

# Encontro RNCA 2023

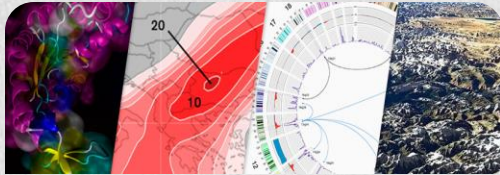
07 e 08 de novembro de 2023  
UTAD, Vila Real



# Access to MareNostrum5 and other European HPC infrastructures

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Barcelona Supercomputing Center

# Barcelona Supercomputing Center – Centro Nacional de Supercomputación



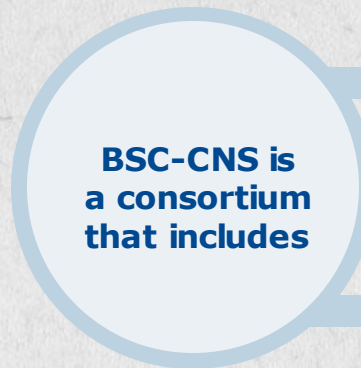
R&D in Computer,  
Life, Earth and  
Engineering Sciences



PhD programme,  
technology transfer,  
public engagement



Supercomputing and data  
services to Spanish and  
EU researchers



**Spanish Government**

**60%**



**Catalan Government**

**30%**



**Univ. Politècnica de Catalunya (UPC)**

**10%**



# Barcelona Supercomputing Center – Centro Nacional de Supercomputación



## Computer Sciences

To influence the way machines are built, programmed and used: programming models, performance tools, Big Data, computer architecture, energy efficiency



## Earth Sciences

To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications



## Life Sciences

To understand living organisms by means of theoretical and computational methods (molecular modeling, genomics, proteomics)



## CASE

To develop scientific and engineering software to efficiently exploit super-computing capabilities (biomedical, geophysics, atmospheric, energy, social and economic simulations)

# MareNostrum 4

Total peak performance: **13.9 Pflops**

General Purpose Cluster:	11.15 Pflops	(1-07-2017)
CTE1-P9+Volta:	1.57 Pflops	(1-03-2018)
CTE2-Arm V8:	0.65 Pflops	(12-2019)
CTE3-AMD:	0.52 Pflops	(12-2019)



## MareNostrum 1

2004 – 42.3 Tflops  
1<sup>st</sup> Europe / 4<sup>th</sup> World  
New technologies

## MareNostrum 2

2006 – 94.2 Tflops  
1<sup>st</sup> Europe / 5<sup>th</sup> World  
New technologies

## MareNostrum 3

2012 – 1.1 Pflops  
12<sup>th</sup> Europe / 36<sup>th</sup> World

## MareNostrum 4

2017 – 11.1 Pflops  
2<sup>nd</sup> Europe / 13<sup>th</sup> World  
New technologies

# MareNostrum 5

## A European pre-exascale supercomputer

- **>314 Petaflops** peak performance ( $314 \times 10^{15}$ )
- World-changing scientific breakthroughs such as the creation of digital twins and the advancement of precision medicine
- Total investment: **>200 M€**

Hosting  
Consortium



Spain



Portugal



Turkey



European  
Commission

The acquisition and operation of the EuroHPC supercomputer is funded jointly by the EuroHPC Joint Undertaking, through the European Union's Connecting Europe Facility and the Horizon 2020 research and innovation programme, as well as the Participating States Spain, Portugal, and Turkey



EuroHPC

# MareNostrum 5

GPP - General Purpose

Intel Sapphire Rapids

Peak performance: 45.4 Pflops

Sustained HPL:

ACC – Accelerated

Intel Sapphire Rapids

NVIDIA Hopper

Peak performance: 260 Pflops

Sustained HPL:

NGT GPP - Next Generation

NVIDIA Grace

Peak performance: 2.82 Pflops

Sustained HPL:

InfiniBand NDR 200  
Fat Tree

Spectrum Scale 248 PB HDD  
File System 2.81 PB NVMe  
402 PB tape

NextGen, Accelerated

Technology under evaluation  
Peak performance >6 PFlop/s

90 racks, 72 nodes per rack, 6480 nodes, peak performance 45 PFlop/s  
Node configuration:

- 2x Intel Sapphire Rapids 8480+ processors, 56 cores at 2GHz
  - 6192 nodes with 256GB DDR5
  - 216 FAT nodes with 1TB DDR5
- 2x Intel Sapphire Rapids 03H-LC processors, 56 cores at 1.7GHz
  - 72 nodes with 128GB HBM + 32GB DDR5
- All
  - 960GB NVMe local storage
  - NDR200 shared by two nodes
  - DLC and RDHX cooling



# MareNostrum5 – Accelerated Partition

35 racks, 32 nodes per rack, 1120 nodes, peak performance 260 PFlop/s

Node configuration:

- 2x Intel Sapphire Rapids 8460Y+ processors, 32 cores at 2.3GHz
  - 512GB DDR5
  - 480GB NVMe local storage
- 4x NVIDIA Hopper 64GB HBM
- 4x NDR200
- DLC cooling

7 racks, 68 nodes per rack, 408 nodes, peak performance 2.8 PFlop/s

Node configuration:

- 2x NVIDIA Grace processors, 72 cores at 2.6GHz
  - 240GB LPDDR5
  - 128GB NVMe local storage
- NDR200
- RDHX cooling

# MareNostrum5 - Storage

## Hard-drive storage

Spectrum Scale File System. 25 racks with RDHX cooling. In total:

- 20.400 HDDs, 18TB each, 1.6TB/s read, 1.2 TB/s write. Total Net Capacity 248PB
- 20 NVMe Flash, 15TB each, 600GB/s read&write. Total Net Capacity 2.8 PB

