

Barcelona Supercomputing Center Centro Nacional de Supercomputación



ATTENTION

This is NOT the application form to access RES resources. This document has been created only as a guide showing the information needed to fill the application form online. All the applications must be presented through the online form available at https://www.bsc.es/res-intranet/.

1. General Information

a) Activity Title

b) Area (select):

Astronomy, Space and Earth Sciences

Life and Health Sciences

Physics

Engineering and Mathematics

Homogeneous Chemistry

Heterogeneous Chemistry and Solids

2. Research Project Description

a) Is this a Test Activity?

Yes / No

b) Is this a Long Term Activity that will extend over two application periods?

Yes / No

c) Brief description of the Project

If this Activity takes place in the context of a Scientific Research Project, give a brief description of the Project, including the reference of National or International grants which support it. Summarize the research in the context of the current state-of-the-art, including references if appropriate. (Maximum 5000 characters).

d) Grant References

e) Brief description of the Project (If this Activity takes place in the context of a Technology or Industrial Project)

If this Activity takes place in the context of a Technology or Industrial Project, give a brief description of the Project, including the potential impact resulting from this activity, in measurable terms (potential for patent applications, competitive advance, prototypes, new products, economic impact, etc.). (Maximum 5000 characters).

f) Specific Activity proposed

Describe the specific Activity proposed. Discuss the need for Supercomputing facilities. Describe in detail the specific calculations you plan to do, and their relevance to the Research Project. If the Activity is a 'Long Term Activity' (which will extend over several applications periods), you must clearly specify which calculations will be done in this period, and which ones will be done in following periods. (Maximum 10000 characters).

g) Computational algorithms and codes outline

Outline the computational algorithms and codes, and their suitability for supercomputing facilities. Describe any benchmarks performed on HPC systems. (Maximum 3000 characters).

3. Software and Numerical Libraries

Software components that the project team requires for the activity.

Please select any software components that the project team requires for the activity.

a) Applications + Libraries

ABINIT	DESMOND	LAMMPS	OPENFOAM	SLEPC
ABYSS	DISPERSE	LAPACK	OPENMPI	SOAPdenovo
AMBER	FFTW	MAYA	OPENMX	SPARK
ARNOLD	FHI-AIMS	MKL	PETSC	SWIG
ATLAS	GDL	MPIBLAST	PLUMED	SZIP
BEDTools	GROMACS	NAMD	QIIME	TABIX
BLAS	GSL	NCO	QUANTUMESPRESSO	UDUNITS
BOOST	GTK+3	NETCDF	R	VASP
BWA	HDF5	NWCHEM	RAxML	VTK
CP2K	HEALPIX	OCTOPUS	RRDTOOL	WRF
CPMD	HMMER	OPENBLAS	SCALAPACK	
CRYSTAL	INTELMPI	OPENCV	SIESTA	

b) Compilers and Development Tools

GCC	INTEL	LLVM	POE
GDB	JAVA	MVAPICH2	TOTALVIEW

c) Utilities + Parallel Debuggers and Performance Analysis Tools

AUTOCONF	EXTRAE	NCVIEW	PERL	SCOREP
CFITSIO	GNUPLOT	OCTAVE	PICARD	SPADES
СМАКЕ	GREASY	OMPSS	PYTHON	VALGRIND
COMPSs	IMAGEMAGICK	OPENBABEL	SAMTOOLS	VAMPIR
CUBE	MOCAT	PARAVER	SCALASCA	
DIMEMAS	NCL	PARAVIEW	SCONS	

d) Other requested software

(Additional information might be requested by the Access Committee)

e) Proprietary software

In case of proprietary software, you should include software name, short description, link to web page with full software description.

4. Research Team Description

* Activities not including a researcher in a Spanish research center will not be eligible for review.

a) Personal data

Name of Team Leader

Institution

e-mail

Phone

Nationality

□ The employment contract of the activity leader with the research organization is valid at least 3 months after the end of the allocation period.

b) Curriculum Vitae of the Team Leader

Please, provide a brief Curriculum Vitae of the Team Leader, including any relevant information that may help in demonstrating his/her qualifications to lead the proposed activity. (Maximum 2500 characters)

c) Names of other researchers involved in this activity

Include only name, institution and e-mail.

d) Relevant publications

List the five most relevant publications, in the last five years, from the members of the research team that guarantee the scientific quality of the proposed Activity and demonstrate the qualifications of the team to complete it.

