

CALL NOTICE FOR ADVANCED COMPUTING PROJECTS

IN ALL SCIENTIFIC DOMAINS

4th edition

Ref.: FCT/CPCA/2023/01

According to the Regulations for Advanced Computing Projects, published under No. 10/2022 in *Diário da República* (Official Portuguese Law Gazette), the allocation of computing resources of the <u>National Network for Advanced Computing (RNCA)</u> is carried out following a competitive tendering procedure whose terms are published on the page of the <u>Foundation for Science and</u> <u>Technology, I. P.</u> (FCT).

This Call notice, henceforth designated as AAC, was drawn up under the terms of the provisions of article 12 of the <u>Regulations for Advanced Computing Projects</u>.

1 Objectives and priorities

The consolidation and strengthening of the National Scientific and Technological System (SCTN) are priorities of the science and technology policy made in Portugal. These priorities aim to contribute to the national and international competitiveness of science and technology, and its contribution to innovation and knowledge transfer, as well as to contribute to the achievement of global aspirations set out in the United Nations Sustainable Development Goals (ODSs). In this context, it is particularly important to promote and strengthen the skills of scientific and technological institutions through their participation in advanced computing projects.

It is with these objectives that FCT opens this <u>Call for Advanced Computing Projects</u> (CPCA) to technologically support advanced computing projects in all scientific domains.

FCT manages the <u>National Network for Advanced Computing</u> (RNCA) seeking to aggregate national advanced computing resources, promoting cooperation between the various centres involved and developing national and international partnerships with other entities.

RNCA was integrated in the National Roadmap of Research Infrastructures of Strategic Interest by Order No. 4157/2019, from the Minister of Science, Technology and Higher Education. Know more about RNCA at <u>https://rnca.fccn.pt/en/</u>.

Keywords: RNCA, CPCA, Advanced Computing, High Performance Computing, HPC - High Performance Computing, SCC - Scientific Cloud Computing, VRE – *Virtual Research Environment*.

2 Type of beneficiaries

Computer resources can be allocated in the form of Individual or Institutional Support, i.e. by individuals or institutions, individually or in co-promotion, as referred to in articles 3, 4 and 6 of the Regulations for Advanced Computing Projects.

Regarding applications from companies as beneficiaries, advanced computing projects must:

- a) take place in the context of pre-competitive research and innovation, where the goods or services that are the subject of this research or innovation have not yet been assigned a commercial value.
- b) not exceed, for all applications of this type, 50% of the total computing budget to be allocated in this call.

3.1 Computational models and types of access to be supported

This call aims at allocating computational resources to Projects in all scientific and innovation domains, with reference to international technology standards.

The following computational models are available to applicants:

- High Performance Computing (HPC)
- Scientific Cloud Computing (SCC) or Virtual Research Environment (VRE)

3.1.1 High Performance Computing (HPC)

For the purposes of this call, each HPC¹ architecture is made up of the following elements:

- a) A set of compute nodes operating jointly and temporarily dedicated to a single application, which together can execute at least 40 x 10^{12} [²] strongly dependent floating-point operations each second, executed on generic, non-specialised microprocessors [³].
- b) A file system accessible from each compute node at a shared rate of at least 40 Gbps
 [⁴] with multiple concurrent access streams [⁵] in each compute node.

Compute nodes are typically managed by a batch system like Slurm or similar. HPC systems are generally accessed by SSH for one or more input nodes, from which you can submit jobs to the batch system. In the context of this call, requests to use visualization resources (e.g. dedicated GPUs) are also accepted from teams with or without previous experience.