4xNDR200 per module

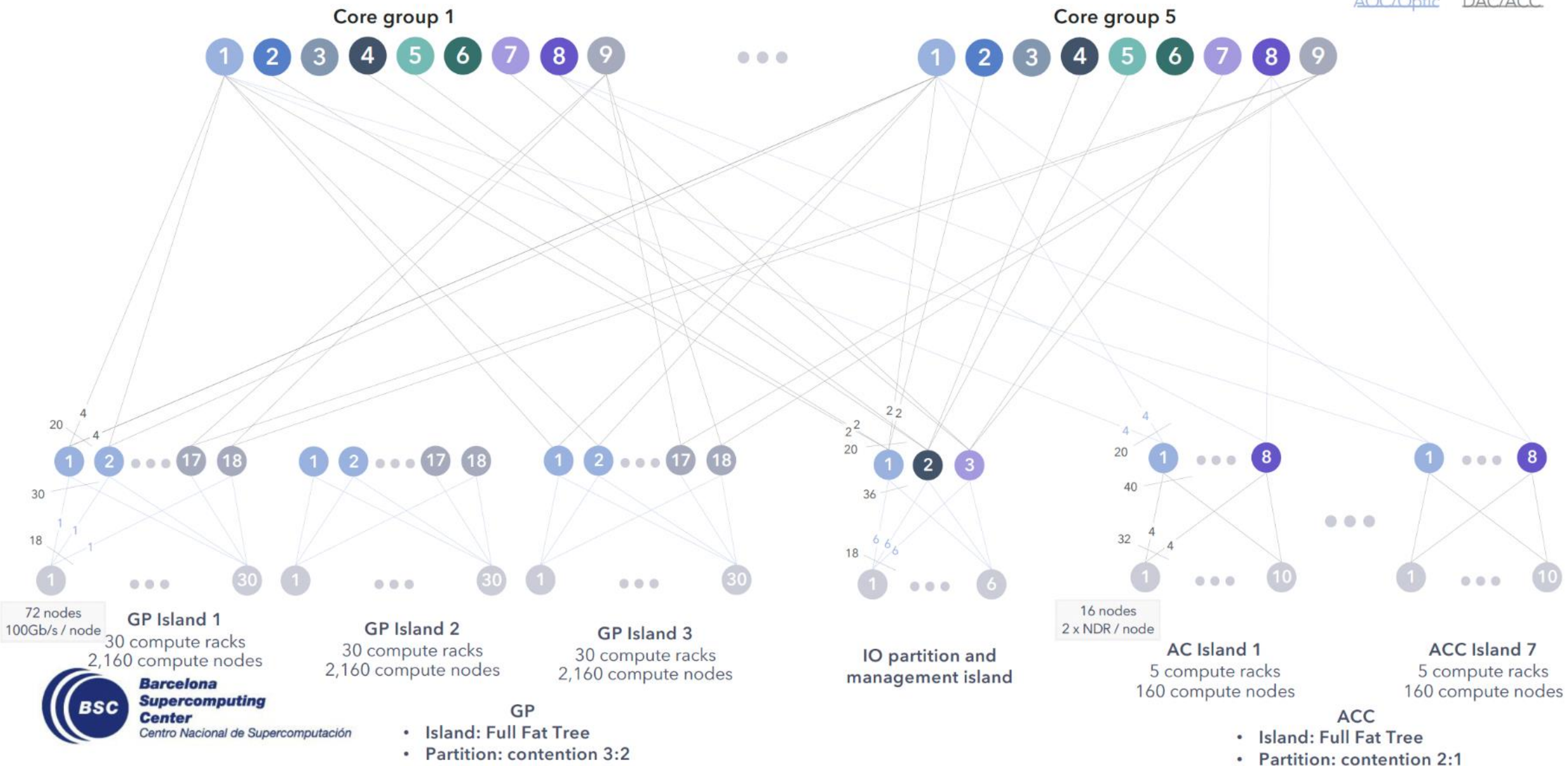
## Tape-based storage

Two tape libraries, 13 racks each library:

- Total 20,100 tapes, 20TB per tape, 402PB Net capacity
- 64 drives, 400MB/s per drive

# High performance network

AOC/Optic DAC/ACC



# Access to MareNostrum5



# Access to MareNostrum5

## EuroHPC JU access programmes

Extreme Scale Access, 2 calls per year

Regular Access, 3 calls per year

Benchmark and Development Access, rolling call

## Red Española de Supercomputación

3 calls per year, for HPC and IA access

## RNCA


Call for Advanced Computing Projects

All open to  
Portuguese  
researchers

# EuroHPC JU – Access

← → ↻ eurohpc-ju.europa.eu/index\_en

An official website of the European Union How do you know? ▾

 **EuroHPC**  
Joint Undertaking

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The European High Performance Computing Joint Undertaking (EuroHPC JU)

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**Leading the way in European Supercomputing**

EuroHPC JU is a joint initiative between the EU, European countries and private partners to develop a World Class Supercomputing Ecosystem in Europe.

[https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls\\_en](https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls_en)

- **Benchmark Access:** to test applications on EuroHPC systems prior to applying for an Extreme Scale or Regular Access project
- **Development Access:** to develop, test and optimise applications on EuroHPC systems
- **Regular Access:** to serve research domains, industry open R&D and public sector applications that require access to substantial computing and storage resources
- **Extreme-scale Access:** targets HPC applications with high-impact and high-gain innovative research from academia, industry and public sector

[https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls\\_en](https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls_en)



