 35.000   | 15.000  | BSC/MN5-GPP       |
| Lucía Sanchis Sánchez   | Modelling of fast-ion transport in fusion plasmas with symmetry-breaking fields                                                                   | 14.623        |               | 5.000    | 10.000  | BSC/MN5-GPP       |

| Líder                             | Título                                                                                                                | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-----------------------------------|-----------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Luis Artiles                      | Quantum Machine Learning for cybersecurity and healthcare                                                             | 0,02             |                  | 1.000    | 1.000   | BSC/MN-ONA   |
|                                   |                                                                                                                       |                  | 10               | 1.000    | 1.000   | BSC/MN5-GPP  |
| Luis de Pedro<br>Sánchez          | Network Traffic Anomaly Detection by Quantum Machine Learning                                                         | 0,01             |                  | 1        | 1       | BSC/MN-ONA   |
| M. Verónica<br>Ganduglia Pirovano | DFT and ML-Driven Exploration of DRM over Sm-Doped Ni/CeZrO4 Catalysts                                                | 9.925,24         |                  | 10.000   | 100.000 | BSC/MN5-GPP  |
| Maedeh Rassekh                    | Spin-orbit torque and thermoelectrical effects in 2D van der Waals materials                                          | 1.814            |                  | 16.000   | 2.000   | UV           |
| Maite Alducin                     | Role of Hot Electrons in the Photoinduced Chemistry of O and CO on Ru(0001) Surface                                   | 2.620            |                  | 10.000   | 2.000   | SCAYLE       |
| Maite Melero<br>Nogués            | Adaptation of Machine Translation LLMs to New Languages and Writing Scripts                                           | 1.200            |                  | 20.000   | 20.000  | BSC/MN5-ACC  |
| Maite Mendioroz<br>Iriarte        | Exploring Brain Liquid Biopsy for Neurodegenerative Disorders (Amyotrophic Lateral Sclerosis and Alzheimer's Disease) | 45               |                  | 2.048    | 10.312  | NASERTIC     |
| Manuel Alcamí<br>Pertejo          | Prediction of chemical degradation routes of pesticides                                                               | 2.400            |                  | 4.096    | 2.048   | BSC/MN5-ACC  |
| Marc Garcia Borràs                | Unraveling electrostatic contributions on the catalytic efficiency of laboratory evolved retroaldolases               | 345,60           |                  | 250      | 250     | CSUC/PIR3    |

| Líder                             | Título                                                                                                                               | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Marc Garcia Borràs                | Unraveling electrostatic contributions on the catalytic efficiency of laboratory evolved retroaldolases                              | 230,40        |               | 5.000    | 5.000   | CSUC/PIR3-GPU     |
| Marco Marazzi                     | Design of anticancer strategies based on the structural photo-control of non-canonical i-motif DNA                                   | 73            |               | 8        | 15      | NASERTIC          |
| Marco Miguel Aguado Acevedo       | Development of Demonstrators for Real-World Applications in the context of ARQA Network                                              | 0,01          |               | 10       | 10      | CESGA/FT-QMIO-QPU |
|                                   |                                                                                                                                      |               | 10            | 10       | 10      | CESGA/FT-QMIO-cpu |
| María Camarasa Gómez              | Surface excitons within many-body perturbation theory and time-dependent density functional theory with hybrid functional frameworks | 3.367,43      |               | 32.000   | 32.000  | BSC/MN5-GPP       |
| Maria de Lluc Planas Llompart     | Towards precessing eccentric waveforms: First end-to-end parameter estimation studies                                                | 700           |               | 2.500    | 6.500   | SCAYLE            |
| Maria Luisa Salvador Senent Diez  | Pollutants and greenhouse gases in the atmosphere                                                                                    | 283,56        |               | 200      | 200     | CESGA/FT3         |
| Maria Veronica Ganduglia-Pirovano | Fine-tuning of the water/Fe3O4(001) neural network potential to address H2O2 decomposition at the solid-liquid interface             | 2.499,84      |               | 10.000   | 10.000  | BSC/MN5-GPP       |
| Marina Corbella Morató            | Engineering substrate specificities towards the enzymatic production of universal type O blood                                       | 201           |               | 6.000    | 6.000   | BSC/MN5-ACC       |

