INCoDe.2030: Portuguese National Initiative on Digital Skills
(Iniciativa Nacional Competências Digitais)

Advanced Computing Portugal 2030

ACP.2030

A science, innovation and growth strategy to foster Advanced Computing in Portugal in the European context, oriented towards building a world-reference high-performance computing ecosystem.

FCT Fundação para a Ciência e a Tecnologia
Computação Científica Nacional
FCCN

Promoted through the Coordination Office of INCoDe.2030 in close cooperation with the Portuguese Science and Technology Foundation, FCT – National Scientific Computing Unit

ADVANCED COMPUTING PORTUGAL 2030
a dynamic and evolutive process:

• **September 2016:** initial preparation of INCoDe.2030, a national initiative to foster digital skills;
• **April 2017:** formal launching of INCoDe.2030, with 5 lines of action: inclusion, education, qualification for employment; specialization, research;
• **November 2017:** establishment of the terms of reference for ***MACC-Minho Advanced Computing Centre - MACC-FCT***, by the Portuguese Government through FCT and in the context of the national initiative INCoDE.2030, exploiting a former partnership with TACC (Texas Advanced Computing Centre) of the University of Texas at Austin, under the "UT Austin-Portugal Program";
• **7 December 2017:** 1st National Forum on Digital Skills - INCoDe.2030, including specific sessions on advanced computing;
• **January 2018:** Portugal participates actively in the preparation of the "EuroHPC" planning, with EC´s DG Connect;
• **March 2018:** launching of a "FCT´s Mobilizing programme to foster AI in public administration", through a competitive call for R&D projects promoted by FCT;
• **April 2018:** Portugal signs the **"EuroHPC declaration"**, during the 2nd EU digital Day, Brussels;
• **November 2018 – Spain-Portugal Summit, Valladolid:** agreement between Portugal and Spain to jointly develop an **"Iberian Advanced Computing Network - IACN"**, with the coordination of the Barcelona Supercomputing Center (BSC-CNS) with FCT->DCC;
• **November 2018:** starting phase of the installation of MACC with a low peta-scale High Performance Computer (HPC system, with a section of the former Stampede 1 of the Texas Advanced Computing Centre, U T Austin), with 800 compute nodes installed in the state-of-the-art datacenter facility of REN, located in Minho, at Riba de Ave, in close collaboration with NOS;
• **12 February 2019:** presentation and public discussion of the advanced computing and AI strategies at INL, Braga, with EC´s Deputy DG Connect;
• **25 February 2019:** presentation and public discussion of the advanced computing and AI strategies in Porto, together with the presentation of OECD 2018 S&T Outlook;
• **5 April 2019:** working meeting and visits for planning the advanced computing strategy and the installation of MACC at the datacenter facility of REN (Riba de Ave, Minho) in close collaboration with NOS, as well as the installation of "MACC User and Visualization Centers"; It included a visit to first "User and Visualization Center of MACC", at the University of Minho in Braga;
• **10 April 2019:** submission of a joint proposal to the EuroHPC JU Call EUROHPC-2019-CEI-PE-01, (Call for Expression of Interest for the selection of Hosting Entities for pre-exascale Supercomputers), coordinated by the Barcelona Supercomputing Center (BSC-CNS) and involving FCT, to install a **pre-exascale machine in BSC-CNS**, to be operated in close interaction with Portugal and under the "Iberian Advanced Computing Network - IACN";

- **15 April 2019:** submission of a joint proposal to the EuroHPC JU Call EUROHPC-2019-CEI-PT-01, (Call for Expression of Interest for the selection of Hosting Entities for Petascale Supercomputers), coordinated by FCT and involving the Barcelona Supercomputing Center (BSC-CNS), to install a **petascale supercomputer at MACC**, hereafter referred as Deucalion, to be operated in close interaction with Portugal and under the "Iberian Advanced Computing Network - IACN";
- **July 2019:** inauguration of the Supercomputer Bob at MACC;
- **November 2019:** contract signed between FCT and EuroHPC to host the Deucalion supercomputing in Portugal;
- **February 2020:** inauguration of Supercomputer Oblivion at the University of Evora.
- **March 2020:** FCT open the first call for R&D projects that includes the possibility of using advanced computing resources of the National Advanced Computing Network (RNCA) – Call for projects on Data Science and Artificial Intelligence in Public Administration;
- **March 2020:** EuroHPC opens the public tender for Acquisition, Delivery, Installation and Maintenance of Hardware and Software of a High-Performance Computing, 10 PetaFLOP Supercomputer, named Deucalion, to be installed in Portugal. This will be the most powerful supercomputer to be installed in Portugal;
- **April 2020:** Started the Portuguese program GO Portugal – Global Science and Technology Partnerships Portugal. It included a partnership with UT Austin University, with a specific area in Advanced Computing, with focus on joint projects and training actions on high performance and high throughput computing systems, quantum computing, data management and visualization, in a variety of domains, such as cities, agriculture, fisheries, space-earth observation, security and health applications;
- **June 2020:** FCT approved a regulation for projects for advanced computing, after a public consultation period. This enables FCT to open calls specific for using advanced computing resources, by academic and innovation communities, complementing other calls that may require the use of advanced computing resources and follow other regulations;
- **July 2020:** The preliminary result for the Deucalion acquisition public tender, found Fujitsu as the best qualified company for suppling this HPC machine.

INTRODUCTORY NOTE

By Manuel Heitor, Minister for Science, Technology and Higher Education

Advanced Computing Portugal 2030 is a dynamic and evolutive process aimed to promote and expand Advanced Cyberinfrastructure (ACI) in Portugal by a factor of 20 in the coming decade and until 2030. It considers close international collaborative actions and has been planned in a way to foster all advanced scientific computing fields, as well as mobilising data processing in an effective and diversified way, among industry and academic communities and in all areas of knowledge and the economy, including health, climate, energy, mobility, and the study of social processes.

It has been prepared and is promoted under the Portuguese National Initiative on Digital Skills (Iniciativa Nacional Competências Digitais), INCoDe.2030, and in close articulation with the recently created national strategy on Artificial Intelligence, "AI Portugal 2030". The ultimate goal is to widespread access to scientific information and create conditions for cooperation between laboratories based on advanced scientific computing networks, as well as promote international collaboration to foster advancements in knowledge and in the economy, with emphasis on the following five lines of action:

1. **Health bit:** promoting advanced computing networks for health applications, in a way to foster health services to patients in association with the massive use of datasets and data processing tools by physicians and health care units;
2. **Earth-Space bit:** promoting advanced computing networks for earth observation and the sustainable development, in a way to foster the preservation of biodiversity through data services to citizens, government organizations and industry, in association with data banks and data processing tools for agriculture, forests, fisheries and climate-energy interaction, among other fields;
3. **Mobility bit:** promoting advanced computing networks for mobility patterns, in a way to foster data services for citizens, government organizations and industry in association with data banks and data processing tools for maritime transportation (including space driven autonomous shipping), road transportation and urban environments (including car to car communication), among other fields;
4. **Social bit:** promoting advanced computing networks for people communication (involving online translation), social networks, behaviours and attitudes, in a way to foster social wellbeing through data services to citizens, government organizations and industry, in association with data banks and data processing tools for public services, among other fields;
5. **Scientific bit:** promoting advanced computing networks for new challenges in the frontiers of knowledge, including in particle physics, plasma physics, chemistry, astronomy, fluid dynamics and molecular modelling and cellular processes, among others;

This strategy overviews and is driven by three recent actions to stimulate and foster advanced computing capacity in Portugal, as follows:

1. The establishment of ***MACC-Minho Advanced Computing Centre - MACC-FCT***, by the end 2017, as promoted by the Portuguese Government through FCT and in the context of the national initiative INCoDE.2030, exploiting a former partnership with TACC (Texas Advanced Computing Centre) of the University of Texas at Austin, under the "UT Austin-Portugal Program". It includes a low peta-scale High Performance Computer (HPC system, with a section of the former Stampede 1), with 800 compute

nodes installed in a state-of-the-art datacentre facility located in the north of the country (Minho, at Riba de Ave), which should be operational by the summer 2019. **The installation of MACC-FCT in 2018-19 has increased the computer capacity of Portugal by a factor of six.**

2. The agreement between Portugal and Spain of November 2018 to jointly develop an **"Iberian Advanced Computing Network - IACN"**, which has been promoted by the two Governments and through the coordination of the Barcelona Supercomputing Center (BSC-CNS), together with a set of well-structured proposals to the EuroHPC program to facilitate the installation of **two new machines until 2021 to considerably increase the computer capacity of Portugal and Spain, as follows:**
   a. a joint proposal to the EuroHPC JU Call for the selection of Hosting Entities for pre-exascale Supercomputers, coordinated by the Barcelona Supercomputing Center (BSC-CNS) and involving FCT, to install a **pre-exascale machine in BSC-CNS**;
   b. a joint proposal to the EuroHPC JU Call for the selection of Hosting Entities for Petascale Supercomputers, coordinated by FCT and involving the Barcelona Supercomputing Center (BSC-CNS), to install a **petascale supercomputer at MACC**, referred as **Deucalion**;

3. The development of the ***QUANTA Lab*** at, a consortium between University of Minho, the *Iberian International Nanotechnology Laboratory (INL)*, INESC TEC and CEIIA, oriented towards the development of quantum science and technology, including materials, with potential applications to emerging sensing devices, and quantum computing. ***QUANTA Lab*** is an IBM Q Hub with research activity in quantum software engineering.

These actions should be considered and understood in terms of the evolving national capacity in advanced computing, which has acquired an ample operational experience over the last two decades through the cooperation of FCT-DCC and a number of research and associate laboratories, bringing together a coherent coordination and operation, with several advanced computing systems already installed, as follows:

- The *Portuguese Distributed Computing Infrastructure* - INCD, together with large heterogeneous computing clusters made operational through LIP (Experimental Particle Physics Instrumentation Laboratory, Associated Laboratory) and in close articulation with CERN. LIP and INCD have extensive experience in providing HPC (small scale), HTC, cloud computing (including HPC on cloud) and data oriented services to the academic and research community and operates an infrastructure with 4.2PBytes of online storage, 1.4PBytes of offline storage and more than 4000 CPU cores, installed at LNEC in Lisbon;
- The Laboratory for Advanced Computing at the University of Coimbra (UC-LCA) – is the Portuguese representative in the PRACE (Partnership for Advanced Computing in Europe) research infrastructure. LCA has been providing high performance computing (HPC) services to the scientific community at large since 2007 and more recently is involved with the ENGAGE SKA research infrastructure. Over the years U.Coimbra has also been involved in the creation of several HPC and HPDA consortia and organization of events, namely for training in HPC tools and programming. LCA and University of Coimbra are also working with SMEs in Centro Region of Portugal to engage them in HPC usage, as part of the activities of a regional Digital Innovation Hub. The LCA currently houses the Navigator supercomputer with a peak performance of 85 TFlop/s. A supplementary HPC system is currently being acquired which will raise the total peak performance to 250 TFlop/s, the size of total shared storage to 1,5 PB and the total core count to more than 5300 cores. This will also include several high-memory nodes and a SMP node.