# EuroHPC JU – Regular Access

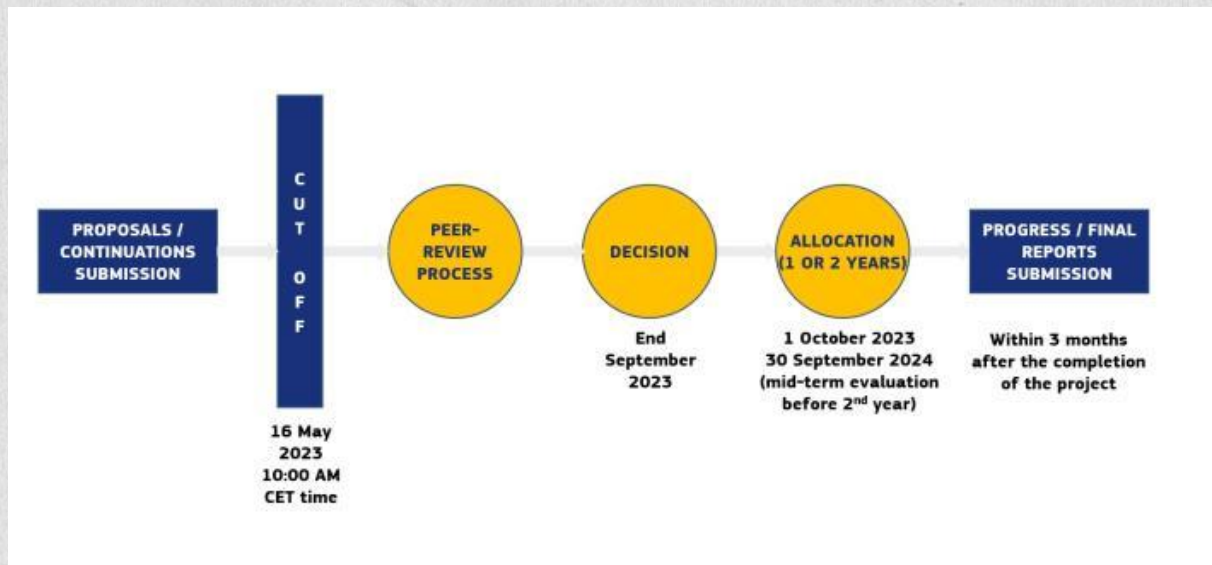


⇒ Three calls per year  
⇒ Four months from deadline to allocation

SYSTEM*	SITE (&COUNTRY)	ARCHITECTURE	PARTITION	TOTAL RESOURCES**	MINIMUM REQUEST
<b>MN5</b> MARENOSTRUM	BSC (ES)	Lenovo ThinkSystems SD650	<b>MN5 GPP</b>	376 719	38 000
		Atos BullSeqwana XH3000	<b>MN5 ACC</b>	300 563	20 000
<b>LEONARDO</b> CINECA	CINECA (IT)	Atos BullSeqwana XH2000	<b>Leonardo DCGP</b>	132 347	13 000
			<b>Leonardo Booster</b>	300 563	20 000
<b>LUMI</b>	CSC (FI)	HPE Cray EX	<b>LUMI-C</b>	376 719	37 000
			<b>LUMI-G</b>	738 665	50 000
<b>DISCOVERER</b> Sofia Tech Park (BG)	Sofia Tech Park (BG)	Atos BullSeqwana XH2000	<b>Discoverer CPU</b>	812 500	80 000
<b>MELUXINA</b> LuxProvide (LU)	LuxProvide (LU)	Atos BullSeqwana XH2000	<b>Meluxina CPU</b>	511 719	80 000
			<b>Meluxina GPU</b>	173 438	30 000
<b>KAROLINA</b> IT4I VSB-TUO (CZ)	IT4I VSB-TUO (CZ)	HPE Apollo 2000 Gen10 Plus x86_64Atos	<b>Karolina CPU</b>	468 750	80 000
		HPE Apollo 6500	<b>Karolina GPU</b>	16 875	8 000

[https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls\\_en](https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls_en)

# EuroHPC JU – Extreme-scale Access



➡ Two calls per year  
➡ Five months from deadline to allocation

SYSTEM*	SITE (COUNTRY)	ARCHITECTURE	PARTITION	TOTAL RESOURCES**	MINIMUM REQUEST
<b>MN5</b> MARENOSTRUM	BSC (ES)	Lenovo ThinkSystems SD650	<b>MN5 GPP</b>	3 955 550	400 000
		Atos BullSequana XH3000	<b>MN5 ACC</b>	4 207 883	420 000
<b>LEONARDO</b> CINECA	CINECA (IT)	Atos BullSequana XH2000	<b>Leonardo DCGP</b>	1 852 863	185 000
			<b>Leonardo Booster</b>	4 207 883	420 000
<b>LUMI</b>	CSC (FI)	HPE Cray EX	<b>LUMI-C</b>	3 955 550	390 000
			<b>LUMI-G</b>	7 755 983	775 000