| Líder                  | Título                                                                                                                       | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|------------------------|------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Marina Corbella Morató | Engineering substrate specificities towards the enzymatic production of universal type O blood                               | 860              |                  | 6.000    | 6.000   | BSC/MN5-GPP  |
| Marta Colleoni         | Exploiting new advancements in gravitational waveform models for ground-based detectors                                      | 2.900            |                  | 6.500    | 12.000  | UMA          |
| Marta Melé Messeguer   | Development of computational workflows for the analysis of ribosomal RNA expression variation across tissues and individuals | 1.500            |                  | 2.000    | 20.000  | BSC/MN5-GPP  |
| Marta Reynal Querol    | Predicting Conflicts and other Disruptive Events                                                                             | 15               |                  | 4.000    | 1.000   | BSC/MN5-ACC  |
|                        |                                                                                                                              | 150              |                  | 6.000    | 1.000   | BSC/MN5-GPP  |
| Marta Villegas         | Open European LLMs                                                                                                           | 4.177,92         |                  | 2.000    | 2.000   | BSC/MN5-ACC  |
| Martin Calvelo Souto   | Impact of Lipid Cell Composition on Beta-Amyloid Aggregation: Exploring Novel Therapeutic Targets for Alzheimer's Disease    | 432              |                  | 1.500    | 1.500   | CESGA/FT3    |
| Martin Croce           | Preparing the cosmological analysis of Euclid Data Release 1                                                                 |                  | 16.200           | 25.000   | 100.000 | BSC/MN5-GPP  |
| Martin Obergaulinger   | Magneto-rotational core collapse: resonant gravitational wave modes and 3D topology of the magnetic field                    | 5.000            |                  | 2.000    | 100.000 | BSC/MN5-GPP  |

| Líder                                | Título                                                                                                                                                       | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina  |
|--------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|---------------|
| Mercedes Boronat<br>Zaragozá         | Optimizing the CeO <sub>2</sub> support in Pt/CeO <sub>2</sub> catalysts to overcome the inverse activity/stability correlation in the CO oxidation reaction | 1.300            |                  | 120      | 1.200   | UMA           |
| Michael Gabler                       | Exploring low-mass Supernova explosions with Prometheus-HotBubble                                                                                            | 2.200            |                  | 2.000    | 60.000  | BSC/MN5-GPP   |
| Miguel Alonso<br>Pruneda             | Electron-phonon interactions at interfaces of nanostructures                                                                                                 | 2.500            |                  | 1.000    | 1.500   | BSC/MN5-GPP   |
| Miguel Alonso<br>Pruneda             | Phonon trapping and relaxation at grain boundaries in nanocrystalline silicon.                                                                               | 2                |                  | 500      | 500     | CESGA/FT3-GPU |
|                                      |                                                                                                                                                              | 1.800            |                  | 1.000    | 1.000   | BSC/MN5-GPP   |
| Miguel Ángel<br>Escobedo<br>Espinosa | Study of heavy quarkonium suppression with improved Qtraj                                                                                                    | 20               |                  | 1.000    | 100     | UZ            |
| Milton Ruiz                          | The role of magnetic fields in r-process nucleosynthesis from neutron star binary mergers                                                                    | 9.999            |                  | 50.000   | 200.000 | BSC/MN5-GPP   |
| Milton Ruiz                          | Black holes mergers in gaseous disks                                                                                                                         | 6.000            |                  | 150.000  | 200.000 | BSC/MN5-GPP   |
| Miquel Solà Puig                     | Nanographenes for Li-S battery applications                                                                                                                  | 1.398            |                  | 900      | 1.000   | BSC/MN5-GPP   |
| Miquel Solà Puig                     | Solvent Effects in Hydrogen Evolution on Dual-Atom Catalysts                                                                                                 | 1.310            |                  | 500      | 500     | BSC/MN5-GPP   |