• In addition to the above two major *infrastructures*:

a. The University of Minho installed and manages CLOUDinha, a cluster infrastructure for data processing composed of 200 cores and 40TBytes of hybrid (HDD+SSD) shared nothing storage, with some servers equipped with the Intel SGX technology. Together with dedicated software, CLOUDinha serves as a cloud-based testbed and to provide computational support to research and development activities.

b. The University of Evora manages the supercomputer (OBLIVION) of the ENGAGE SKA research infrastructure [ ] (the University of Evora is a node), the Portuguese interface to the Square Kilometer Array [ ] telescope project. The University participates in PRACE as a third party to the UC-LCA and is a Benchmark Code Owner (BCO) for PRACE. The supercomputer (in Phase I) is composed of 68 compute nodes, and storage and login/management nodes, EDR infiniband, and the BeeGFS parallel file system [ ]. It has a peak performance of 234 TFLOPS and a storage capacity of 576 TB. Phase II comprises an upgrade to 88 compute nodes, 1.73 PB of storage, and a peak performance of 300 TFLOPS. The machine has been designed to be a high performance/low cost facility using the latest Intel SKL processors. Tests using the particle and grid codes parallel codes (using the Message Passing Interface model) carried out in a similar machine show a scaling (for up to 2048 compute cores) near to that of the Marenostrum4 [ ] and JUWELS [ ] supercomputers, but better than the Mont-Blanc 3 Prototype Dibona [ ] (using the Marvell' ThunderX2 ARM based processors [[7]]) and the Marconi2 KNL supercomputer [[8]].

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1 http://engageska-portugal.pt
2 https://www.skatelescope.org
3 https://www.beegfs.io/content/
4 https://www.bsc.es/marenostrum/marenostrum/technical-information
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1. FOREWORD

BY NUNO FEIXA RODRIGUES, INCODE.2030 GENERAL COORDINATOR

Scientific knowledge and technological development have been built up over the centuries in many different ways. In the beginning, man had little more than his brain, paper and pencil. And though limited as they may seem at first sight, these resources produced some of mankind greatest scientific and technological achievements.

The construction of physical systems to conduct experiments is another great pillar of the scientific method and still much in use today. A significant part of the technological advance has been achieved at the expense of building (scale) models of airplanes, cars, ships, skyscrapers, trains and rockets; tested under the most extreme conditions simulated in complex apparatus, the likes of wind tunnels, earthquake simulators, compressors and mechanical tensioners.

However important, this route has several practical problems that hinder scientific development. First, it is difficult to set up physical systems that accurately simulate complex phenomena, such as sea waves or the behaviour of rivers in flood situations. It is also very expensive and often environmentally unsustainable to build complex and large physical systems, like ships or passenger jets, to perform experiments under different circumstances and then throw away the entire device. In many cases it is too slow, for instance when experiences must wait for certain natural phenomena to occur, as happens with comet passages or the alignment of planets. In other cases, experiments take very long periods of time before one may draw conclusions, like climate change or the evolution of galaxies. No less relevant is the danger that this path may involve as a knowledge creation process, particularly in cases of weapons development, nuclear energy study or the development of new drugs.
The third path is computational science, which essentially consists of a virtual version of the second. The only resource of this method of creating scientific and technological knowledge are computers, often very big ones. The general process of computational science involves the construction of digital models of the systems to be study, the environment where they operate, and algorithms that reliably simulate the behaviour of the system under diverse conditions. It is a technique that is solving most of the limitations found in the way of building physical models, therefore being applied today to solve problems in a growing number of areas, noteworthily in the design of physical structures (e.g. aircraft wings, ship propellers, car design), simulation of geophysical phenomena, weather forecasting, noise reduction and study of astronomical phenomena.

The expectation has never been so great for the application of computational science methods, supported by ever more powerful computing resources, to solve a large part of todays scientific and technological problems. While until recently, Advanced Computing (AC) was an exclusive resource of an elite club with selected members from governments, R&D institutions, universities and large companies, today we are witnessing the democratization of high performance computing, with several efforts on the ground, not only to increase the supply of advanced computing, but also to bring it to new areas, institutions and users.

The reasons behind this expectation are based on the convergence of 3 developments that are taking place in the AC ecosystem and in the world's economy. It starts with a worldwide investment in computing infrastructures, realized not only by the main centres of AC, but more recently by the entry of large cloud platform operators, who promise to offer AC resources in an unprecedent simple and cheap way. On the other hand, new AC software tools are exploring AI and Big Data techniques, reaching application areas never explored before and increasing along the way the number of users and organizations that begin to systematically use this resource in their activities. No less relevant is the context of rapid digitalization of economy and society, which is producing massive amounts of digital data ready to be processed by AC in order to produce new insights, products and services.

But if expectations on the potential of AC are great, the challenges to rip the benefits are even greater. As with many other technologies of general application and great potential added value creation, the greatest challenge lies not in access to the technology, but in its dissemination and efficient use by scientific, technological, economic and public administration actors.

There are many barriers to greater application and exploitation of AC for the creation of knowledge, economic value and welfare. In Europe, and particularly in Portugal, some of the greatest challenges lie in the shortage of qualified professionals to meet all the skills needs of the AC ecosystem, in the lack of software tools with high levels of abstraction that facilitate the application of AC to new areas, in the need to develop more efficient platforms for managing AC resources, and in the creation of initiatives and structures that support the entry of new users, particularly SMEs and public administration.

The National Strategy for Advanced Computing 2030 identifies the main actors and infrastructures needed to leverage Portuguese science and innovation through advanced computing. It establishes a path, privileging advanced training of human resources and creating the necessary conditions for these professionals to apply their knowledge and capacity throughout the AC value chain in the most diverse fields of application.
It is now up to companies, government, higher education institutions, research centers, technology transfer organizations and public administration, to tread this path together towards building a better future.

The implementation of this strategy would not have been possible without the generous contribution of many people who have sent me, as mere editor of this work, several opinions, articles, reviews and comments, which ended up becoming the main guidelines of this strategy.
To all of them, my most sincere thanks and recognition.

2. INTRODUCTION

The challenge presented by the Advanced Computing Portugal 2030 (ACP.2030) strategy for this decade is the creation of national value chains resorting to Advanced Computing (AC) activities that increase innovation and productivity in every economic sector. Such a goal is only achievable if on top of providing an appropriate infrastructure and qualified human resources, the implementation of this strategy is also capable of producing a research and enterprise cultural shift, one where AC is considered upfront as an elementary building block to consider in every research, innovation, production and service delivery process. This is a very ambitious goal considering that Portugal has just started in 2020 to operate its first supercomputer and there are currently no relevant value chains identified where AC plays a significant role in a continuous and sustained setting.

ACP.2030 adopts a wide definition of Advanced Computing (AC), referring to the capability of processing digital information at very fast speeds, one that is not available in desktop PCs, commercial service-oriented data centres, nor small computer clusters or servers. The concept includes strict high-performance computing (HPC) instances, but also other models such as High Throughput Computing (HTC), Grid Computing, and other emergent advanced computing models mentioned throughout the document.

Until recently, AC was a resource used almost exclusively by academia to solve research problems, although with notable exceptions of practical application, such as weather forecasting and mining and oil prospecting. However, the pervasiveness and rapid spread of digitalisation to every economic activity opens new opportunities to include AC in the chain of activities of companies that lead to the creation of products and services. Techniques of data analysis, AI and simulation are already game-changing elements in the production processes of the most innovative companies in the world. While all these digital processes can be greatly accelerated and improved by AC, many actually depend completely on AC to deliver useful results. The increasing applicability and contribution that AC can provide to a wide range of digital processing is elevating it to the status of a general purpose technology with potential to create added-value in all economic sectors, much like what the combustion engine or the electric motor achieved for mechanical tasks in the past.

Recent developments in AC have widened considerably the range of applications where it provides a significant contribution for the improvement of results. The first type of high economic value solutions that modern AC application provides concerns the simulation of complex physical systems for product optimization. The field of application of this type of solution is very wide, extending to all products that have to guarantee high levels of performance (quality), such as, in the textile sector, the manufacture of sportswear with high aero, hydro and thermal dynamic performance in different use environments; in the sustainable energy sector, for the optimisation of the operation of wind mills; or in the pharmaceutical sector, for the modelling of molecular structures of new drugs. The second type regards the achievement of analytical goals, often through the processing of large amounts of data and AI techniques. Typical applications in this domain are the construction of models of return on investment in marketing and advertising or to discover sources of performance loss in industrial processes, as well as for reasoning about sociological problems involving very large samples. In the third type, CA is itself the production process of the final product, as it happens in the entertainment industry with the rendering of 3D films or the production of digital special effects, and also in the industrial sector for the creation of digital twins.

One may ask about the relevance and opportunity of a national strategy based on a single tool and one that seems to be available everywhere, from desktop PCs, to cars, mobile phones and even electronic wearables. The answer certainly lies in many aspects, but perhaps the most important stems from the increasing value that can be extracted by processing data and the massive spreading of the so-called digital processing devices. In fact, these devices are packed with sensors and interfaces that generate much more data than they can process to extract value from. It's also interesting to note that even when these devices process information, they do so by producing more information, thus creating a never-ending data production cycle.

Data has already proven its value in many sectors and is today considered one of the most valuable assets for modern economies to explore. But, the extraction of this value, in a significant and sustained way, poses a series of complicated challenges that must be tackled with combined efforts in multiple fronts. One of the most rewarding, but also difficult, processes of value extraction from data, concerns the use of AC resources to solve complex multivariate problems that cannot be handled by any other means.

Advanced Computing Portugal 2030 (ACP.2030) stems from the political initiative Portugal INCoDe.2030 and constitutes a collaborative effort from a multidisciplinary team, ranging from the advanced computing user community, service managers, computer architecture experts, to service developers and operators. It begins by describing the motivational framework and principal objectives of a strategy for advanced computing in Portugal, followed by an analysis of the state of the art of the global advanced computing landscape, and also on the national resources and established partnerships available to the research and innovation communities. It then proposes a global strategy for advanced computing in Portugal, accompanied by a comprehensive set of tactical goals for the next two years.

The envisioned strategy is the result of a team effort and will be open to public comments leading to a final document which will be revised periodically, taking into account the achievements, necessary adjustments and new developments in the advanced computing global environment.

3. WHY ADVANCED COMPUTING IN PORTUGAL? A VISION FOR SUSTAINED GROWTH

The achievement of the ACP.2030 goals depend on the promotion and expansion of the national advanced computing capability, both in terms of cyber infrastructure as well as its data management, by a factor of 20 in the coming decade.

The envisioned physical infrastructure will facilitate the widespread access to data at an unprecedented scale and speed (in what is named info-structure), thus enabling the creation of competences (human resources) leading to the development and, in some cases, the extension of existing know-how and products in various domains.

Of particular interest in the national context are 5 key application areas where Portugal already has base know-how and critical mass to extend its knowledge and promote further innovation, potentially leading to high economic impact both domestically and worldwide.

These key application areas are identified as instances of value chains where AC can today provide important contributions to its improvement. Figure below depicts these areas as key "bits" on health and wellness, environment, urban and global mobility, social and community networking and scientific knowledge. The proposed advanced computing infrastructure will enable the development of these keys areas, by promoting advanced computing, networking and data services at a large scale for at least the following aspects:

1. **Health Bit:** fostering novel and advanced health services and devices in terms of observation of trends in public health, supporting national public health policy making and, with this, increasing social well-being, productivity and overall enhancing the citizens' quality of life.

2. **Earth Bit:** expand earth observation capabilities to enhance terrain analysis, climate modelling, sea analysis and weather prediction in support of innovation activities and sound governmental policies for the sustained development and preservation of biodiversity and the environment in general.

3. **Mobility Bit:** enable the development of applications for the management of maritime/land transportation and urban mobility, leading to a more effective management of physical infrastructures while minimizing environmental impacts, in particular in large urban areas.

4. **Social Bit:** support social and networking services and enhanced access to services and information by the government or third-parties to foster social well-being.

5. **Scientific Bit:** expand the frontiers of knowledge including the research of new materials and energy sources, key to meet the growing needs of modern societies.