[https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls\\_en](https://eurohpc-ju.europa.eu/access-our-supercomputers/eurohpc-access-calls_en)

Home > Access to Our Supercomputers > Awarded Projects

## Awarded Projects

### Filter by

#### Keywords

#### Access Mode

#### Call Cut-off

#### Country

#### Domain

### Awarded Projects (6)



Showing results 1 to 6

COUNTRY Portugal



#### Coherent Radiation Mechanisms in Extreme Plasma Physics

Astrophysical observations reveal that disorganised plasmas around compact objects produce coherent radiation. How orderly processes can arise from such conditions and give place to coherent dynamics still eludes us. Several mechanisms have been proposed to explain these phenomena.



#### EVPCC- ElastoViscoPlastic fluids flow Past Confined Cylinder

Complex fluids which simultaneously have elastic and plastic behaviors are ubiquitous in every day life (ketchup, chocolate), nature (fluids and materials in the human body), and various industries such as food, process, chemical and pharmaceutical.



## Red Española de Supercomputación (RES), created in 2007

- Member of the Spanish Unique Scientific and Technical Infrastructures network (**ICTS**)
- Composed of 14 members, offering access to:
  - 16 High-Performance Computing systems
  - 9 Data Management facilities





## RES in numbers

- Combined computing capacity above 22 PFlop/s
- Combined storage capacity above 180 PBytes
- High-speed network (RedIRIS)
- Periodic competitive calls for access

>20% through RES

### Annual statistics (2023)

- Nearly 1.000 million core hours distributed
- ~400 activities/experiments enabled
- ~240 scientific papers acknowledging RES
- More than 1.000 regular users



# RES Competitive Services

## Computing SERVICES

- Quarterly calls and allocations
- Submissions by Jan, May, Sept
- Up to 30M core hours per year

## Data Management SERVICES

- Yearly call
- Open from November to January
- Duration 3 to 5 years
- From 200TB to 1PB
  - + VMs

## Artificial Intelligence SERVICES

- Quarterly calls and allocations
- Submissions by Jan, May, Sept
- Mentored activities
- Test activities

Home > List of application activities

## List of application activities

All Areas

2023-3 (November 1st - February 29th)

Search

### Search Results

**Area:** Astronomy, Space and Earth Sciences

**Title:** Modelling the impacts of green infrastructure on air quality and climate change at the urban scale.

**Leader:** Gara Villalba Méndez

**Institution:** Associate professor at the Dept. of Chemical, Biological, and Environmental Engineering, Universitat Autònoma de Barcelona and senior researcher at the Institute of Environmental Science and Technology

**Assigned machine(s):** Picasso (UMA)

**Assigned khours with priority:** 700

#### Abstract:

The computational activity proposed takes place in the context of the ERC Consolidator project URBAG: Integrated System Analysis of Urban Vegetation and Agriculture 2019-2025). Given the need of cities to increment green areas and local agriculture to promote urban sustainability, URBAG aims to provide the knowledge and tools to evaluate which combinations of urban/peri-urban agriculture and green spaces result in the best performance in terms of air quality, heat wave and climate change mitigation, as well as ecosystem services provided to urban dwellers. To do so, URBAG uses, develops, and improves atmospheric transport models at the urban scale with the aim to evaluate 1) the efficacy of green areas on heat wave episodes using WRF and 2) how urban and peri-urban agriculture and vegetation affect air quality and climate change using WRF

<https://www.bsc.es/res-intranet/abstracts>

# Access to MareNostrum 5

Up to 1Mh

1Mh to 10Mh

10Mh to 100Mh

More than 100Mh

RES

RNCA

EuroHPC



# Access to European HPC systems