| Líder                                         | Título                                                                                                                         | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina         |
|-----------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|----------------------|
| Modesto Orozco                                | Fitting the Newly Developed Nucleic Acid Force Field with the NMR constraints from RNA Tetraloops                              | 400           |               | 10.000   | 2.000   | BSC/MN5-ACC          |
| Modesto Orozco López                          | Optimizing Xenonucleotide-Based Enzymes by Cation Exchange                                                                     | 9.696         |               | 5.120    | 3.072   | BSC/MN5-GPP          |
| Mohit Kumar                                   | Observing the self-assembly of a new phospholipid molecule                                                                     | 1.200         |               | 3.000    | 2.000   | UAM                  |
| Mònica Aragüés Peñalba                        | Quantum and hybrid quantum-classical algorithms for power system applications                                                  | 80            |               | 1        | 1       | CESGA/FT-QMIO-QULACS |
| Mònica Aragüés Peñalba                        | Quantum and hybrid quantum-classical algorithms for power system applications                                                  | 0,06          |               | 1        | 1       | BSC/MN-ONA           |
| Montserrat Costa Surós                        | Improving ice nucleation and mixed-phase cloud processes in the EC-Earth Earth System Models for enhanced climate projections. | 3.700,48      |               | 51.440   | 155.000 | BSC/MN5-GPP          |
| Néstor Balcázar-Arciniega, and Joaquim Rigola | DNS of Drag Force and Mass Transfer in Gravity-Driven Bubble Swarms in Inclined Pipes: Effect of Density and Viscosity Ratios  | 3.100         |               | 3.072    | 3.072   | BSC/MN5-GPP          |
| Nicolas Moreno                                | Advancing LHMM-Based Multiscale Simulations of Viscoelastic Instabilities in Complex Polymer Flows                             | 3.400         |               | 200      | 2.000   | BSC/MN5-ACC          |

| Líder                   | Título                                                                                                                                                                                | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Noelia Ferruz           | ProtGPT3: Aligning Protein Language Models to Fitness Landscapes                                                                                                                      | 62               |                  | 10.000   | 15.000  | BSC/MN5-ACC  |
| Núria López             | Reactivity of Highly Correlated Materials as Photo-electrocatalysts                                                                                                                   | 399,60           |                  | 6.144    | 6.144   | BSC/MN5-ACC  |
| Núria López             | Reactivity of Highly Correlated Materials as Photo-electrocatalysts                                                                                                                   | 4.527,36         |                  | 6.144    | 6.144   | BSC/MN5-GPP  |
| Nuria Lopez             | Dynamic Structural Evolution of Metal and Alloy Catalysts using ML-based Grand Canonical Simulations                                                                                  | 633,60           |                  | 6.144    | 6.144   | BSC/MN5-ACC  |
|                         |                                                                                                                                                                                       | 8.017,92         |                  | 6.144    | 6.144   | BSC/MN5-GPP  |
| Oier Lakuntza           | First-Principles Study of the Impact of Fe/Li and Mn/Li Defects on the Performance of LiFe <sub>0.9</sub> Mn <sub>0.1</sub> O <sub>2</sub> as a Cathode Material for Li-Ion Batteries | 573              |                  | 700      | 600     | CSUC/PIR3    |
| Oriol Lapiedra González | Unravelling Predation-Driven Rapid Evolution: Genomic and Ecological Insights from Two Lizard Systems                                                                                 | 600              |                  | 20.000   | 150.000 | BSC/MN5-GPP  |
| Pablo G. Lustemberg     | Unveiling MgO(001) Surface Defects via CO Vibrational Signatures: A DFT Study                                                                                                         | 2.086            |                  | 1.000    | 5.000   | BSC/MN5-GPP  |

| Líder                         | Título                                                                                                                              | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina  |
|-------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|---------------|
| Pablo Gamallo                 | A Generative Language Model for the Galician-Portuguese Diasystem                                                                   | 120              |                  | 3.500    | 1.500   | CESGA/FT3-GPU |
| Pablo Gamallo                 | Carvalho-TA: Advancing Machine Translation for Low-Resource Iberian Languages through Galician-Centric LLMs                         | 4,80             |                  | 3.000    |         | CESGA/FT3-GPU |
| Pablo Gamallo<br>Belmonte     | CO2 hydrogenation on 2D and 3D Nickel clusters supported on Ceria, Ni7/CeO2 vs Ni10/CeO2.                                           | 2.094            |                  | 900      | 1.500   | BSC/MN5-GPP   |
| Pablo Ordejón                 | Realistic modeling of graphene-like structures for designing new sensing platforms                                                  | 4.000            |                  | 2.000    | 3.500   | BSC/MN5-GPP   |
| Pedro José<br>Martínez Ferrer | Comparisons of different chemistry and transport modelling approaches with direct numerical simulations of lean hydrogen-air flames | 6.623,23         |                  | 6.000    | 3.000   | BSC/MN5-GPP   |
| Petia Radeva                  | Scaling Data-centric Deep Learning Towards Comprehensive Food-Centric Multimodal Understanding                                      | 879,36           |                  | 16.384   | 16.384  | BSC/MN5-ACC   |
| Prof Eduardo<br>Miranda       | Generative Quantum AI for Computer Music                                                                                            | 0,01             |                  | 5        | 5       | BSC/MN-ONA    |
|                               |                                                                                                                                     |                  | 10               | 5        | 5       | BSC/MN5-GPP   |
| Prof. Maciej<br>Lewenstein    | Investigation of localization and optical properties of quantum many-body systems                                                   | 2.300            |                  | 4.000    | 5.000   | BSC/MN5-GPP   |