¹ <u>https://www.incd.pt/?p=servicos/hpc</u>

² 40 Tera-FLOP

³ An example of a class of specialized processors is the GPU

⁴ 1Gbps= 1 Giga bit per second

⁵ Parallel file system, like Lustre or BeeGFS

3.1.2 Scientific Cloud Computing (SCC) or Virtual Research Environment (VRE)

Both SCC and VRE models are carried out through a computational architecture of virtual servers:

3.1.2.1 Scientific Cloud Computing (SCC)

In the context of this notice, each *SCC*⁶ architecture is integrated by the following elements:

- a) A set of computing nodes shared by several users and applications, made available in a self-service system with maximum quotas for the use of physical resources, through a virtualization software layer in cloud computing IaaS [⁷].
- b) The virtual servers (VM Virtual Machines) provided will access the virtual disk through local devices, or by mounting a remote file system.

The creation of VMs can be done through a web dashboard, command-line tools or using APIs. The service is based on Openstack. SCC is best indicated for scientific data processing in cloud computing environment. This model allows the instantiation of fully user defined VMs, both in the Linux operating system, as well as in the configuration of hardware and software, providing great flexibility in the configuration and use of the means to perform computational tasks.

3.1.2.2 Virtual Research Environment (VRE)

In the context of this notice, VREs are defined by the following elements:

- a) Set of interoperable online tools that contribute to facilitate the management, storage, processing and visualization of research data between one or more groups or institutions.
- b) Like SSC they require a set of compute nodes, memory capacity and data storage, and the possibility to create VMs see points a) and b) of point 3.1.2.
- c) VREs can make use of SSC resources, which can be supplemented by HPC for the performance of heavier processing tasks.

VREs are platforms for computing, processing, and accessing data, typically available through portals or web interfaces based on cloud computing. They aim to facilitate research and collaboration between researchers from one or more organisations. Unlike SCC, this model aims to provide environments as services that will be available to researchers continuously during the execution of the project. VREs are optimized to provide access to databases, workflow systems, or for production, availability and sharing of data products.



⁶ <u>https://www.incd.pt/?p=servicos/cloud</u>

⁷ See cloud IaaS definition in: https://csrc.nist.gov/publications/detail/sp/800-145/final.

3.2 Types of access

The present call includes the following access types, the limits of which are defined in table 1:

- A0 Experimental Access
- A1 Development Access
- A2 Regular Access
- A3 Larger Access

Table 1. Summary of access typologies with duration and maximum limits per application.

| | A0 | A1 | A2 | | | A3 |
|-----------------------------------|------------|---------|--|---------|-----|-----------------------------|
| Computational model | НРС | | | SCC | VRE | НРС |
| Platforms | Todas | | Navigator, Oblivion, Vision, Cirrus | Stratus | | Deucalion Mare Nostrum 5 |
| Duration (months) ^a | 6 | 12 | 12 | 12 | 24 | 12 |
| CPU core. hours ^b | 50.000 | 100.000 | 100.000 a 3.000.000 | _ | | 100.000 a 20.000.000 |
| vCPU.hours ^b | | | 1.200.000 | | | - |
| GPU. hours ^b | 730 | 4.380 | 8.760 | | | 100.000 |
| Quota ^c | 10% | 10% | 80% | | | |

^a Maximum duration, extendable for a further 3 months (A0/ A1) or 6 months (A2/ A3 Deucalion) in duly justified and approved cases; There will be no extensions for A3 Projects in MareNostrum 5. ^b Minimum and Maximum limits of computational resources, if the capacity punctually installed in the operational center does not allow the above mentioned ceilings. For projects that request SCC or VRE candidates should consider the maximum limit of 256 GB RAM (memory) and 5 TB storage per project. The allocation of GPU.hours may be lower depending on the number of requests and the capacity available at the time of project approval;

^c Quota of resources reserved for each type of access. If the resources requested do not meet one of these quotas, the remainder may be allocated to other typology(ies).

3.2.1 A0 – Experimental Access

This type of access is recommended for scientific or innovation projects whose work team has no prior experience in advanced computing or who has no history of use in RNCA computing resources. It is intended for experimentation, testing and pilot access to platforms.

Applications for this type of access will be subject to administrative validation and technical suitability.



3.2.2 A1 – Development Access

This type of access is recommended for conducting software performance tests, code optimization, scalability testing, benchmarking, re-factoring⁸ and short-scale projects.