To support this vision, ACP.2030 is structured over three pillars, namely, the infrastructure, the info-structure and people, as depicted in figure 1 below.

Figure 1. Advanced computing ecosystem

While these three pillars support the core strategy in the development of the 5 key application areas mentioned above, other organizations will not only tap into the resources of the ACP.2030, hence increasing the need for advanced computing and processing services, but also serve as incubators for newer AC-based activities that will spawn new applications.

This strategy will rely on the development of new competences in selected areas that are underrepresented in the national AC landscape and/or by enhancing existing ones through the collaboration between established organizations. These include, but are not limited to, Colabs, Research Centers, Higher Education Institutions and SMEs. Many of these organizations already have their own internal resources (either physical or human) which can be leveraged in various ways by ACP.2030. In turn, they can also rely on the access to a computing infrastructure with a much larger scope, as well as enhancing the technical know-how of their own staff through collaborations.

Figure 2 below depicts in more detail the envisioned interactions inside ACP.2030, involving government, industry, academia and European HPC organizations (such as EuroHPC and PRACE). While an initial funding model of the infrastructure will rely on a large governmental investment, a challenge will be to develop a sustainable funding model that relies heavily on industrial involvement, either through the use of the advanced computing infrastructure data processing capabilities and/or by the creation of a self-sustaining based market.

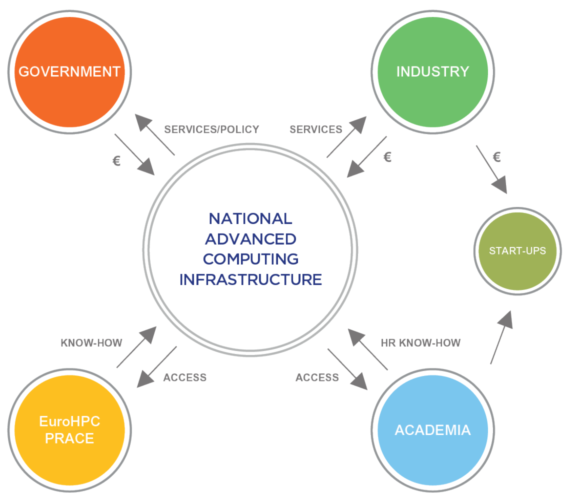


Figure 2. Interactions between the National Advanced Computing Infrastructure, government, industry, academia and European organizations.

4. OBJECTIVES

The last decades have witnessed a growing need for advanced computing to support the creation of added value across many industries and social activities. To support this effort in a sustainable fashion, the INCoDe.2030 program has defined specific objectives for the increase of the national computational, storage and visualization capabilities. These efforts are focused on increasing the capabilities of specific AC centers across the network (or smaller regional) and on the staffing of centers with qualified personnel, as well as the continued education in advanced computing-related data processing technologies of the national workforce both in the public and - more importantly - in the private sectors.

Specifically, ACP.2030 establishes the following objectives:

• **Increase the offer and availability of advanced computing resources and services to research, innovation, industry and public administration.** The foundation of the strategy will rely on the availability of professionally operated advanced computing services, accessed through a clear and agreed policy. These services must be well characterized, predictable and reliable, to allow user communities to plan their projects.

• **Increase the advanced computing skills of the various user communities.** Education in various computing skills at all levels of the workforce is paramount for the sustained growth of a digital-based economy. AC has specific challenges for the user community but also for management and operations personnel, namely in operating large-scale complex systems with high energy efficiency. Within this context there is a clear need for an additional investment in the education of the workforce from academia to support the establishment of SMEs and start-up companies.

• **Increase the advanced computing usage by the various user communities.** Overall and across many industries, access to AC resources is hampered by either lack of knowledge and/or lack of qualified human resources. Understanding the value of advanced computing in processing large volumes of data to extract information and knowledge is key to many service-based industries. Lowering the barrier for adoption of AC and incentivizing the uptake is key to bootstrap and sustain its use.

• **To increase R&I in Portugal in Advanced Computing**. The establishment of a national advanced computing infrastructure provides a solid foundation to establish new and more efficient research methods in emerging scientific areas of significant impact, such as new materials for engineering, pharmaceutical drug research, climate modelling and weather prediction.

Democratizing the access to this advanced computing infrastructure from academia and industry will foster the creation of diverse ecosystems that will leverage the computing resource in the short- and medium-term and contribute to its sustainability in the long-term via the continued creation of technical know-how in emerging computing technologies (such as quantum) and/or alternative or more efficient (e.g., “greener”) AC substrates or architectures.

5. TODAY'S AC LANDSCAPE: COMPUTING, NETWORKING AND DATA STORAGE

The term Advanced Computing (AC) is also used in these strategy as an inclusive concept that encompasses the ability to (i) solve computational problems that cannot be solved in a reasonable amount of time by traditional single-user computing systems (e.g., a desktop or a small cluster of PCs), or to (ii) provide high capacity computational resources, unavailable within single organizations, to solve scientific, technological and societal problems of great complexity and impact, which require a very large calculation capacity. For the sake of clarity, the following categories of advanced computing are distinguished:

• **HPC - High Performance Computing.** These large-scale systems, reported in the TOP500 Supercomputer Sites list [ ], are capable of executing billions of floating-point operations per second, and consist mostly of clusters of tightly coupled computers connected through a local high capacity and low latency network. Some system variants include Graphics processing units (GPU) nodes, as these support the efficient execution of many parallel floating-point operations (albeit with a restricted execution model) in terms of raw power. Even more specialized, and power efficient, hardware architectures can be fitted with Field-programmable Gate Arrays (FPGAs) and in some extreme cases with Application-Specific Integrated Circuits (ASICs). These customized architectural variants invariably exhibit trade-offs in terms of usage difficulty, high cost, prolonged development cycles and reduced flexibility.

• **HTC - High Throughput Computing.** Unlike typical HPC architecture, HTC jobs don't require very frequent data transfers between concurrent tasks. As such, they can be mapped to nodes in a grid-like structure geographically distributed across organizations or across independent machine clusters. HTC architectures therefore involve very sophisticated virtual mechanisms to share resources and can therefore be distributed over a very large scale, including many processor clusters, and thus resulting in very high aggregated throughput computing.

• **VRE - Virtual-Reality Environments.** Orthogonal to these computing categories, advanced computing centres typically also include facilities for advanced visualization and analysis. These visualization resources include multi-screen high-resolution video walls, immersive visualisation rooms (or "caves"), virtual and augmented reality, often coupled to the computational resources via dedicated high-performance data links for on-line or quasi-real time display of simulations.

In addition, to these more classical computing and visualization resources, emerging alternative technologies such as neuromorphic computing architectures and quantum computing machines promise to deliver even higher performance for selected application domains. While these computing paradigms are still in an exploratory and/or research phase, existing HPC centres are already offering access (albeit restricted) to these resources currently in research facilities associated with these centres.

[9] https://www.top500.org/

The classical model in which large HPC resources are made available is through an insourced model, in which the HPC operator buys, installs and operates the computers. However recent new models are available through commercial cloud operators that are starting to incorporate HPC service offers in publicly available service portfolios. Referential examples include Amazon's AWS [[10]] and Microsoft's Azure [[11]]. Such services typically offer dedicated high capacity physical servers coupled with a low latency and fast network, along with pre-installed software, such as Lustre and Slurm. Current users report that (1) such offers are in fact of high quality, but have a very high cost premium for long term usage as is the norm for large HPC resources; (2) regular offers top off at about 1 peta FLOP; (3) data confidentiality must be carefully analysed on a case by case offer; and (4) service characteristics are limited to what is available on the cloud operator, which limits special requirements such as usage of a particular piece of hardware. For these reasons, HPC on cloud is not yet a mature solution for large, long term, HPC offers. That could change in the upcoming years and it is therefore important to closely follow commercial cloud HPC offers, in particular to assess their viability as complement local offers for temporary usage scenarios or when these operators offer discounted accesses, even if temporary or with very stringent schedules.

5.1. EXISTING ADVANCED COMPUTING RESOURCES

The Portuguese Roadmap of Research Infrastructures of Strategic Interest includes the following initial computing infrastructures:

• The ***Portuguese Distributed Computing Infrastructure* - INCD**, together with large heterogeneous computing clusters is operated by LIP (Experimental Particle Physics Instrumentation Laboratory, Associated Laboratory) and in close articulation with CERN. LIP and INCD have extensive experience in providing HPC (small scale), HTC, cloud computing (including HPC on cloud) and data oriented services to the academic and research community and operate an infrastructure with 4.2PBytes of online storage, 1.4PBytes of offline storage and more than 4000 CPU cores, installed at LNEC in Lisbon. INCD is part of the EGI initiative and IBERGRID, the last of which was born out of the Iberian Common Plan for distributed infrastructures released in 2007. EGI delivers advanced computing services to support scientists, multinational projects and research infrastructures. The EGI Services are provided by EGI's federated cloud providers and data centres.

• The **Laboratory for Advanced Computing at the University of Coimbra (UC-LCA)** – is the Portuguese representative in the PRACE (Partnership for Advanced Computing in Europe) research infrastructure. LCA has been providing high performance computing (HPC) services to the scientific community at large since 2007 and more recently is involved with the ENGAGE SKA research infrastructure. Over the years, University of Coimbra has also been involved in the creation of several HPC and HPDA consortia and organization of events, namely for training in HPC tools and programming. LCA and University of Coimbra are also working with SMEs in Centro Region of Portugal to engage them in HPC usage, as part of the activities of a regional Digital Innovation Hub. The LCA currently houses the Navigator supercomputer with a peak performance of 85 TFlop/s. A supplementary HPC system is currently being acquired which will raise the total peak performance to 250 TFlop/s, the size of total shared storage to 1,5 PB and the total core count to more than 5300 cores. This will also include several high-memory nodes and a SMP node.

[10] https://aws.amazon.com/hpc/

[11] https://azure.microsoft.com/en-us/solutions/high-performance-computing/

Later the National Advanced Computing Network (RNCA) was added to the Portuguese Roadmap of Research Infrastructures of Strategic Interest. RNCA includes two other large-scale computing systems:

a. Bob HPC cluster. Officially inaugurated in July of 2019 the "Stampede 1" supercomputer (provided by the Texas Advanced Computing Centre) of the University of Texas at Austin, under the "UT Austin-Portugal Program") is now installed in a state-of-the-art datacenter facility located in the north of the country (Minho, at Riba de Ave). This system, shown in the picture below, is composed of 800 compute nodes connected through a FDR Infiniband network, and with a Lustre parallel file system.

Figure 3. The 'Bob' HPC Cluster at Riba d'Ave, Minho, Portugal.

b. Oblivion cluster. The University of Evora hosts and manages the OBLIVION supercomputer of the ENGAGE SKA research infrastructure, where the University of Evora is a node of this network and the Portuguese interface to the Square Kilometer Array (SKA) telescope project. The University participates in PRACE as a third party to the UC-LCA and is a Benchmark Code Owner (BCO) for PRACE. This system (in Phase I) is composed of 68 compute nodes, and storage and login/management nodes, EDR infiniband, and the BeeGFS parallel file system [beegfs. It has a peak performance of 234 TFLOPS and a storage capacity of 576 TB. Phase II comprises an upgrade to 88 compute nodes, 1.73 PB of storage, and a peak performance of 300 TFLOPS. The machine has been designed to be a high performance/low cost facility using the latest Intel Skylake (SKL) processors.

Current usage of existing advanced computing resources

Currently the Oblivion cluster is being installed and has no production usage indicators. It is projected to begin operations in the second semester of 2020.

The Bob HPC cluster, although a machine from the year 2013, running with significant cooling limitations at the datacentre level, presents significant usage levels as the following infographic shows.