| Líder                        | Título                                                                                                                                       | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina      |
|------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|-------------------|
| Prof. Max Garcia-Melchor     | High-throughput Screening of Novel Molecular Catalysts for the Oxygen Evolution Reaction                                                     | 1.368         |               | 2.000    | 6.000   | BSC/MN5-GPP       |
| Prof. Max García-Melchor     | High-Throughput Screening of Bimetallic Alloys for C–N Coupling                                                                              | 1.458,60      |               | 1.000    | 6.000   | BSC/MN5-GPP       |
| Prof. Max García-Melchor     | Computational Screening of Liquid Organic Hydrogen Carriers for Sustainable Hydrogen Storage                                                 | 1.596,98      |               | 2.000    | 6.000   | BSC/MN5-GPP       |
| Rafael Franco Fernández      | Molecular dynamics of five odorants and 3 microbiota metabolites on two olfactory receptors detected in microglia                            | 5             |               | 2.000    | 2.000   | BSC/MN5-ACC       |
| Rafael Sanjuán Verdeguer     | Uncovering viral receptors using deep learning.                                                                                              | 300           |               | 20.000   | 2.000   | BSC/MN5-ACC       |
| Raffaele Bernardello         | Response of the Earth System to overshoot, Climate neUtrality and negative Emissions. Earth System Model simulations for the RESCUE project. | 9.430         |               | 7.500    | 7.500   | BSC/MN5-GPP       |
| Ramón Beivide Palacio        | Evaluation of topologies, routing algorithms and allocation technics for interconnection networks for HPC and Data Centers.                  | 232           |               | 40       |         | BSC/MN5-GPP       |
| Raúl Ignacio Guerrero Avilés | Quantum Chemistry in Novel Quantum Hardware                                                                                                  | 0,01          |               | 300      | 300     | CESGA/FT-QMIO-QPU |

| Líder                         | Título                                                                                                                     | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina         |
|-------------------------------|----------------------------------------------------------------------------------------------------------------------------|------------------|------------------|----------|---------|----------------------|
| Raúl Ignacio Guerrero Avilés  | Quantum Chemistry in Novel Quantum Hardware                                                                                | 10               |                  | 300      | 300     | CESGA/FT-QMIO-QULACS |
| Raúl Ignacio Guerrero Avilés  | Quantum Chemistry in Novel Quantum Hardware                                                                                | 0,01             |                  | 300      | 300     | BSC/MN-ONA           |
| Raúl Ignacio Guerrero Avilés  | Quantum Chemistry in Novel Quantum Hardware                                                                                |                  | 10               | 300      | 300     | BSC/MN5-GPP          |
| Raúl Pérez Soto               | Towards a deeper understanding of proton shuttle catalysis                                                                 | 180              |                  | 150      | 200     | CESGA/FT3            |
| Reisel Millan                 | Optimization of Cu-CHA Catalysts for the Partial Oxidation of Ethane to Ethylene                                           | 1.380            |                  | 200      | 1.200   | UMA                  |
| Ricardo Serafín Alonso Rincón | Regev Algorithm implementation for integer factorization problem                                                           | 0,01             |                  | 256      | 256     | CESGA/FT-QMIO-QPU    |
| Ricardo Serafín Alonso Rincón | Regev Algorithm implementation for integer factorization problem                                                           | 0,01             |                  | 256      | 256     | BSC/MN-ONA           |
| Riccardo Rurali               | Accelerating the Design of Sodium Superionic Conductors Through the Integration of Phonon Band Theory and Machine Learning | 14.112           |                  | 2.000    | 4.000   | BSC/MN5-GPP          |
| Riccardo Rurali               | Intercalation strategy for boosting TMDs thermoelectric performances                                                       | 3.225,60         |                  | 1.000    | 4.000   | CESGA/FT3            |