As candidaturas a este tipo de acesso serão sujeitas a validação administrativa e de adequação técnica Applications for this type of access will be subject to administrative validation and technical suitability.

3.2.3 A2 - Regular Access

This type of access is intended for the use of HPC, SCC or VRE in the LCA-UC, HPC-UÉ and INCD operational centers and is recommended for scientific or innovation projects whose working team has previous experience in HPC or Cloud.

To assess the appropriate software scalability, the operational teams of the platforms may request A0 or A1 access before using A2 project resources.

Applications for this type of access will be subject to evaluation of technical suitability by elements of the RNCA operational centers that administer the requested resources and the evaluation of scientific merit by external evaluation panels invited by FCT.

3.2.3 A3 – Larger Access

Este tipo de acesso destina-<u>se exclusivamente à utilização de recursos HPC nas plataformas</u> <u>Deucalion ou MareNostrum 5</u> e está recomendado para projetos científicos ou de inovação cuja equipa de trabalho tenha experiência prévia em HPC.

To assess the appropriate software scalability, the operational teams of the platforms may request A0, A1 or A2 accesses before using A3 project resources.

Applications for this type of access will be subject to evaluation of technical suitability by elements of the RNCA operational centers that administer the requested resources and the evaluation of scientific merit by external evaluation panels invited by FCT.

3 Form of support

The support to be granted under the procedure of this call is exclusively the way of allocating time to use advanced computing resources, not providing funding of any kind or human resources to develop or support computer applications.

4 Computer resources global allocation

The allocation of computational resources of this call is described in table 2 and its notes, and the FCT can reinforce the available resources, if justifiable. The sum of the total available capacity is **400 million CPU core.hour/vCPU.hours and 275,000 GPU.hours.** The total financial value allocated to the call is 300,00 euros.

⁸ Refactoring the computer project to meet the specific conditions of the platform on which it will run.



Table 2. Resumo dos centros operacionais e respetivas plataformas computacionais disponíveis no presente concurso. Informações detalhadas sobre o hardware e software podem ser encontradas na ficha técnica do presente concurso.

| ос | Plataform | Model | System | Available Typologies |
|--------|-------------------------|-------|--|-------------------------|
| - | Deucalion | | ARM: 1 632 compute nodes, each node with Fujitsu ARM A64FX x86: 500 compute nodes, each node with AMD EPYC GPU (in x86): 33 GPU Nvidia boards | A0*, A1*, A3 |
| - | MareNostrum 5 | | GPP – 6408 compute nodes, each node with 2x Intel Saphire Rapids 8480+(112 cores each node) @2 GHz ACC – 1120 compute nodes, each node with 2x Intel Saphire Rapids 8460Y(64 cores each node)@2,3 GHz e 4 GPUs NvidiaHopper 2 extra partitions, including NGT GPP with Nvidia Grace | |
| LCA-UC | Navigator Navigator+ | HPC | 164 compute nodes, each with two Intel Xeon E5-2697v2 (12 cores each CPU) @2.7 GHz 32 compute nodes, each with two Intel Xeon Gold 6148 (20 cores each CPU) @2.4 GHz; 4-8 GB-RAM/core; 8 GPU type Tesla V100; 2 GPU Nvidia A40 for visualization | |
| HPC-UÉ | Oblivion | _ | 88 compute nodes, each with two Intel Xeon Gold 6154 (18 cores each CPU) @3.0 Ghz; 5.33 GB-RAM/core | A0, A1, A2 |
| | Vision | | 16 GPU type Tesla A100 | |
| INCD | Cirrus-A | | CPU type AMD EPYC 7501, each with 500GB-RAM e 64 cores; CPU type AMD Opteron 2356, each with 32 GB-RAM e 8 cores; amongst others (check technical sheet); 5 GB-RAM/core; 8 GPU type Tesla T4, V100, A100 | |
| | Stratus SCC ou VRE | | vCPU in AMD EPYC 7501, each with 500GB-RAM and 64 cores | |

Notes: The computing resources per RNCA platform are detailed in the call's technical data sheet and correspond to the best projection that is possible to perform at the time of publication. * only from batch B of A0 and A1 application submissions.