5. Resources

a) To which machine(s) are you requesting access?

Select a machine:

MareNostrum 4	Altamira	Picasso	Tirant
Memento	La Palma	MinoTauro	Power9
Caléndula	Pirineus	Canigó	Lusitania II
Cibeles	FinisTerraell	Urederra	

Please, try to estimate in terms of resource consumption, the typical run as well as the largest case (the most resource demanding experiment) for your simulation.

Interprocess communication

Null / Tightly Coupled / Loosely Coupled

Typical Job Run

Number of processors needed for each job

Estimated number of jobs to submit

Average job duration (hours) per job

Total memory used by the job (GBytes)

Largest Job Run

Number of processors needed for each job

Estimated number of jobs to submit

Average job duration (hours) per job

Total memory used by the job (GBytes)

Total disk space (Gigabytes)

Minimum / Desirable

Total scratch space (Gigabytes)

Minimum / Desirable

Total Requested time (Thousands of hours)

If this activity is asking for more than 10 Million CPU hours, you need to justify the amount of resources requested for the activity. (max 1000 characters)

Please select:

□ The required resources have to be executed in the selected machines, the other architectures do not fit the requirements to execute the proposal.

** this option implies that if no hours in this machine/these machines are available, the access committee will reject the full application.

□ The architectures selected for the requested resources are only a suggestion. If no hours in this machine/these machines are available, please grant resources in any other similar architecture where the codes used for the application may run efficiently.

** this option implies that if no hours in this machine/these machines are available, the access committee will reject the full application.

If the Activity is a **'Long Term Activity'** (which will extend over two Application Periods), give an estimate of the total resources that the Activity will require until it is completed.

b) Estimate of the total resources that the Activity will require until it is completed (including the present and the following Application Periods)

Number of application periods expected to complete this Activity

1 period / 2 periods

Total Requested Time (thousands of hours) expected to complete this Activity (sum of both periods)

6. Abstract for publication

Max. 850 characters, ready for publication in the web page in case the proposal will be accepted.

7. Contact with CURES during last year

User has contacted the CURES during last year:

Yes / No

8. Usage Terms & Conditions

You will have to read and accept the Usage Terms & Conditions:

- As a non-profit organization, RES policy is to make use of the centers resources with an exclusive research purpose and non-profit aims. If you intend to use RES resources with profit purposes, we should occur into commercial agreements, either you belong to a non-profit or for-profit organization.
- You will be given a username and password to access RES facilities. You should maintain them strictly secret and not share them with other users, in order to avoid the infiltration in our facilities.
- All data stored in disks will be removed 1 week after the project is completed. Please take this into account in order to get your data before this date.
- The RES is not responsible of user data. Users are encouraged to backup his/her own data.
- The RES requires that you mention the use of RES facilities in any of your publications with the sentence "The author thankfully acknowledges the computer resources at *MachineName* and technical support provided by the *NodeName* (RES-ActivityID).", and requests you to send a copy or a link to it (dissemination@res.es).
- You authorize RES to publish the subject of your research done using RES facilities, if no NDA signed.
- Personal data protection:
 - For the purposes stipulated in General Data Protection Regulation 2016/679, we inform you that the personal data provided in this form shall be included in a file, created under our direction, in order to communicate with you and to be able to conduct the

process of selection of projects you are registered in. Moreover, we guarantee confidentiality in the processing of your personal data.

- Such data is furnished voluntarily. Nevertheless, you are entitled to access the information about you compiled in our file, correct it if erroneous, or cancel it, as well as oppose processing of such data.
- As regards the personal data referring to other natural people you must communicate to Barcelona Supercomputing Center Centro Nacional de Supercomputación as a result of this selection process, prior to such communication, they should be informed of the particulars set forth in the previous paragraphs by you.
- As acknowledgement and acceptance thereof, you hereby expressly consent and authorize Barcelona Supercomputing Center - Centro Nacional de Supercomputación to process the personal data furnished voluntarily, according to the aims set forth herein.
- This authorization is valid until revoked by the data owner.