| Líder                  | Título                                                                                                                         | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina |
|------------------------|--------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|--------------|
| Robert San José        | Numerical simulations for assessing climate change adaptation and mitigation strategies in support of the EU DISTENDER project | 4.106         |               | 20.000   | 30.000  | BSC/MN5-GPP  |
| Roberta Farris         | Unveiling the reaction mechanism of quasi-solid-state Li-O2 batteries using nano-sized MoS2-X @ CNT cathode Materials system   | 500           |               | 400      | 200     | BSC/MN5-GPP  |
| Roberto Lázaro Gastón  | Variational Quantum Regression for Wind Energy Forecasting                                                                     | 0,01          |               | 256      | 256     | BSC/MN-ONA   |
| Rocco Ballester        | Harnessing Quantum Computing for Advancements in Federated Learning and Optimization                                           | 0,30          |               | 250      | 300     | BSC/MN-ONA   |
|                        |                                                                                                                                |               | 10            | 250      | 300     | BSC/MN5-GPP  |
| Rodolfo Ostilla Monico | Blade-Vortex Interactions in the Bending Regime                                                                                | 350           |               | 20       | 2.000   | SCAYLE       |
| Roger Guimerà Manrique | Training of deep generative model for graph and molecular structures.                                                          | 345,60        |               | 500      |         | BSC/MN5-ACC  |
| Rosana Colleparado     | Multiscale simulations of chromatin phase transitions and their regulation by the microenvironment                             | 460,80        |               | 10.000   | 10.000  | BSC/MN5-ACC  |
|                        |                                                                                                                                | 2.580,48      |               | 10.000   | 10.000  | BSC/MN5-GPP  |
| Ruben Perez            | Conformational Transitions of the Spike originated by the Interaction with Manifold Polarizable-Surface Interactions           | 18,50         |               | 7.000    | 7.000   | BSC/MN5-ACC  |
|                        |                                                                                                                                | 460,80        |               | 14.000   | 14.000  | BSC/MN5-GPP  |

| Líder                       | Título                                                                                                              | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina  |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|---------------|
| Santi Roca Fabrega          | HARKONENS, the Arrakihs simulations II: unveiling the nature of DM and constraining the baryonic physics parameters | 16.000        |               | 500      | 200.000 | BSC/MN5-GPP   |
| Santiago Gonzalez de la Hoz | ATLAS production and simulation jobs running on HPC facilities (IFIC Phase XIII)                                    | 4.650         |               | 4.000    | 4.000   | BSC/MN5-GPP   |
| SARA RASTELLO               | Stellar Evolution Matters: Simulating Black Hole Multiples with PeTar and SEVN                                      | 2.000         |               | 3.000    | 3.000   | UZ            |
| Sascha Husa                 | Joint Spanish Contributions to the LISA Distributed Data Processing Centre                                          |               | 100           | 2.000    | 4.000   | BSC/MN5-ACC   |
|                             |                                                                                                                     | 2.100         |               | 2.000    | 5.000   | BSC/MN5-GPP   |
| Sergi Vela                  | Stability and structural study of non-symmetric pristine and O-terminated M2C MXene flakes                          | 3.404         |               | 1.000    | 1.000   | BSC/MN5-GPP   |
| Sergio Chiva Vicent         | CFD simulations and ML models convergence for creating digital twins of complex physical systems.                   | 268           |               | 1.024    | 2.048   | CESGA/FT3-GPU |
|                             |                                                                                                                     | 1.400         |               | 1.024    | 2.048   | BSC/MN5-GPP   |
| Sergio Mendoza Fariña       | KOIOS: Frugal Learning and Human-AI Workflows                                                                       | 863,84        |               | 10.000   | 10.000  | BSC/MN5-ACC   |
| Sergio Mendoza Fariña       | KOIOS: Frugal Learning and Human-AI Workflows                                                                       | 161,28        |               | 1.500    | 1.500   | BSC/MN5-GPP   |