5 Eligibility criteria for projects and beneficiaries

The eligibility conditions for applications are those indicated in Article 6 of the Advanced Computing Project Regulations and those indicated in this AAC.

6.1 Advanced Computing Project

Applications are accepted individually or in co-promotion, in the form of Individual or Institutional Support:

- to one or two computational models;
- to one or more platforms for the same project;
- to one or more different types of access (A0, A1, A2 or A3) see limits in point 9

Regarding A2 and A3 access types:

- The presentation of a scalability graph of the software to be used, obtained from real or estimated data, is eligibility criteria for the HPC computational model. It is also recommended to present previous experience, namely in the use of this computational model or previous projects in advanced computing (e.g. in the RNCA network, PRACE network, EuroHPC, etc.).
- Eligibility in the SCC and VRE computer models for commercial and/or profit-making entities is limited to the availability of physical computer resources after these have been allocated to non-commercial or profit-making entities, and is also subject to the application of any costs indicated in the computer project acceptance term.

6.2 Responsible Investigator (IR)

The IR of the project:

- a) Should, at the moment of application update and make available **their CienciaVitae**, **associated to CiênciaID**, to FCT;
- b) In access types A2 and A3, the IR must identify a researcher who is co-responsible for the project, known as the Co-investigator in Charge (co-IR), and who will replace the IR in his/her absence.

6 Allocation of computer resources

As stipulated in article 9 of the Advanced Computing Projects Regulation, access to resources will be using computer resources from RNCA's operational centres. Access to resources will be provided for a limited period indicated in this notice, namely in points 3.2.

7 Evaluation criteria

Pursuant to Article 14 and 15 of the Regulation of Advanced Computing Projects, all applications received will be evaluated according to the criteria described in 8.1 and 8.2 which are densified and detailed in the evaluation guide.

For each batch of applications and type, a **ranked list** of applications will be generated. If two or more A2/A3 applications have the same final score after applying the evaluation criteria, the tiebreaking criteria will be applied.



In the event of AO/A1 applications having the same final assessment after applying the criteria, preference will be given to the application with the oldest submission date and time.

For the A2 and A3 access typologies, and after gathering the evaluations of the applications, the RNCA access committee (composed of elements from FCT and Operational Centers, as defined by the Internal Regulations, published in the Official Gazette under no. 1049/2020) will integrate and distribute the computational resources into the reserved resource quotas.

8.1 Evaluation of scientific merit

Only A2 and A3 applications will be subject to scientific merit evaluation by external evaluation panels invited by FCT, I.P. A0 and A1 applications will only be validated for their technical suitability by the technical teams operating the RNCA computing platforms.

Evaluation criteria:

- S1: Scientific relevance (40%);
- S2: Innovation and impact (30%);
- S3: Project planning and implementation (30%);

Formula, weights and score:

Final score = $40\% \times S_1 + 30\% \times S_2 + 30\% \times S_3$

General aspects of the evaluation process:

The scientific merit of the applications will be assessed by external evaluation panels, according to the scientific sub-area of each application. Each application will be evaluated by 2 independent evaluators from the corresponding panel. The following panels will be set up to assess the above criteria, each coordinated by a member appointed by FCT, I.P.:

- P1 Physics and Mathematics;
- P2 Chemistry and Materials;
- P3 Engineering and Technology;
- P4 Life and Health Sciences;
- P5 Earth and Environmental Sciences;
- P6 Social and Economic Sciences.

The score is based on a quantitative scale of 0 to 10. The minimum score for awarding resources is 5. If two or more applications have the same score after the evaluation criteria have been applied, the one with the highest score in the following criteria will be considered the best-ranked, in order of preference: S1 >>>S2 >>>S3.