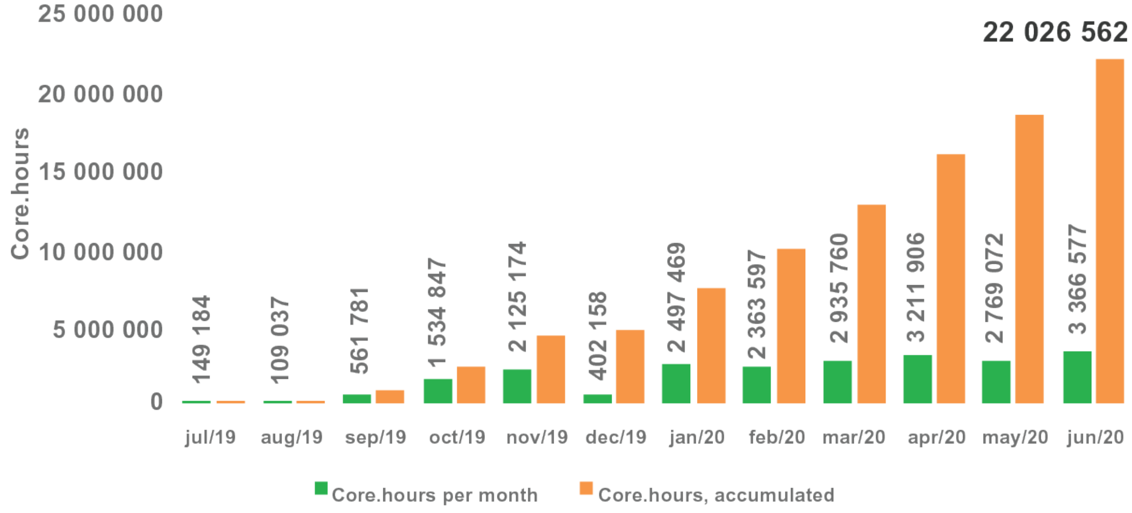
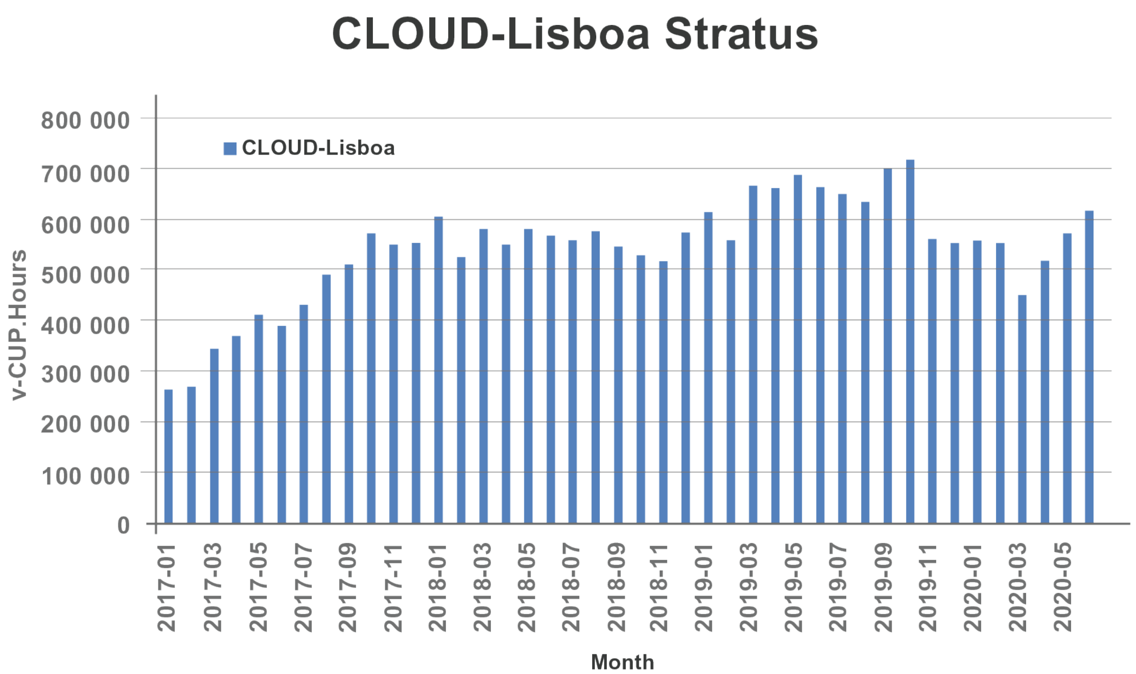


Figure 4. Bob Cluster usage

The green bar shows the number of core.hours usage per month, that is, the number of CPU cores used times the number of hours that they were used. In June, 3,3 million core.hours of CPU time were used. The orange bars show the accumulated value since the cluster was first started, in July 2019. In December the machine did heavy maintenance at the storage system, that took an impact on the usage level. The usage was due to approximately 24 scientific projects running on the machine.

The Portuguese Distributed Computing Infrastructure – INCD – is constituted as a legal entity since 2013 and is the current center with more variety of computational clusters and established user base. The most central and flexible cluster is a cloud computing cluster, capable of running High-Throughput Computing and VRE- Virtual Research Environment applications. The following infographic shows a monthly evolution of CPU time usage, which is slightly below real usage due to limitations of the accounting system.



The vertical scale of the graphic is based on virtual CPU time, since it is a virtual server environment, that loosely maps to CPU_core on and HPC system. The usage was due to approximately 42 projects running on the cluster.

5.2. LARGER SYSTEMS

The following two systems will be accessible in the short term to users of the national advanced computing infrastructure. While the first will be located in Portugal and operated by the Minho Advanced Computing Centre (MACC), the second, will be installed and operated by BSC-CNS in Barcelona:

Deucalion, a peta scale system: In April 2019 Portugal and Spain successfully won an EuroHPC's bid for procuring in 2020 and hosting in Portugal an HPC 10 peta FLOP machine, called Deucalion. This supercomputer is envisaged to include several computing technologies namely leading edge x86 and ARM processors, as well as accelerating coprocessors, with more than 266 TBytes of RAM and 10 PBytes of high-performance storage, targeting a peak performance of 10 PFlops and with an anticipated maximum power consumption of 1 MWatt.
Deucalion will be operated by the Minho Advanced Computing Center (MACC), with 65% of its capacity time allocated to Portuguese access and the remainder to be used by European computing projects.

Mare nostrum 5, a pre-exa scale system: Shortly before the Deucalion proposal, Spain, Portugal, Turkey and Croatia applied and won an EuroHPC's call for hosting in Spain a pre-exascale machine, called Mare nostrum 5. Mare nostrum 5 will be operated by BSC in Barcelona, Spain and Portugal will have a reserved capacity of 5%.

5.3 SHARED PORTUGAL -SPAIN RESOURCES

At the 30th Portugal-Spain summit that took place in Valladolid (Spain) in November 2018, it was established an agreement between Portugal and Spain to jointly develop an Iberian Advanced Computing Network (IACN or RICA), through the coordination of the Barcelona Supercomputing Center (BSC-CNS). This initiative led to the submission of two proposals for HPC machines to the EuroHPC, designated as "Deucalion" and "Mare nostrum 5", that will significantly increase the computer capacity of Portugal and Spain. The principles established in the Valhadolid agreement will allow deepening the cooperation processes at the IACN level, beyond these 2 initial HPC machines, in particular for the investment and development of training and harmonised resource access offers.

5.4. SHARED EUROPEAN RESOURCES

European peta and pre-exascale landscape is rapidly evolving, working towards a common environment where Portugal should be a key member, sharing all computational resources in a collaborative manner. Amongst the most important entities that encompass and promote this massive effort are PRACE and EuroHPC. PRACE stands for Partnership for Advanced Computing in Europe and offers advanced computing resources to academic and industry users through a peer-review process, enabling scientific discovery and innovation. With PRACE, Tier-0 and Tier-1 systems are made accessible to single or multi-year projects in periodic calls as well as training sessions and events in all areas. Noteworthy is the fact that, 10% of total available PRACE resources are also prioritized for an Industry Access Track. So far, in recent calls, several Portuguese researchers have been granted millions of computational hours, while

LCA at University of Coimbra is still in active collaboration as a general partner in PRACE 2 network. On the other hand, Portugal will soon become a contributor, with LCA offering some of its resources to PRACE DECI (Distributed European Computing Initiative) Tier-1 calls.

Portugal is a founding member of EuroHPC, a 1 billion Euro joint initiative between the EU and European countries to develop a World Class Supercomputing Ecosystem in Europe. One of EuroHPC key objectives is to fund and co-sponsor European HPC projects - like Deucalion and MareNostrum 5, where Portugal will hold 65% and 5%, respectively. Apart from these own resources, Portugal will also have access to EuroHPC remaining shared quotas, through peer-reviewed calls that will allocate up to 50% of all pre-exascale and 35% of all petascale resources.

In summary, both PRACE and EuroHPC infrastructures are strongly committed to enhance shared computational resources and boost European competitiveness for the benefit of society.

Several other European platforms are in place to provide support, education and build up capacity – such as the European Technology Platform for High Performance Computing (ETP4HPC, part of EuroHPC), the European Extreme Data & Computing Initiative (EXDCI) and European joint Effort toward a Highly Productive Programming Environment for Heterogeneous Exascale Computing (EPEEC). INESC-ID (Instituto de Engenharias de Sistemas e Computadores), a National Associate Laboratory for Electronics and Informatics, is a main partner of EPEEC.

As exascale class systems are not far in the future, initiatives and infrastructures like these are key to place Europe - and Portugal as part of - at the vanguard of advanced computing in the World.

5.5. OTHER RESOURCES AND PARTNERSHIPS

Portugal has established international partnerships, namely with the University of Texas at Austin (UTAustin) and Carnegie Mellon University (CMU), that are closely related to HPC, although not directly providing physical HPC resources such as computer time. However, these partnerships constitute very important opportunities to increase national competence in the operation and application of AC, namely through joint R&D projects and mobility of researchers.

UTAustin has a special program dedicated to Advanced Computing to promote and support joint projects and training actions on high performance and high throughput computing systems, quantum computing, data management and visualization, aiming at better exploiting the use of advanced computing facilities, at the Texas Advanced Computing Center, Portugal and Europe in a variety of domains, including cities, agriculture, fisheries, space-earth observation, security, and health applications.

CMU main areas of cooperation include the area of Information and Communication Technology, with a particular emphasis in areas related to the processing of large-scale data sets, including Data Science and Engineering, Artificial Intelligence, Machine Learning, Language Technologies, Data Analytics, Cloud Computing and Engineering and Public Policies. These are areas that are envisioned to have more and more contacts with HPC disciplines, as data intensive applications and AI are progressively power users of HPC resources.

5.6. CURRENT INFRASTRUCTURE SHORTCOMINGS

While over the last decade the national advanced computing infrastructure has been upgraded both in terms of hardware and various operational aspects, it still exhibits various shortcomings. In addition, the anticipated expansions will clearly exacerbate them or expose newer issues.

Specifically, the following operational and/or capability shortcomings need to be addressed in the emerging AC infrastructure:

- **Governance and Coordination.** While such an infrastructure exists, it is focused on a handful of physical resources and is ill-equipped to manage the access of a diverse user basis and their diversified needs, as well as to keep up with market evolution by anticipating and even fostering new potential users and needs. Also, acquisition of newer hardware is often not done under a global and coherent policy or strategy. Competence centres often duplicate resources with similar features, thus preventing an increase of diversity of hardware that could benefit the whole infrastructure.

- **Sustainability of Operations.** Reflecting the current lack of a strong governance, it is impossible to establish global usage policies to meet the needs of all users. Allocating the right resources to the right job under such an environment is very hard, if not impossible. As a result, some resources are undersubscribed whereas others are oversubscribed leading to overall resource use inefficiency. Similarly, there is a lack of a solid financial sustainability model that can ensure the continued operations and renovation of the various aspects of the advanced computing infrastructure from new hardware, updated software and human resources.

- **Geographical Coverage.** Because of its history, the current national advanced computing infrastructure is centred around a handful of competence centres, often co-located with the specific hardware resource and its own supporting staff. This severely limits the widespread access to the ACI and hence the experimentation and adoption of computing-based competences.

- **Qualified Staff and Supporting Engineers.** There is a chronic shortage of qualified staff who can operate large supercomputing centres and applications engineers who can advise potential users on how to best use the resources at hand. Portugal is no exception, and the few capable human resources are often only familiar with the operational aspects of their own local resource and thus cannot provide adequate support regarding other centres. Furthermore, there is a lack of qualified engineers prepared to provide guidance and advice in specific HPC application areas, namely for the industry sector. This makes for a very bridle infrastructure where nationwide expertise is not leveraged.

- **International Integration**. Despite various international agreements and memoranda between selected universities and/or the Portuguese government and European supercomputing centres, the exchange of resource usage across centres is not yet a reality as it requires a pro-active exchange of know-how and thus hinges on the availability of qualified human resources.

As it is clear from the various issues outlined above, while the expansion for hardware resources of various kinds (computing, storage and visualization) can be remedy with adequate funding levels, the issues related to human resources (qualified people) require not only immediate attention regarding funding, but a longer term approach and strategy in terms of recruiting, training and the creation of conditions for retaining them.

6. STRATEGY FOR A DYNAMIC AND SUSTAINABLE ADVANCED COMPUTING ENVIRONMENT

The ACP.2030 strategy is structured in three main pillars, namely the infostructure, infrastructure and people. A detailed description of these pillars is provided, followed by the presentation of the vision for supporting effective AC systems in what is referred to as Green HPC and the support for various research aspects related to HPC. Similarly, a vision is outlined to support innovation and industrial development using the AC infrastructure. Lastly, it is addressed the paramount importance of continuing to engage in European and international collaborations to foster AC uptake by all domains of activity. Last, but not the least, some key aspects are provided for the financial sustainability of the ACP.2030 effort in the short and medium terms.

The core of ACP.2030 is built around 3 pillars, namely the infrastructure, the people (or human resources) and the infostructure, as summarized next.

6.1 INFRASTRUCTURE

The current national advanced computing infrastructure operates a series of operational centers (OC), that will provide in the short term a combined capacity of 12 Peta FLOPS. In 2020, EuroHPC and FCT will procure a 10 Peta FLOP machine, Deucalion, to be installed in Portugal, greatly expanding the national supercomputing capability.

In addition, Portugal has a standing partnership with Spain, Turkey and Croatia which also grants access to 5% of a pre-exascale class machine to be procured and operated by BSC in the coming year of 2021. Physical resources of ACP.2030 consist of a mix of clusters, computing grids as well as supercomputers, the latter installed in Riba d'Ave in the northern region of the country. The national operational centres and the international centres providing computational resources through established partnerships will be hyperconnected and coordinated by the National Advanced Computing Network (the Portuguese NREN - National research and education network). Together, these centres will provide a combined computational capacity of 20 Pet FLOPS by the end of 2022, representing an unprecedented growth and availability of computing power. Such resources represent a great national trial to which companies and the research community must rise to the challenge to reap off the benefits by creating a new wave of innovative and added-value services and products.

A variety of competence centres will be installed nationwide, with the specific mission of actively promoting the use of advanced computing and supporting research groups and industry with high specialization in different scientific and application areas. To accomplish this mission, each competence centre will be equipped with local storage capacity, visualization infrastructures and equipment that best suits the specialisation areas covered as well as with very high bandwidth connections to the operational centres. It is anticipated that such installed capacity, together with a body of qualified human resources, will enable these local centres to actively promote the use of AC and provide expertise in the analysis and visualization of large computational data sets.

The strategy rests on the aforementioned AC resources that should evolve in the near future from the current loosely organized governance setting defined by the national advanced computing network to a more cohesive and integrated national computing centre.

6.2 PEOPLE

There is a recognized shortage of human resources with competencies related to advanced computing, be it at the programming level, or application development, or in data analysis and visualization. In this context, this program will support a series of actions towards building a reliable and stable advanced computing workforce, leveraging existing long-term collaborations such as EGEE and PRACE, and newer ones, such as the UT Austin - Portugal collaboration, involving the upskilling and/or reskilling of the current workforce and also people who will make the transition from academia to a services-based industry in the domain of advanced computing.

In addition, the strategy will also promote the creation of education and training efforts that aim at increasing the offerings of advanced computing expertise in academia in the topics of parallel and distributed computing programming as well as resilience and data analysis plus visualization. While these offerings tend to be generic in nature, FCT, through the EuroCC and similar projects, will promote the development of short courses focusing on specific industry needs to accelerate the uptake of AC-based techniques.

Competence centres also have an important role to play in attracting and supporting human resources with diverse AC specialisations, in particular by developing efforts to facilitate the access to RNCA resources for education and training programmes as well as by promoting sensibilisation initiatives presenting the career opportunities and potential that AC activities has to offer.

Establishing a productive community of AC experts to exploit the available computing resources depends on a combination of formal education, constant short training and exchange of specific techniques and best-practices. The latter can only be achieved by leveraging on the many international partnerships Portugal has with universities and computing centres from countries with greater experience in the different fields of specialisation. To this extent, ACP.2030 will promote the creation of education, training and internship partnerships to foster the creation of new partnerships and direct existing one to serve the national AC qualification effort.

The near and long future of AC technology education is also considered by promoting the earlier experimentation and adoption of newer models of computation (e.g., quantum and neuromorphic), particularly at high education levels, so that future human resources are better prepared to face upcoming challenges.

6.3 INFOSTRUCTURE

Infrastructure availability and people qualification are two fundamental aspects of ACP.2030, but these will have little effect in the creation and strengthening of value chains without proper instruments that generate fruitful and enduring collaborations between the two. The infostructure is therefore a comprehensive set of catalyser actions geared towards the engagement of people, companies, education and research institutions to create long-term endeavours of smart use of the available AC infrastructure.

AC applications are spreading to almost every economic and research areas, pushed by an ever-increasing availability of computing resources and the fast-paced developments in

AC software. For the infrastructure to perform its mission of triggering and promoting the many advancing fronts of AC application, a diversified set of actions must be put in place. Chiefly among these, is the eligibility of AC expenses in research and innovation projects in all areas that apply for incentives from the state. Another action related to this is the creation of a program specifically designed to support the introduction of AC tasks in existing business and production processes. These incentives must not only reach the final beneficiaries of the AC resources but also the entire chain of intervenients, namely the operational centres, competences centres and research and development entities.

The value chains using AC being fostered here will have different arrangements in the field, depending on a myriad of factors. Some end-users will make heavy use of AC and will need in-house qualified teams of professionals, while others will have fewer AC activities and may rely more on third-party services. No matter what the usage level or expertise location, much of the success of AC applications ultimately depend on the experience and ingenuity of the professionals working in the different specialization areas needed to deliver added-value results. The importance of increasing the education and training of these professionals has already been discussed, but one must also create the right conditions in AC entities to receive and host this highly qualified human resources. The infostructure must therefore take actions to create stable and rewarding environments, where AC professionals can continuously improve their skills and apply them in ever more challenging projects.

The AC market will of course evolve under these and other variables, but at this early stage of development it is paramount to put in place instruments aiding the principal players in this market, namely the end-users in the different economic sectors, the AC infrastructure providers and the AC service provider intermediaries. Each of these players have different needs and expectations of the value chains to be created in the AC market, and all must be considered to trigger virtuous cycles in the AC national economy. The role of end-users and AC infrastructure providers has already been addressed under the different ACP.2030 pillars, as well as how actions must be implemented to stimulate their engagement with AC.

AC intermediaries provide AC specialised services to other companies and institutions, often in a limited set of applications areas, typically being involved in the installation and customisation of software and AC platforms, software integration, job tuning, parallel programming, data analysis and visualisation. Standing between the end-users and infrastructure providers, these agents have an important role to play in the AC market, which is particularly relevant for the introduction of AC to new companies and sectors. The potential of the intermediary actors can go well beyond the increase and strengthening of a national AC market. There is a thriving international market for these services, where national players can certainly become capacitated to intervene, especially after gaining experience and having results to show from the national market.
The infostructure includes actions to provide incentives for the development and delivery of intermediary activities, considering not only the triggering role of these players in the creation of AC value chains, but also as an opportunity to create a new AC services sector.

In ACP.2030, software is even more important than the infrastructure, because if the latter demands investments that are beyond Portugal dimension, the former depends on conditions where the country is particularly well positioned to invest and realize relevant results. The increasing number of ICT graduates, a thriving digital entrepreneurial environment and a growing ICT economic activity are just but a few of the elements positioning the country in a favourable position to tackle the highly dynamic AC software market.

The infostructure pillar also addresses the software dimension of the AC ecosystem, often designated as the software stack, which includes among other components, the job managing software, the operating system, the networking software and machine-level management tools. This element is particularly relevant in the current AC setting, where hybrid AC solutions are emerging, resorting to smart combinations of AC and standard computing solutions. Furthermore, it is of utmost importance to invest on the development and maintenance of a well-articulated software stack running on the operational centres that facilitates as much as possible the entrance of new AC users. This is an effort to be carried in close cooperation with more experienced advanced computing centres in other countries, through the established AC international partnerships in place.

In the HPC landscape there are different types of systems and solutions, with a clear distinction being drawn between the classical centralized Peta-scale and pre-exascale class of systems (a.k.a. supercomputers) and the grid-oriented. In terms of the operating systems both classes of systems are dominated by the Linux variants. For example, in the TOP500 supercomputers, 95% use Linux. In the grid world the ratio between Linux and non-Linux based (e.g., Windows) machines is more balanced.

Focusing on HPC systems (not grid-based), it is common for the adoption of advanced computing libraries/frameworks, such the MPI and OpenMP libraries given the hierarchical storage and close connectivity between nodes. Typically, CPU cores share physical memory within nodes (and in some cases the same is true across nodes), but distance nodes on the same HPC machine interact via message passing using the popular MPI library.

In grid-based computing, where several distributed sub-clusters are federated on to a common architecture and resource pool, it is common to use application workflows. These environments export a programming model akin to message passing where a computation is partitioned into disjoint tasks or jobs assigned to different clusters across the network, and whose inputs and outputs are exposed to the workflow software that orchestrates their execution and communication. Typically, they include a web interface that the end user can utilize with minimum parametrization time.

Initiatives, such as the European EGI have developed the Unified Middleware Distribution (UMD) software suite that is an integrated set of software components packaged for deployment as production quality services in EGI. UMD has a comprehensive set of more than 50 software products, for functions such as usage accounting, storing and retrieving huge amounts of data, job management, distributed database caching system, and many other categories.

Lastly, at the application level, the user needs to run his applications in the physical resources. The user normally has its own software that needs to be compiled at the local environment on the HPC cluster. There are currently hundreds of Advanced Computing applications and variants, distributed alongside the broad spectrum of scientific and technological domains, as is the case of LAMMPS for Molecular Dynamics) simulations, Hadoop for Big Data computing or TensorFlow for Deep Learning.

Above this application level, there is an additional layer that deals with the management of the physical resources themselves. Currently, and at a national level, there is a layer of management of the overall advanced computing infrastructure between FCT and the operational centres in terms of the used energy, overall use of the machines and allocation of time on these machines by research groups who must compete for them. There is also an effort to ensure data protection and privacy.

6.4 GREEN HPC

By 2030, it is expected that the power usage of ICT (Information and Communications Technology) related services will reach 3% at the planet level, with a substantial portion attributed to large scale computing centres. Peta-scale and exascale class of facilities also raise the issues of delivery of power and cooling solutions to support the facilities that house these systems. The growing reliance on information derived by advanced large-scale data mining and AI-based techniques of current industrialized economies will only exacerbate these power and energy issues.

In this context, and not surprisingly, energy efficiency is a paramount concern in the European supercomputing agenda, as it is clearly patent on EuroHPC's multiyear strategic agenda. In addition to more efficient computing devices taking advantage of GPU-based processing units and emerging storage technologies, custom and application specific architectures (e.g., FPGA-based) are also being sought. Orthogonal to these efforts, there has also been a recent push towards fitting large-scale computing centres with "greener" energy sources thus attempting to reduce the carbon footprint of these large computing centres. While one of its largest machines – "Bob" – currently operates with a Power Utilization Effectiveness (PUE) of 1.7, Portugal is committed to operate its newer super-computer, Deucalion, under a fully sustainable energy management and consumption strategy.

As part of the INCoDe.2030 strategy for the expansion and promotion of HPC-based technologies that can support various economic activities and markets, the development of greener HPC should rest on the following aspects:

1.Privileging the use of energy efficient computing, storage and connectivity systems. While in the past most of HPC class systems have exclusively used x86 computing architectures, emerging more energy efficient nodes are contemplating other architectures such as ARM. In addition, GPU-based nodes and even custom computing nodes are being investigated to substantially improve energy efficiency, not only for general class of application but also for specific application domains.

2. Designing and leveraging node cooling solutions, either air- or water-based that are more efficient than today's solutions. In addition, promote the use of renewable energy sources (e.g., eolic and/or thermal) for the operation of the computing centres in a synergistic fashion with the cooling techniques themselves.

3. Promoting the development and use of "greener" operational management techniques such as the use of dynamic voltage frequency scaling (DVFS) to best match the application needs and pre-defined power/energy and thermal budgets (e.g., ref Green-Queue from SDSC) either at a job-allocation stage of within the scope of each job. Similarly, suggest, either based on ML techniques the use of queues with selected resource characteristics. For instance, submit selected applications to specific pool queues with a selected mix of GPU-based and x86-based nodes.

4. Promoting and training users in best programming practices regarding a) the identification of inefficient code sections; b) reorganization of code sections to best exploit concurrency and matching to the native available parallelism at the node level and c) use of accelerator-based programming techniques to improve application energy efficiency.

Despite the obvious benefits of each of these techniques in isolation, a substantial technical challenge lies in the effective integration of some of these practices in the deployment and daily-operation of these centers. In addition, a non-trivial effort is required in the education of the workforce to be aware and exploit the various opportunities for energy efficiency in their applications. A major and very effective driver is cost where energy efficient computations that use less overall energy and exhibit lower power peaks will cost substantially less than less efficient ones.

6.5. RESEARCH

An important aspect of the INCoDe.2030 program is the support for research in advanced computing architectures, programming and visualization related to big-data analytics, and in particular in making HPC very energy efficient. In this context, one may anticipate the use of the advanced computing infrastructure as a testbed for the exploration of the following aspect of computing via either prototypical nodes or via the access to other facilities under European agreements (e.g., PRACE):

1. Evaluation of advanced computing architectures, including the use of ARM-based processors or the RISC-V open source processors, in the design of power efficient computing architectures. In this context, solutions will appear evaluating prototype systems using commercially emerging storage technologies (such as phase-change memories).

2. Exploration of alternative (still silicon-based) computing architectures, such as custom-computing architecture based either on FPGA or DSP aimed at drastically reducing power and even processing-in-memory (PIM) techniques.

3. At the operational level, the use of aggressive application-dependent DVFS for enhanced power and energy efficiency in the context of large scale multi-threading codes.

4. At the programming level the use and development of communication-free and/or communication-oblivious algorithms that are less reliant on long communication delays in large scale computing.

In a not so distant future, it is anticipated that the infrastructure will be expanded with experimental nodes exploiting alternative computing technologies such as the use of analogic and digital technology in what is currently named neuromorphic computing and even include offering (in a variety of access modes) of quantum computing.

These research efforts will clearly involve not only the national academia but also industry via focused programs that aim at creating the conditions for emerging high-value start-ups companies in AC-related techniques and services.

6.6. INNOVATION & INDUSTRIAL DEVELOPMENT

Involving industry and actively promoting its uptake of AC-based services and technology, is key for promoting innovation in various technology-based domains, and, ultimately, for sustained development of industry.

In this context, the INCoDe.2030 program will undertake the following specific actions:

1. Promote and finance partnerships between academia and industry for the development and use of existing applications in support of specific domains. In addition, it will promote the use of RNCA services in their production processes.

2. Promote the creation of financial conditions from the creation and growth of start-ups oriented toward AC-based services and technology, in particular on the development of novel AC software for data mining, engineering and visualization.

3. Support the creation of short courses for specific AC techniques and technologies oriented towards industry needs.

A key, preliminary action item in this context, is a survey of existing academia and industrial capabilities in terms of know-how and competences in HPC domains, and needs in manufacturing or emerging markets.

6.7. INTERNATIONAL COLLABORATION

Given the limited national resources, Portugal is leveraging existing partnerships and striking new collaborations within the EU and worldwide, in particular with Spain and Brasil, respectively. In Europe, FCT will leverage historical collaborations within the PRACE and EGI.EU programs, which aim mainly at securing computing time in infrastructure maintained by these consortia. Similarly, as previously mentioned, FCT is procuring a new petascale class machine funded by the EuroHPC program and to have access to a preexascale class machine to be operated by BSC starting 2021.

Complementary to these efforts, FCT has established partnerships with other organizations and HPC centres, most notably, the Barcelona Supercomputing Center (BSC), with whom is seeking to enhance its expertise in operational aspects of large scale computing centres by engaging with the staff of these centres and exchanging know-how, experiences and technical competence in management tools in use at BSC. Elsewhere, for example, in the USA, FCT has also engaged the Texas Advanced Computing Center (TACC) with whom several of its staff members have exchanged experiences and are actively replicating part of the "Bob" machine info-structure in support of this machine's operation in Portugal. At a more academic level, FCT is engaged with US academia, specifically CMU and UT Austin, where research-oriented programs in application areas akin to HPC (such as ML and AI) are underway.

At a national level, FCT, is also seeking to extend its partnership with the newly created AIR Center and PT Space to broaden the user base of HPC to the domains supported by these centres such as weather prediction and climate modelling, key areas of great societal impact. A similar stance is being pursued with other institutions in Brazil, Latin America, Africa and Asia, leveraging Portugal's privileged political relations with those countries or regions.

6.8. SUSTAINABILITY

With a typical life cycle of 5 years or less, and costs that range in the millions of Euros, Advanced Computing resources are expensive to install and maintain. Main sources of operational costs are energy consumption cost and support staff. As an example, the first (non-accelerated CPU-only) machine on the TOP 500 list with an energy dissipation below 1M Watt ranks 50 on this list (the Oakridge-CX machine) whereas the top spot is taken by a 10 M Watt machine (the Oakridge-Summit machine with CPUs and GPUs). In Portugal, an HPC machine that dissipates 1M Watt of electric power (by current standard not even a very large system) has a yearly direct energy cost of more than 1 million euros, even when operated in a highly efficient datacentre.

The cost of support staff who need to keep the machine running smoothly and help users run computer jobs is also high. Technical staff are in high demand and often have very lucrative offers from other branches of industry. Recruiting (typically from academia), training and retaining staff for the operation of these large scale centres and supporting a broad and diverse user community is, perhaps, a bigger financial challenge than the procurement of the system itself.

Advanced Computing is therefore not possible to perform without investing significant financial resources, to install, operate and evolve its machines. Portugal will need a mix of funding sources to make advanced computing a sustainable activity, from European structural funds, to the national budget and cost recovery fees from direct usage. All these potential funding sources need to be articulated, as it is not likely that one single source could provide a sustainable source. In order to allow cost recovery fees from direct use, the organizational architecture in place should allow for efficient accounting, billing and charging processes.

Even though HPC demands significant financial investments, the economic benefits opportunities it opens far exceeds the costs, in particular within the context of the current fast-growing digital economy. In a study carried out by research firm IDC it was found that for each dollar enterprises' investment in HPC systems, it generates $515 in revenue and $43 in profits and/or cost savings. The same study found even higher values for European Union HPC projects that generated financial returns, asserting that, on average, for each euro invested in HPC, €867 were generated in increased revenue and €69 in profits. The 59 European projects analysed reached a combined increased revenue of €133.1 billion, amounting to about €230 million per project on average.

7. ACTION PLAN (2020-2022)

Having set out the national and international AC panorama and the main guidelines of the strategy, it is important to set out an operational plan of comprehensive actions in support of the objectives for the INCoDe.2030 program, specifically addressing actions towards increasing national capacity in terms of the AC infrastructure, info-structure and human resources. Given its importance, selected educational actions have been included, specifically geared towards industry as well as technical support to facilitate the adoption of HPC-based services and applications by industry.

The specific aims each action is supporting are included for each of the three pillars of the national ACP.2030 strategy.

INFOSTRUCTURE

OBJECTIVE 1 – IMPLEMENT A MANAGEMENT AND OPERATIONAL MODEL FOR RNCA

Considering the current macro economical context, as well as the scarcity of qualified human resources for the management and operation of computational infrastructures, which are operated by various entities, it is essential to create mechanisms that allow an articulation of all services offered to the interested communities. Since its inception, the national advanced computing network(RNCA) will increasingly articulate all operational and competence centres (OC and CC), offering a service catalogue, access policy and transparent mechanisms to be opened to national and international participants, with relevant capacity and compatible access policies. This network allows the maximization and efficient use of the available resources in terms of equipment housing, communication resources, computational services and data storage. The following actions contribute to this purpose:

ACTION 1.1

Create mechanisms for RNCA governance.
In order to have a fully functioning national advanced computing network, it's crucial to implement a clear, inclusive and well-balanced governance model. That model should be the result of public consultation and should guarantee the transparency of all processes as well as providing guidance for the evolution of the network. It is envisaged that RNCA should evolve to become an autonomous legal entity fully dedicated to the advancement of advanced computing in Portugal. As an autonomous legal entity, RNCA could more easily apply for public funding, with the possibility of partnering with private entities, and also rely on a set of efficient cost recovery processes.

ACTION 1.2

Manage operational teams at the RNCA centres, allowing computational services to be provided in a continuous and professional manner. This action is the bedrock of all other developments. It's fundamental to work towards having stable and professional teams operate the computing resources and giving support to the different user communities, ranging from those more apt and specialized to those with less skills in using advanced computing systems. This action should include the design and periodic review of service management processes, such as providing user documentation, terms of use, access policies and other similar necessities.

ACTION 1.3

Create mechanisms of regular consultation of the user communities, in order to implement constant improvement procedures and assure fully transparent and accessible processes of awarding computing resources. Implementation of independent and verifiable mechanisms for consulting the user communities about the delivered quality of computational resources and support to its proper and efficient usage. In more practical terms, there should be proper channels for user complaints and compliments as well as a specific position for a service compliance officer, focused on the user experience and satisfaction.

OBJECTIVE 2 – PROMOTE RNCA SUSTAINABILITY

In order to provide reliable, sustainable and high-quality advanced computing services, several requirements must be met, namely technical, human and financial capabilities. RNCA should move towards a professional management model, with specialized and dedicated operational teams, maintaining close proximity to the communities served. The following actions contribute to this specific objective:

ACTION 2.1

Implement state of the art green computing measures to increase efficiency and environmental sustainability. Higher efficiency systems allow for more computing power to be provided with less consumed energy. This does not by itself guarantee environmental sustainability, as the extra margin gained by increased efficiency, can quickly be consumed by newer applications that were not possible before [[12]]. However, since new advanced computing applications are considered beneficial to science, society and the environment, this strategy does focus on increased efficiency, that should be obtained by the following 4 goals:

• Procure high efficiency data centres for hosting advanced computing systems, with Power-Use-Efficiency (PUE) ratios ideally below or equal to 1,1.

• Procure high efficiency computing systems, with optimized performance in terms of FLOPS per Watt ratio and with power capping mechanisms by varying performance characteristics.

• Provide user (programmer) education and training in using advanced computing resources with the least energy impact as possible, using accelerator libraries whenever possible, optimizing code and adhering to general resource exploration rules, such as an economic resource usage as a mandatory principle.

• Develop specific service management processes, considering such initiatives as showing the final user energy consumption by specific usage, or promoting formal processes as ecological footprint measurement or environmental code of conduct.

ACTION 2.2

Explore diverse opportunities in national and international funding systems for RNCA's sustainability and development, starting with the following sources of funding for the operation of the advanced computing network in Portugal:

• European structural funds, that are more applicable for investment expenses, such as new advanced computing machines for European user communities. These funds can be specific for advanced computing, like EuroHPC's calls for hosting HPC machines in European countries, or can be for other purposes, that allow advanced computing as an eligible expenditure for the original project goals.

• While several research and innovation projects require advanced computing resources today, many more haven't been designed to do so,

[12] Jevons paradox

wasting great opportunities for R&D cost and time reductions as well as improved quality results. These persistent inefficiencies in the national research and innovation system must be addressed by putting in place programs to clearly present direct benefits of HPC for each economic sector and to demand a self-diagnose procedure of potential AC improvements in specific sector project proposals.

• National budget funds, that must close the gap left by structural funds, especially with regards to operating expenses, such as energy and personnel costs.

• Paid services.

To best explore these opportunities, the following sub-actions should be realized: (i) Maintain an updated record, by the end of each year, of expenses incurred by all partners in providing services within the scope of RNCA; (ii) By the beginning of each year provide a forecast cost plan, together with a list of identifiable funding systems and gap analysis for RNCA funding requirements at various levels, namely necessary investments and operational expenses. Provide a critical analysis of the impact of lack of funding; and (iii) Develop administrative and accounting processes that allow for smooth operation of paid RNCA services.

OBJECTIVE 3 – ALIGN DATA MANAGEMENT WITH EOSC: EUROPEAN OPEN SCIENCE CLOUD

The National Advanced Computing infrastructure (RNCA) seeks to strengthen and align its internal processes and mechanisms for the management and protection of data across all domains of knowledge with accepted and proven international practices. To this effect, FCT will implement the following actions.

ACTION 3.1

Ensure, whenever applicable, federation of AC resources with the European Open Science Cloud (EOSC).

ACTION 3.2.

Ensure the existence of large volume data storage services (Big Data) according to the FAIR principles (Findable, Accessible, Interoperable, Reusable) as well as the possibility to federate in the EOSC the services as well as the data.

ACTION 3.3.

Ensure the integration with other national infrastructures for access and curation of research data, enabling interoperability as well as resource reuse.

ACTION 3.4.

Operate as a national competence centre in what concerns the access and preservation of FAIR research data, inside RNCA's scope of action.

OBJECTIVE 4 – DATA SECURITY AND PRIVACY

There is a growing concern worldwide about data security and privacy, not only for the individual, but equally important in industry and at a governmental level. Threats vary from hampering the availability of services to data breaches. To ensure an adequate level of protection to all RNCA users, the following actions will be pursued.

ACTION 4.1

Elaborate a cybersecurity plan for RNCA, in conformity with recent European laws.

Although a certified implementation of a security policy may lead to a bloated and expensive process, current practices should be followed such as asset identification, security objectives definition, controls and an overall organized process. Practices should include compliance mechanisms with General Data Protection Regulation (GDPR) and other relevant norms. A fully certified security process may be required for parts of RNCA that have special requirements, namely those that relate to process and storage of clinical data, or other sensitive information.

ACTION 4.2

Implement articulation processes of RNCA with RCTS CERT, concerning cybersecurity.

RCTS CERT are security services in place for the Portuguese NREN - National Research and Education Network. RCTS CERT has been a FIRST (Forum of Incident Response and Security Teams) member since 2011 and earned a Trusted Introducer (https://www.trusted-introducer.org/) certification in January 2015, becoming the first batch of national teams to be certified. RCTS CERT should assume a very important role in defining RNCA security policy, coordinating compliance analysis and supporting RNCA in all matters concerning cybersecurity. RCTS CERT should handle all security incidents related to RNCA. Furthermore, It should be clear what parts of RNCA have different levels of security; ideally, every RNCA resource should have a cybersecurity statement issued by RCTS CERT.

ACTION 4.3

Implement privacy mechanism to support industry requirements and procedures.

Industry innovation processes may involve trade secrets that are to be protected within RNCA resources and operational processes. As a first stage of approaching this potential difficulty, RNCA should conduct a sensitivity analysis with industry representatives regarding privacy issues and other cybersecurity related requirements. With that information and knowing RNCA's assets and position, a gap analysis should be conducted, and a balanced improvement roadmap implemented. At all times it should be clear to industry users what the implemented level of security is.

INFRASTRUCTURE

OBJECTIVE 5 – ACQUIRE AND MODERNIZE COMPUTATIONAL RESOURCES FOR RNCA

The following actions aim at greatly enhancing the aggregate computational and storage capacity of the RNCA by the end of 2021 through the modernization of existing resources and acquisition of newer computational, storage and communication systems.

ACTION 5.1

Promote technical and physical conditions at the RNCA operational centres, required for a sustainable and professional computational service. Procure and acquire modern computational systems fitted with state-of-the-art processor and storage architectures to increase the computational and storage capability of individual systems.

ACTION 5.2

Develop a communications network that includes all competence centres (CC), articulated with the operational centres (OC), that combines diverse equipment and technical skills and resources in support of academia and industry in all domains of application.

ACTION 5.3

Increase quantity and quality of long-term storage capacity for research and industrial datasets.

ACTION 5.4

Physically connect operational centres (OC) to competence centres (CC), and these to the national network (RCTS - Rede, Ciência

Tecnologia e Sociedade (Science, Technology, Society Portuguese network), connecting the whole network to similar and wider European and World networks. This connectivity must support the exchange of large scale and large volume data.

ACTION 5.5

Integrate the national AC resources with other national and international authentication and authorization infrastructures, such as Ciência ID, RCTSaai/eduGAIN.

ACTION 5.6

Conduct a requirements assessment for the industry sector in terms of advanced computing and define a clear path to meet specific requirements.

OBJECTIVE 6 – INTEGRATE THE NATIONAL AC INFRASTRUCTURE AT AN INTERNATIONAL LEVEL

This integration will promote the sharing of resources, bring new opportunities and promote mobility and research in an extended international network. National participation at the main international networks of advanced computing requires a constant effort of technological progress, as well as best practices development and integration in national context. This will only be possible through an active and qualitative participation of all parts. The following actions contribute to this aim:

ACTION 6.1

Develop an Iberian Advanced Computing Network (IACN or RICA - Rede Ibérica da Computação Avançada), in articulation with Spain. Pursuant to the Valladolid agreement between the governments of Portugal and Spain, where an advanced computing iberian network has been created, both countries (FCT in Portugal) will coordinate policies and initiatives in supercomputing, distributed and quantum computing enabling advances in areas such as medical, pharmaceutical and biotechnology industry, agriculture, new materials energy security and communications.

ACTION 6.2

Participate with other European advanced computing institutions and their initiatives: EuroHPC, PRACE, EGI, BDVA and ETP4HPC, centres of excellence and centres of competence. In this context, FCT will facilitate the access to its advanced computing infrastructure to research and development projects funded vehicles such as H2020's European Commission RIA and CSA actions.

ACTION 6.3

Develop partnerships with other World regions to share computational resources and collaborate in funding grants. Specifically, FCT will encourage research projects where researchers collaborate in the context of various international organizations (such as the AIR Centre or the SKA) either funding personal or computing time in the national computing infrastructure. Other selected collaborative efforts headed by selected educational institutions in Portugal will be supported extending their reach in South America and Asia.

OBJECTIVE 7 – EXPLORE EMERGING ADVANCED COMPUTING TECHNOLOGIES

The existence of state-of-the-art computational facilities as part of the RNCA will enable experimentation and early evaluation of alternative and/or emerging computing paradigms. Examples include the use of hybrid computing solutions that make use of FPGAs for the implementation of custom and thus highly energy-efficient computing solutions and/or early evaluation of emerging computing paradigms such as neuromorphic computing for selected application domains or quantum computing. Within this context the following actions are proposed:

ACTION 7.1

To make available, on a national level, experimental advanced computing platforms and resources, based on emerging technologies, for researchers to use. RNCA should establish partnerships with existing institutions that run state of the art facilities, such as quantum computing hardware or simulators. These resources and accompanying processes, such as usage instructions and documentation, should be made available to the research community under different arrangements targeting both the application and research of these novel computational systems.

Whenever there are no available high-quality partnerships possible, RNCA should procure or subcontract the procurement, installation and exploration of these advanced resources.

ACTION 7.2

To engage in national and international efforts and projects aimed at promoting the development and piloting of the next generation of computing solutions. FCT should support national initiatives that enable specialists to have a relevant role within these contexts. This is better performed at two different levels: national management contacts and field specialists contacts, that should be engaged in such projects.

ACTION 7.3

RNCA should include in its communication plan the aggregation, promotion and facilitate the dissemination of knowledge about novel and emerging solutions in all areas of advanced computing.

PEOPLE

OBJECTIVE 8 – ADVANCED COMPUTING EDUCATION AND TRAINING

Recruiting, training and educating a high-value workforce in advanced computing technologies is key for the sustainability of the various aspects of the RNCA, from the day-to-day operation of the network to its efficient use and adaptation to emerging technologies (e.g., quantum or custom computing architectures) that need to be integrated in its fabric. People training is the single most relevant aspect to maximize effectiveness, achieve optimizations at various levels and extract the most value from the computing infrastructure. To this extent, the following actions are established:

ACTION 8.1

Set up a national program of educational and training actions for AC researchers and RNCA users in particular. The need for continuous education for all HPC users is critical to promote the best use of programming and execution techniques that are best fitted to each application domain and computing system.

ACTION 8.2

Set up a national program of education and training actions for trainers and mentors, focusing on selected user communities who are heavy users of HPC computing cycles. These include, but are not limited to, Computational Hydraulics, Bioinformatics and Applied Mathematics communities. Various educational and training actions will be carried out with their endorsement and support to increase the reach and effectiveness of these actions.

ACTION 8.3

Create funding programs to financially support actions articulated with existing international educational programs, namely RES.ES, PRACE, Portugal-UTAustin, Portugal-CMU, Ibergrid, EGI, amongst others. These programs are designed to support short-term training missions where human resources will attend existing refresher or educational programs at the selected international institutions.

ACTION 8.4

Promote awareness and facilitate the use of RNCA services, through the development of e-learning resources such as webinars and MOOC modules. These resources should cover various aspects of the RNCA systems (e.g., covering the various types of computing and storage resources) and services (e.g., covering a wide range of services from access to visualization and archival) and be updated regularly to reflect the modernization of the RNCA.

OBJECTIVE 9 – PROMOTE ADVANCED COMPUTING THROUGH RNCA AND BEYOND

To ensure the widespread use of the advanced computing resources, a broad effort needs to be made to increase the awareness in various communities about the advantages AC brings to many economic sectors. Such an objective will be procured through the following actions:

ACTION 9.1

Develop and implement a communication plan for RNCA and its services, documents and results, through the website and other media. Strategically promote RNCA to national research, development and innovation institutions, as all other interested entities. Bring together the best use cases and testimonials and share the massive potential of AC infrastructure through a myriad of resources, such as audio-visual and digital media, digital archive with MOOCs and webinars, website, newsletters and all means necessary to increase the awareness of RNCA and advanced computing to all communities.

ACTION 9.2

Produce regular reports, news and information regarding the usage of advanced computing resources. As the usage of AC resources takes shape and steadily increases, collect all input/output data in the form of performance indicators, statistics, users feedback, published data and any other relevant information. Convert all numbers, facts and figures and use them in monthly graphs published on the website, RNCA annual reports, other media outreach documents and events. This data stack will be key to quantitatively evaluate performance, outreach capabilities and set the future direction of ACP.2030.

ACTION 9.3

Promote communication and dissemination efforts among user communities at large. Beyond RNCA, efforts to increase advanced computing awareness may start independently at schools, universities, science awareness promotion agencies, public administration, civil protection action, under thematic contexts of major catastrophes, driverless cars platforms, manufacturing with new materials or prevention of disease outbreaks. As everyone and all organisations may be involved, it is imperative to recognize and spread word about such cyberinfrastructure and its powerful nature, with infostructure and infrastructure joining efforts to help people understand the positive impact of advanced technology in everyday life.

ACTION 9.4

Engage innovation & industry sectors with a strong communications strategy. Following INCoDe2030 principles, AC resources could easily reach research and public institutions, but they should also play a key role in private companies too. Synergies and partnerships with SMEs and innovations agencies (eg.: ANI - National Innovation Agency) should be encouraged, with RNCA taking the leadership in showcasing national AC infrastructure, best case studies, funding opportunities and attribution of computational resources through regular and competitive calls. This can well be achieved by promoting RNCA in strategic events, established protocols and digital media. Both parties benefit from this approach, as companies also gain in technology awareness and training as in competitiveness in national/international markets.

8. ACRONYMS AND DEFINITIONS

AC	Advanced computing
ACI	Advanced CyberInfrastructure
ACP 2030	Advanced Computing Portugal 2030 is strategically aimed to promote and expand ACI by a factor of 100 until 2030
AI	Artificial Intelligence
AI Portugal 2030	National strategy on Artificial Intelligence until 2030
AIR CENTER	Atlantic International Research Center
ARM	CPU based processor based on RISC (reduced instruction set computer), acronym for Advanced RISC Machine, originally Acorn RISC Machine
ASIC	Application-Specific Integrated Circuits
AWS	Amazon Web Services are comercial on-demand cloud computing services
BCO	Benchmark Code Owner
BDVA	Big Data Value Association **http://www.bdva.eu/**
BSC-CNS	Barcelona Supercomputing Center - Centro Nacional de Supercomputación **https://www.bsc.es/**
CERN	*Conseil Européen pour la Recherche Nucléaire*, also known as European Organization for Nuclear Research **https://home.cern/**
CSA	Coordination and support actions included in Horizon 2020 program
DECI	Distributed European Computing Initiative integrated in PRACE ecosystem of Tier-1 HPC facilities and services **http://www.prace-ri.eu/deci-projects/**
Deucalion	Supercomputer approved by EuroHPC, to be installed in 2020 at MACC
DSP	Digital signal processor
CC	competence centers
CPU	Central Processing Unit
CMU	Carnegie Mellon University **https://www.cmu.edu/**
DVFS	Dynamic voltage frequency scaling
DSP	Digital Signal Processor
eduGAIN	The eduGAIN interfederation service simplifies access to content, services and resources for the global research and education community **https://edugain.org/**
EGI	European Grid Infrastructure
Engage SKA	Enable Green E-Sciences for the Square Kilometre Array **https://engageska-portugal.pt/**
EOSC	European Open Science Cloud
EPEEC	European joint Effort toward a Highly Productive Programming Environment for Heterogeneous Exascale Computing **https://epeec-project.eu/**
ETP4HPC	European Technology Platform for High Performance Computing **https://www.etp4hpc.eu/**
EU	European Union
EuroCC	HPC Competence Centers, call EuroHPC-04-2019
EuroHPC, EuroHPC JU	EuroHPC Joint Undertaking is a 1 billion Euro joint initiative between the EU and European countries to develop a World Class Supercomputing Ecosystem in Europe **https://eurohpc-ju.europa.eu/**

Exascale, pre-exascale	Refers to methods and processes for using supercomputers capable of performing at least 1 EFLOPS or storage systems capable of storing at least 1 EB. Pre-exascale is the precursor of exascale, with performance well above 1PFLOPS but still under 1EFLOPS.
EXDCI	European Extreme Data & Computing Initiative **https://exdci.eu/**
FAIR	FAIR principles - Findable, Accessible, Interoperable, Reusable
FCCN, unidade FCCN	FCCN - National Scientific Computing unit of FCT IP **https://www.fccn.pt/**
FCT, FCT IP	Scientific and Technology foundation - Public Institution (acronym for Fundação para a Ciência e Tecnologia, Instituto Público) **https://www.fct.pt/index.phtml.pt**
FLOP(S), TFLOPS, PFLOPS, EFLOPS	FLoating-point Operations Per Second. TFLOPS or teraFLOPS - 1012 floating points per second. PFLOPS or petaFLOPS - 1015 floating points per second. EFLOPS or exaFLOPS - 1018 floating points per second.
FPGA	Field-programmable Gate Arrays
FTE	Full-time Equivalent
GPU	Graphic Processing Unit
HPC	High Performance Computing
HPDA	High Performance Data Analytics
HTC	High Throughput Computing
IACN	Iberian Advanced Computing Network, same as RICA - Rede Ibérica de Computação Avançada
IB	InfiniBand
IBERGRID	Iberian grid infrastructure **https://wibergrid.lip.pt/site/**
IBM	International Business Machines Corporation
ICT	Information and Communication Technology
INCD	National Infrastructure for Distributed Computation (acronym for Infraestrutura Nacional de Computação Distribuída) **https://www.incd.pt/**
INCoDe.2030	Portuguese National Initiative on Digital Skills (Iniciativa Nacional Competências Digitais) until 2030 **https://www.incode2030.gov.pt/**
INESC ID	***Instituto de Engenharias de Sistemas e Computadores***
INESC TEC	Institute for Systems and Computer Engineering, Technology and Science
Infiniband, FDR and EDR	InfiniBand™ (IB) is a computer networking communications standard used in HPC that features very high throughput and very low latency. FDR (Fourteen Data Rate) and EDR (Enhanced Data Rate) are 2 types of IB.
INL	Iberian International Nanotechnology Laboratory
LAC-UC, LCA-UC	Laboratory for Advanced Computing at University of Coimbra **https://www.uc.pt/lca**
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator is a molecular dynamics program commonly used in HPC
LIP	*Laboratório de Instrumentação e Física de Partículas*, acronym for Experimental Particle Physics Instrumentation Laboratory
LNEC	*Laboratório Nacional de Engenharia Civil*, acronym for National laboratory for Civil Engineering

MAAC	Minho Advanced Computing Center
ML	Machine Learning
MOOC	Massive open online course
MPI	Message Passing Interface
NOS	NOS, SGPS S.A. is a Portuguese media holding company
Oakridge-CX, Oakridge-Summit	Large-scale Massively Parallel Supercomputer Systems
OC	Operational centers
OpenMP	Open Multi-Processing
Petascale	Refers to methods and processes for using supercomputers capable of performing at least 1 PFLOPS or storage systems capable of storing at least 1 PB
PIM	Processing-in-memory
PRACE	Partnership for Advanced Computing in Europe, funded under the EU's Horizon 2020 Research and Innovation Programme (2014-2020) and an e-Infrastructure on the ESFRI Roadmap **http://www.prace-ri.eu/**
PT SPACE	Portugal Space Agency **https://www.ptspace.pt/**
PUE	Power Utilization Effectiveness
RAM	Random Access Memory
R&D	Research and Development
RCTS, RCTS CERT, RCTSaai/ eduGAIN	Computer security incident response service the source or target of which is RCTS – *Rede, Ciência Tecnologia e Sociedade* or Science, Technology and Society Network. The RCTSaai service provides an authentication and authorization infrastructure which simplifies access for educational and research communities to web services. **https://www.fccn.pt/en/security/rctsaai/**
REN	Rede Eléctrica Nacional, SA
RES.ES	Red Española de Supercomputación, España **https://www.res.es/**
RIA	Research and innovation actions included in Horizon 2020 program
RICA	*Rede Ibérica de Computação Avançada*, same as IACN - Iberian Advanced Computing Network
RISC	Reduced instruction set computer
RNCA	*Rede Nacional de Computação Avançada*, same as National Advanced Computing Infrastructure **https://www.fccn.pt/rnca**
RNIE	Portuguese roadmap for strategic research infrastructures (acronym for ***Roteiro Nacional das Infraestruturas de Investigação de Interesse Estratégico***)
SDSC	University of California San Diego Supercomputing Center **https://www.sdsc.edu**
SKL	Intel Skylake
SME	Small and Medium Enterprises
TACC	Texas Advanced Computing Center **https://www.tacc.utexas.edu/**
Tier 0/1	In PRACE terms, Tier-0 are very largest European Supercomputers, while Tier-1 are national Supercomputers included in DECI proposals
UMD	Unified Middleware Distribution
UTAustin	University of Texas at Austin **https://www.tacc.utexas.edu/systems/stampede**
VRE	Virtual-Reality Environment. May also mean Virtual-Research Environment

9. CONTRIBUTIONS

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White papers written for this strategy, available as appendices:

Scientific area	Title of the paper	Authors
Research: Healthcare	High Performance Computing opportunities and challenges in Healthcare	Sandro Queirós and Nuno Sousa ICVS - Life and Health Sciences Research Institute/3B's – PT Government Associate Laboratory (Braga/Guimarães)
Operational management: User needs	User extreme needs for HPC in the next decade	Pedro Alberto e Manuel Fiolhais (LCA-UC, Coimbra)
Shared Resources: PRACE	An Advanced Computing Strategy for Portugal in the context of PRACE	Pedro Alberto e Manuel Fiolhais (LCA-UC, Coimbra)
Commercial and Industry sector - Renewable energy	Vestas HPC vision	Vestas Wind Systems A/S (Porto)
Research: HPC architectures	Next HPC architectures for science and innovation	Ricardo Fonseca (ISCTE, Lisboa)
Shared Resources: European strategy on advanced computing	Strategies for HPC in Portugal and European collaborations	Maria F. Ramalho (Institute for Advanced Simulation, Jülich Supercomputing Centre at Research Centre Jülich, Germany)

Scientific area	Title of the paper	Authors
Commercial and Industry sector - Communications	HPC opportunities in Digital Communications	Wavecom (Aveiro)
General contributions on HPC, HTC and Cloud computing	Contribution to the Advanced Computing Portugal 2030	Jorge Gomes (LIP, Lisboa)
Commercial and Industry sector - Mobility	HPC opportunities in Mobility	CEIIA - Centre of Engineering and Product Development (Matosinhos)
Research: HPC sustainability	HPC in Portugal: Opportunities and Challenges	Pedro Diniz (INESC TEC, Univ. South California - EUA)
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