| Líder                   | Título                                                                                                                                    | Con prioridad | Sin prioridad | Projects | Scratch | Site/Máquina  |
|-------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|---------|---------------|
| Sergio Posada Perez     | Dual-Atom Catalysts on Carbon Nitride for Nitrogen Reduction: Gas-phase and Solvated Adsorption Study                                     | 1.584         |               | 900      | 900     | SCAYLE        |
| Sergio Posada Pérez     | Mechanistic Study of Hydroformylation on Rh Single-Atom Catalysts Supported on Cerium Phosphates                                          | 699           |               | 500      | 500     | SCAYLE        |
| Susana Puig Sarda       | Multi-Omic Characterization of Pediatric Cutaneous Diseases: Genomic and Transcriptomic Insights into Melanoma and Genetic Skin Syndromes | 53,76         |               | 102.400  | 40.000  | CSUC/PIR3     |
| Tanausú del Pino Alemán | Three-dimensional Radiative Transfer Simulations of the Polarization Observed in the Ca II Lines of the Solar Chromosphere                | 5.000         |               | 2.000    | 2.000   | BSC/MN5-GPP   |
| Toni Gabaldón           | Metagenomic profiling from fecal immunochemical test tubes to identify early players and diagnostic markers in colorectal cancer.         | 2.600         |               | 10.000   | 200.000 | BSC/MN5-GPP   |
| Valentin Diez Cabanes   | In silico Design of Safe and Sustainable Xeroprotectants and Nanomaterials based on Atomistic Simulations                                 | 320           |               | 600      | 500     | CESGA/FT3-GPU |
| Vicent Ribas Ripoll     | Lung CT synthesis with Diffusion Models                                                                                                   | 6             |               | 300      | 80      | CESGA/FT3-GPU |

| Líder                    | Título                                                                                                                      | Con prioridad | Sin prioridad | Projects | Scratch   | Site/Máquina |
|--------------------------|-----------------------------------------------------------------------------------------------------------------------------|---------------|---------------|----------|-----------|--------------|
| Victor Guallar Tasies    | Learning Biomolecular Representations with Topological Neural Networks                                                      | 380           |               | 3.000    | 5.000     | BSC/MN5-ACC  |
| Victor Guallar Tasies    | NextAI: Next Frontier Generative AI in Drug Discovery                                                                       | 105,60        |               | 3.000    | 5.000     | BSC/MN5-ACC  |
| Victor Montal            | Design of constructs for WNV vaccines: promoting E protein dimerization                                                     | 94,80         |               | 1.400    | 150       | BSC/MN5-ACC  |
| Victor Montal Blancafort | ApoE4 homodimerization: A pathogenic interaction relevant for Alzheimer Disease                                             | 154           |               | 2.000    | 150       | BSC/MN5-ACC  |
| Vincenzo Fiorentini      | Multiferroicity in the hafnium-vanadium oxide solid solution                                                                | 900           |               | 500      | 1.000     | BSC/MN5-GPP  |
| Xavier Luri Carrascoso   | Gaia: First iteration run within the final data reduction cycle                                                             | 3.000         |               | 750.000  | 1.000.000 | BSC/MN5-GPP  |
| Xavier Solans Monfort    | Factors controlling the selectivity for urea synthesis through electrocatalytic co-reduction of nitrate and carbon dioxide. | 920           |               | 500      | 3.000     | BSC/MN5-GPP  |
| Xavier Vilasís Cardona   | LHCb-Dirac at the BSC-HPC                                                                                                   | 1.000         |               | 4.000    | 4.000     | BSC/MN5-GPP  |
| Yann Pouillon            | Reference calculations on porphyrins with SIESTA for hybrid classical-quantum workflows                                     | 600           |               | 200      | 200       | BSC/MN5-GPP  |

| Líder     | Título                                                    | Con<br>prioridad | Sin<br>prioridad | Projects | Scratch | Site/Máquina |
|-----------|-----------------------------------------------------------|------------------|------------------|----------|---------|--------------|
| Yumeng Xu | Search and Reconstruction on Eccentric Binary Black Holes | 1.500            |                  | 1.000    | 10.000  | UMA          |



## 6. Siguiendo pasos

Se dispone de un entorno web para poder acceder durante el periodo a toda la información relacionada con la actividad.

Está disponible a través de la web: <http://www.bsc.es/RES>. Es una zona protegida, que puede accederse con el correo electrónico del líder de la actividad, o de la persona que presentó la solicitud.

Desde esta zona, que está en construcción y evolución, se puede:

- Dar de alta a los usuarios/investigadores que participan en esta actividad. Se hace de forma automática, pero es imprescindible firmar el documento y devolverlo por correo antes de 15 días de dar el alta. De otra forma se anulará el acceso al sistema hasta que se reciba la documentación. Esto debe realizarse tanto para los usuarios de actividades de continuación como para actividades nuevas.
- Consultar la información proporcionada por el comité de acceso.
- Consultar los recursos asignados para la actividad. Es importante comprobar que no hay errores en estos datos, ya que serán los que se apliquen en los diferentes sites.
- Analizar el consumo semanal de recursos.

Una vez rellenada la información, el equipo de soporte local del site de asignación se pondrá en contacto con los usuarios para proporcionar la información necesaria.