<u>Note</u>: Only after an assessment of scientific merit will A2 and A3 applications be subject to an assessment of technical suitability (see 8.2)



8.2 Validation of technical suitability:

All applications will be subject to validation of their technical suitability by the technical teams operating the computer platforms listed in the table in point 5 of this CAA, according to the following criteria:

- T1: Technical suitability for RNCA resources
- T2: Reasonableness of the resources requested
- T3: Planning of the use of the resources

This validation is based on the qualitative classification of "accepted" and "not accepted", and does not enter into the final grade calculations in the case of accesses A2 and A3.

9 Submission of Applications

Applications are composed only of the electronic form referred to in paragraphs 9.1., 9.2. and 9.3, and its annexes. The maximum limit of applications by IR or co-IR is as follows:

- Access types A0 and A1: Each IR can submit a maximum of <u>ONE application</u> every 3 months, in non-consecutive batches of applications and always subject to the availability of resources.
- Access types A2 and A3: Each IR and co-IR can submit only <u>ONE application</u> in each of these types. In other words, in each type each person can only appear once, either as an IR or co-IR. Applications submitted in breach of this condition will not be accepted.
- If an A2 application and an A3 application from the same pair IR and co-IR are submitted, even if they are in reverse positions, only one of the applications can be approved. In this situation, the application with the highest classification will be chosen. If both applications have the same classification, only the A2 application can be approved. If the resources for type A2 are exhausted, the application for type A3 will then be approved.

For each type, applications will be dealt with in batches and on a first-come, first-served basis until the defined quota is exhausted.

9.1 A0 – Experimental Access and A1 – Development Access

A0 and A1 Applications must be submitted in English from **26 October 2023 until 13:00** (GMT Lisbon Time) on **30 May 2024**, on the appropriate **form** at:

https://myfct.fct.pt/

>>>> Selecting "Call Advanced Computing Projects (4th ed) - AO Experimental Access"

>>>> Selecting <u>"Call Advanced Computing Projects (4th ed): A1 Development Access"</u>

Every 6 to 8 weeks, the A1 applications received so far will be aggregated into batches and are subject to technical adequacy assessment. Calendar of batch submission dates will be available at https://www.fct.pt/apoios/Computacao/index.phtml.pt



9.2 A2 – Regular Access

A2 Applications <u>must</u> be submitted in English from **26 October 2023** until 13:00 (GMT – Lisbon Time) on **19 December 2023**, on the appropriate **form** at:

https://myfct.fct.pt/

>>>> Selecting "Call Advanced Computing Projects (4th ed): A2 Regular Access"

9.3 A3 – Larger Access

A3 applications for access to **Deucalion** <u>must</u> be submitted in English from the following dates: **19 December 2023** until 13:00 (GMT – Lisbon Time) on **8 February 2024**, on the appropriate **form** at:

https://myfct.fct.pt/

>>>> Selecting "<u>Call Advanced Computing Projects (4th ed): A3 Larger Access</u> - <u>Deucalion</u>"

A3 applications for access to **MareNostrum** 5 have been postponed to the following provisional dates, to be confirmed during the production phase of this system: 28 march 2024 until 1pm (Lisbon time) on 30 may 2024, on the appropriate form at:

https://myfct.fct.pt/

>>>> Selecting the "<u>Call Advanced Computing Projects (4th ed): A3 Larger Access - Mare</u> <u>Nostrum 5"</u>

9.4 Non-depletion of computational resources

Allocation on the platforms will be carried out until the respective quota limit is reached. If applications do not exhaust the available computational resources, FCT may set a new deadline for submission of applications for new batches of applications. This process can be repeated until all resources are assigned or the call is closed.

10 Applications approval

The ranked lists of applications are defined according to the criteria and weightings defined in point 8. In the case of A2/A3 accesses, after gathering the scientific merit assessments of the panels and the validation of technical suitability, the RNCA access committee (composed of elements from FCT and from Operational Centers, as defined by the Internal Regulations, published in the Official Gazette under no. 1049/2020) will integrate and distribute the computational resources by the reserved quota of resources, following the 20-40-40 principle:

- 20% of the applications with the best score in each panel will have recommended access to 50-100% of the resources requested, according to the preference of the platform indicated in the application and its availability.
- 40% of the following applications will have recommended access to 50-75% of the resources requested.
- The remaining 40% of applications will have recommended access to 5-25% of the resources requested, subject to availability on the platform.



Separate rankings will be generated for the A2 and A3 typologies and for each batch of A0 and A1 applications. Each approved application will have a unique reference associated with it, which will be known to the IR. The allocation of computing resources will be formalized by signing a term of acceptance in accordance with article 21 of the Advanced Computing Project Regulations.



10.1 Use of resources allocated to the approved project

Once the project has been approved and resources have been allocated to one of the platforms, it is essential to comply with the rules of the operational center and use the reserved resources within the stipulated deadlines.

- The resources allocated should be used throughout the project, i.e., promoting the use of at least 1/3 of the computational resources up to half the project time. If the beneficiary does not start work by 2/3 of the deadline, he/she may see the assigned computer resources reduced or deleted. In addition, each operational center can use the "sliding window" mechanism to optimize the execution of resources on the platform.
- If the beneficiaries use the resources according to the computer work plan throughout the months of the project, without delays or unjustified stoppages, and if the operational center is available, the projects may be awarded extra resources.
- In case of unforeseen events, such as breakdowns, works, maintenance of platforms or others, users may have to suspend their work with subsequent resumption, or be relocated on another platform of the network, in order to have the least impact on the realization of the project.

10.2 Data Management and results of the approved project

The IR and co-IR are responsible for managing the data generated, as well as backing it up. According to Article 24 of the Regulation, beneficiaries must 1) ensure open access to publications, namely by depositing them in one of the repositories in the RCAAP network; and 2) ensure open access to data, in compliance with the FCT's Research Data Policy.

It is recommended that this plan is created on the *Argos* platform <u>https://argos.openaire.eu/</u> during the submissions phase. If the project is approved, the data management plan must be made public or shared with the FCT within 6 months of signing the Terms of Acceptance. Support contact: <u>helpdesk.polen@fccn.pt</u>

All publications resulting from the use of the computer resources covered by this Regulation and any other results should include in the support section reference to FCT I.P., the platform used and the identifier assigned to the project.

Hence, FCT I.P. may publicize the project information, referenced as public.

11 Documents and further information

This document and other relevant documents and information, namely the Regulations for Advanced Computing Projects, are available at <u>https://www.fct.pt/financiamento/programas-de-financiamento/computacao/</u>.

Additional information and clarifications, including on completing the application form, can be requested at the email address: <u>rnca@fccn.pt</u> with "FCT/CPCA/2023/01" as subject.

It is recommended to read the tender documentation in advance, in particular:

- Advanced Computing Projects Regulations;
- Technical data sheet for computing platforms;
- Applications guide;
- Evaluation Guide



• Panels and scientific areas

11. Acronyms & definitions

- "AAC" = PT: Aviso para Apresentação de Candidaturas ENG: Call Notice
- "core.hour" = Unit of processing time widely used in HPC. Number of CPU colours or vCPU times the time, in hours, that they are used for a given function.
- "HPC" = High Performance Computing
- "HPC-UE" = High Performance Computing Universidade de Évora (Operational centre running the Oblivion and Vision platform)
- "INCD" = National Distributed Computing Infrastructure
- "IP" = Proposing Institution
- "IR" = Responsible Investigator
- "LCA-UC" = Advanced Computing Laboratory of the University of Coimbra
- "MACC" = Minho Advanced Computing Center
- "PRACE" = Partnership for Advanced Computing in Europe
- "SCC" = Scientific Cloud Computing
- "vCPU" = virtual CPU visible inside a VM. Typically corresponds to a CPU core of the VM host server.
- "vCPU.hora" = number of virtual CPUs times the time, in hours, that they are used for a given function.
- "VM" = Machine
- "VRE" = Virtual Research Environment

Resources allocated to the call:



