Infraestrutura
Nacional de
Computação
Distribuída

2022 Activities Report

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EXECUTIVE SUMMARY

In 2022, INCD finished the execution of the contract established with Portuguese Foundation for Science and Technology (FCT) in the Framework of the Portuguese roadmap of research infrastructures. The contract started in 2017 aiming at the INCD infrastructure development and implementation. This contract was further extended until December 2022 to enable completion of the last international public tender to improve the computing and data storage capacity. This tender enabled the reinforcement of the INCD capacity in Lisbon and Coimbra, and the deployment of a new centre in Vila Real.

Fulfilling its mission, the infrastructure continued to support a wide range of scientific users from multiple research domains. In this regard, INCD supported projects from the second edition of the call for advanced computing projects organised by FCT. Under this call organised in the context of the National Advanced Computing Network (RNCA), INCD supported computing projects providing processing time, data storage and user support. In addition, INCD also supported a range of projects, communities and services of national and international relevance. A protocol with FCT for the formal adhesion of INCD to RNCA was signed. Similarly, another protocol with FCT to support the housing of a new computing facility in the north region was renewed and implemented. Overall, in 2022, INCD supported 114 projects and delivered 43,854,961 processing hours to the research community. This research produced 126 peer reviewed publications, 22 conference papers, 8 posters in conferences, 5 PhD thesis, 23 MSc thesis, 19 curated datasets and 1 patent.

The international collaborations continued with the INCD participation in EGI, IBERGRID and WLCG, operating and supporting services federated in these infrastructures. INCD also finalised successfully the participation in the European project EOSC-Synergy, towards the harmonisation and integration of thematic services, computing and data resources in the European Open Science Cloud (EOSC), with a particular focus on quality. Also, within the scope of the EOSC initiative, INCD continued the participation in the European projects EGI-ACE and C-Scale. Through them, INCD expanded its range of activities and collaborations supporting applications and thematic services in areas such as earth observation, artificial intelligence, biodiversity and coastal engineering. The European project iMagine started in September 2022 with the INCD participation focused on the provisioning of cloud capacity for image processing in marine and freshwater science.

Finally, in the context of the FCT call for institutional scientific employment (CEEC) awarded in 2022, INCD started the process to contract a new auxiliary researcher.

1. FEEDBACK FROM THE INCD INTERNATIONAL ADVISORY COMMITTEE

The INCD Board of Directors handed over to the members of the AC the Activities Report of 2022 on May 8th 2023, in preparation for the annual meeting on June 26th. The committee would like to thank the INCD management for the excellent preparation of the report and presentation. Being informed about the activities of the last year, the focus of the meeting was to provide feedback and advice on the future plans for the infrastructure.

The report starts with an executive summary followed by a high-level description of the main topics around infrastructure, services and human resources. Exploitation activities in several areas are also highlighted along the report. The report concludes with the numbers on resource usage and scientific impact measured in publications, PhD and Msc thesis and patents in a very broad set of scientific areas. Medical and Health sciences are leading the usage of INCD, which is a very interesting development, followed by a very impressive catalogue of users: Physics, Biology, Computing, Social, Civil Engineering, Environment, etc. The AC appreciates the large effort that INCD dedicates to allocate resources, as well as integrate user requirements, from the increasing number of research communities it is supporting.

One of the highlights during 2022 has been the substantial increase in the infrastructure capacity in the three INCD operations centres: Lisbon, Coimbra and Vila Real, the last site being a completely new deployment. This expansion amounts to doubling the size of the resources of INCD, which were saturated according to the reported usage of resources. The Vila Real centre is expected to start operating in 2023 delivering HPC, HTC, Cloud and data services complementing the Lisbon operations centre.

Following the previous report recommendations, services have been classified by categories. The Primary Knowledge services reflect the know-how and specific competences of the INCD staff. Software development services, including user engineering, management services and user support and documentation. Computing and Data services have also been separated in two categories, one closely related to the infrastructure as a service, and the other more elaborated services building on the primary knowledge services to generate additional value from the infrastructure.

Resource usage numbers in HTC, Cloud and HPC and scientific output continue being impressive, and growing significantly with respect to previous years. The service model strategy of INCD, based on the realisation that “one size does not fit all”, is proving to be successful to serve the needs of a large number of scientific users in Portugal with different technical requirements and resource needs. The doubling in the resources available will therefore be extremely impactful in many areas of research.

The breadth of the technical contribution of INCD, both in terms of service provision and software development consultancy, continues to be remarkable. The ratio of scientific and technical output with respect to the infrastructure costs is very high compared with even larger infrastructures in other European countries this board is

familiar with. This shows that INCD has put in place an optimal strategy to operate and support scientific users. Strategically, it is advisable to preserve the expertise and know-how of INCD in the future, for the support of research at the national and European level, capitalising on the investments made in the area of recruiting and training of the last few years.

In this respect the AC finds it highly concerning that there is no extension of the funding for national infrastructures in Portugal. Every effort should be made to provide sustainability to INCD in the framework of the RNCA or other similar future national infrastructure.

INCD is leveraging international cooperation to further develop its portfolio on primary knowledge services. Computing federation activities are taking place in the framework of IBERGRID and EGI. INCD provides the computing and data storage capacity for the Portuguese World Wide Computing Grid Tier-2 facility that supports the national participation in the ATLAS and CMS experiments at the CERN LHC. INCD is now also hosting the EGI software repositories and Certification Authorities for the International Grid Trust Federation (IGTF).

In the EOSC context INCD activities are focussed in supporting the Open Science paradigm applied to research data repositories. The team's expertise in these activities has been developed in the context of EU funded projects, which INCD leveraged and applied to two national endeavours with a clear future impact: hosting the National Data Repository of Portugal, and development of a Data Lake for agriculture in Portugal as public service. This strategy provides a path for exploitation of results of EU funded projects, which is a very interesting approach for the sustainability of EU project outcomes.

In the context of the OCRE procurement in EOSC, INCD has teamed up with Google to propose the usage of Google Cloud in conjunction with its own Cloud service enabling the INCD cloud to burst into Google for higher capacity and additional capabilities. This is an extremely interesting development which opens the venue for future collaboration with a true Cloud Hyperscaler to exploit the expertise of INCD at large scale, in particular arising from the primary knowledge services for Science in large scale of resources.

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Danilo Piparo (CERN)

Davide Salomoni (INFN)

2. INTRODUCTION

Infraestrutura Nacional de Computação Distribuída (INCD)[1] provides state-of-the-art advanced computing and data-oriented services to the national research and academic community. INCD supports research across all scientific and technological domains. Internationalisation is a key aspect of the INCD activities both through the participation in European projects, and by linking strongly with digital infrastructures and initiatives such as EGI[2], IBERGRID[3], WLCG[4] and EOSC[5].

The INCD association (*Associação INCD*) was created in 2015 in the framework of the Portuguese roadmap of research infrastructures of the Portuguese Foundation for Science and Technology (FCT)[6]. The INCD association has as core goals performing research, development, promotion and international articulation of advanced computing activities, as well as the development and operation of the INCD infrastructure. The infrastructure activities are performed by the INCD association in partnership with its associates (FCT, LNEC[7] and LIP[8]).

In 2022, INCD through its operational centres supported projects from the calls for advanced computing projects (CPCA) and research in data science and artificial intelligence applied to public administration (DSAIPA) both coordinated by FCT, as well as projects, communities and services of national and international relevance. The research supported by INCD covers multiple scientific domains including among others: life sciences, physics, biodiversity, material sciences, civil engineering, earth sciences, information technology and environment.

3. ABOUT THE INFRASTRUCTURE

The main services provided by INCD encompass high performance computing (HPC), high throughput computing (HTC) and cloud computing complemented by data oriented services. The infrastructure comprises facilities deployed across several geographical locations, providing resiliency, exploiting existing resources and promoting partnerships with research and education organisations in the country. The hosting of the facilities and their network interconnection is performed in close collaboration with the Portuguese National Research and Education Network (RCTS) managed by FCT-FCCN[9]. In particular, INCD leverages the RCTS housing service and RCTS Plus private network service. The housing and the network constitute the foundation layers upon which the INCD architecture is built (Fig 1).

The main INCD services i.e. cloud, HPC, HTC and data oriented, sit immediately above the housing and network layers. These services can be used either directly by the

[1] Infraestrutura Nacional de Computação Distribuída (INCD) web site: https://www.incd.pt/
[2] EGI.eu: https://www.egi.eu/
[3] IBERGRID: https://www.ibergrid.eu/
[4] Worldwide LHC Computing Grid (WLCG): https://wlcg.web.cern.ch/
[5] European open Science Cloud (EOSC): https://eosc.eu/
[6] Fundação para a Ciência e a Tecnologia (FCT): https://www.fct.pt/
[7] Laboratório Nacional de Engenharia Civil (LNEC): https://www.lnec.pt/
[8] Laboratório de Instrumentação e Física Experimental de Partículas (LIP): https://www.lip.pt/
[9] FCT-FCCN the FCT scientific computing unit and Portuguese NREN: https://www.fccn.pt/

end-users or indirectly through other higher level services meant to provide additional capabilities driven by user requirements. These may include, federated access to the computing and data resources, integration in international computing infrastructures, added-value services for computing and data processing, and virtual research environments for specific disciplines or user communities. Common to all layers of the architecture are transversal activities such as security, training, interoperability, support, collaboration, research and innovation.

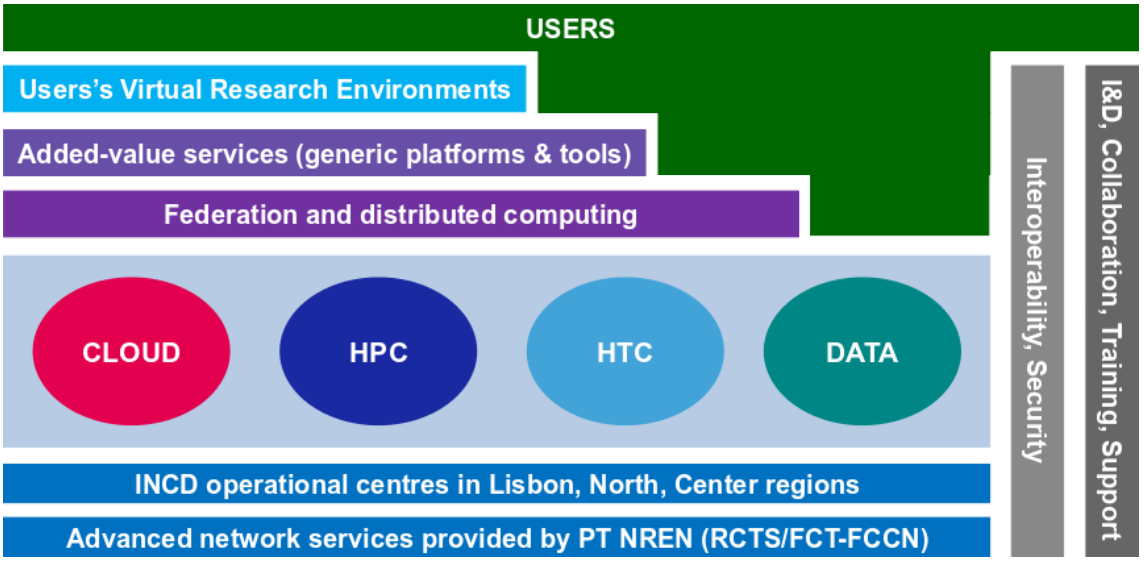

Figure 1: INCD high level architecture.

4. OPERATIONAL CENTRES

The infrastructure operations centre in the Lisbon region was established in the context of the former National Grid Initiative in 2009 and is housed at the Sala-Grid data centre in the campus of the National Civil Engineering Laboratory (LNEC) in Lisbon. The data centre is managed by FCT-FCCN, while the INCD computing equipment and services are managed by LIP. The infrastructure operations centre in the north region was housed at a commercial data centre in Riba-de-Ave sharing capacity from the Bob supercomputer[10] in a partnership with FCT. In the end of 2022 the decommissioning of the Riba-de-Ave centre started and a subset of the Bob supercomputer began to be migrated to the Sala-Grid data centre in Lisbon, where INCD will continue managing part of the system capacity. Simultaneously, a new INCD centre in the north began to be deployed in the University of Trás-os-montes e Alto Douro (UTAD) in Vila Real. The deployment of this centre started in December of 2022 and will ensure the continued presence of INCD in the north region. The Vila Real centre commissioning is delayed due to improvements being introduced in the data centre but is expected to start

[10] HPC resources in Portugal: https://eurocc.fccn.pt/en/hpc-in-portugal/

operating in 2023 delivering HPC, HTC, cloud and data services complementing the Lisbon operations centre. The operations centre in Coimbra is located at the Physics department of the University of Coimbra. The upgrade of the centre also started at the end of 2022 and is expected to begin delivering additional data storage services in 2023. These centres are complemented by the LIP data centre in Lisbon that also provides tape based storage. The infrastructure is managed and supported by personnel based in Minho and Lisbon.

5. INFRASTRUCTURE UPGRADES

In February of 2022, INCD launched an international public tender to increase the capacity of the infrastructure[11] covering the three INCD operations centres in Lisbon, Coimbra and Vila Real. The tender process was complex both due to the administrative and legal steps required for larger public contracts and also due to delivery delays caused by the disruptions in the global semiconductor supply chain. The process finished in December of 2022 with the delivery and installation of the equipment.

In Lisbon the computing cluster capacity was increased with 1920 additional CPU cores AMD Epyc 7643 with a total of 10 TB of RAM, the online data storage was increased with 1920 TB of raw storage capacity for Lustre. The GPU computing capacity was also improved with additional A100 GPUs. The data centre network was improved with additional network switching capacity, and the wide area network connectivity was upgraded to 100Gbps.

The Vila Real centre is a completely new facility that now houses the largest fraction of the equipment purchased by INCD in the international public tender. The installed equipment includes 4992 CPU cores AMD Epyc 7643 with a total of 27 TB of RAM, the online storage includes 960 TB of raw storage capacity for Lustre and 2880 TB of raw storage capacity for Ceph. All systems are interconnected by Infiniband HDR 200 Gbps and Ethernet 10 to 25 Gbps networks. Additional systems for support and management were also deployed. The centre also received additional data storage equipment decommissioned from Riba-de-Ave that will complement the newly acquired storage capacity for Lustre.

The upgrades in Coimbra included the installation of tape library storage equipped with eight LTO-9 fibre channel tape drives and capable of delivering a total capacity of 20 Petabytes when fully populated with LTO-9 tapes. Additional tapes will be purchased as required to complement the initial 1 Petabyte capacity. The tape library is complemented by about 400 TB of online storage capacity for staging. The local network infrastructure was also upgraded.

The computing capacity in Lisbon was also further improved with 816 CPU cores Xeon E5-2680v3 with a total of 2 TB of RAM offered by CERN to INCD to improve the Portuguese Tier-2 in the Worldwide LHC Computing Grid (WLCG). Also in the context of WLCG the Tier-2 storage capacity was upgraded with the addition of 576 TB of raw

[11] INCD upgrades: https://www.incd.pt/?p=noticias/detalhes&id=28&lang=en

storage. These upgrades enabled the removal of old hardware installed in 2009 that was still in operation supporting the Tier-2.

6. INFRASTRUCTURE NETWORK

To interconnect the several centres INCD has established a private wide area network using the advanced network services provided by FCT-FCCN (Fig 2). The centres are interconnected via an Ethernet Layer 2 network, which is itself built upon and connected to the national academic network also operated by FCT-FCCN. All centres have 10Gbps links with the exception of the INCD largest centre in Lisbon at the LNEC campus that in 2022 was upgraded to 100Gbps.

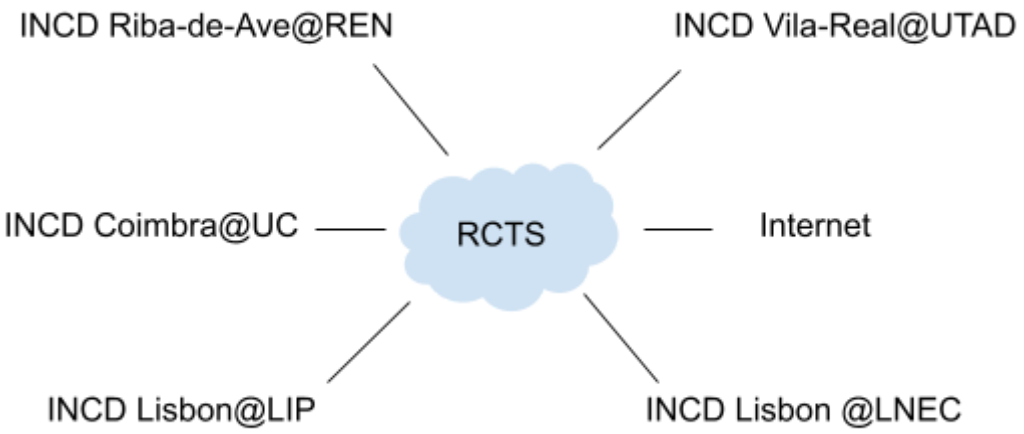

Figure 2: INCD network connectivity.

7. HUMAN RESOURCES

INCD is backed by a technical team that includes twelve LIP researchers, engineers, technicians and communications personnel that also contribute to INCD and that are complemented by one INCD engineer and one INCD administrative assistant. The team members are based in Minho and Lisbon. In addition, as a result of applying to FCT research positions, INCD started the process to contract one additional team member with PhD as auxiliary researcher, the hiring process was finalised already in 2023. The team is further complemented with contributions by researchers from LNEC. In addition INCD has a management board with three directors that are nominated by the members of the association. The coordination of the technical activities and related personnel both from LIP and INCD is performed by the INCD technical coordinator which also coordinates the LIP team contributing to INCD. With the end of the INCD main project funded by the FCT roadmap of research infrastructures, measures have been taken to reduce the human resources costs. Particularly two engineers previously

in INCD established new contracts with LIP where they will continue contributing to INCD, while a new junior engineer was contracted by INCD.

8. INFRASTRUCTURE SERVICES UPDATE

The INCD services catalogue is continuously improved according to the evolution of the technology and user requirements. The catalogue of the services provided in 2022 is summarised in Table 1. The catalogue has been reorganised in three areas covering computing services, data services and knowledge based services. Each of these areas is further divided into primary and secondary services. The primary services are the generic building blocks that constitute the core of the INCD infrastructure, while the secondary services include specific services that are largely built upon the primary services.

Areas	Primary services	Secondary services
Computing	High Performance Computing High Throughput Computing Cloud Computing	Large memory computing Accelerated computing Federated cloud computing Federated HTC/HPC Containerised computing Scientific portals and gateways Value-added services
Data	Cloud Storage File Storage Tape Storage	Data repositories Long term storage Data protection Distributed RO filesystem Federated file storage
Knowledge	Software Development Managed Services Support and Documentation	Integration of software & services Software quality assurance Training and consultancy

Table 1: INCD services catalogue

8.1. PRIMARY COMPUTING SERVICES

The primary services encompass the main computing services namely High Performance Computing, High Throughput Computing and Cloud Computing. They constitute the core of the INCD offering upon which the secondary services are built and provided. The services are further described in the following subsections.

Cloud Computing

The INCD cloud computing service (named *Stratus*) is an infrastructure-as-a-service (IaaS) cloud that provides access to virtual machines on-demand. The cloud service is built-on the Openstack cloud management framework. The cloud computing service is complemented by the INCD cloud storage service that provides block and object storage to the Openstack[12] cloud. The cloud computing service is currently provided by the INCD node in Lisbon. The deployment of a second Openstack installation in the north region is expected to become available in 2023 at the new operations centre in Vila Real. The second installation will provide additional capacity and resiliency for cloud applications. In 2022 the service delivered 16,793,741 vCPU hours of processing time. In 2022 the service had a capacity of 2500 vCPUs cores. The new site in Vila Real will add approximately 3840 vCPUs.

High Throughput Computing

The High Throughput Computing (HTC) service is optimised for the execution of large numbers of individual tasks either single threaded or multi-threaded, targeting massively computational and data intensive applications. Differently from the HPC workloads where the running processes need to communicate with low latency, the HTC computing processes are individual tasks that can be executed separately. For higher efficiency, the HTC and HPC services share the same Slurm[13] batch systems. In 2022 the HTC service delivered 18,113,138 hours of processing time, mainly supported by partitions of the *Cirrus-A* cluster in Lisbon. These partitions are composed of heterogeneous nodes both Intel Xeon and AMD Epyc interconnected via high performance Ethernet networks. The service relies on a Lustre[14] file-system optimised for non-parallel workloads provided by the INCD file storage service. In 2022 the service had a capacity of approximately 2200 CPU cores.

High Performance Computing

The High Performance Computing (HPC) service is optimised for the execution of parallel computing workloads that require inter-process communication with low

[12] Openstack cloud management framework: https://www.openstack.org/
[13] Slurm batch system: https://slurm.schedmd.com/
[14] Lustre distributed file system: https://www.lustre.org/

latency. The service is particularly suitable for MPI[15] applications. In 2022, the service delivered 8,948,082 hours of processing time, backed by partitions of the *Cirrus-A* cluster in Lisbon and *Cirrus-B* cluster in Riba-de-Ave. The *Cirrus-A* cluster features computing nodes equipped with AMD Epyc processors, while the *Cirrus-B* cluster corresponds to a partition of the Bob supercomputer featuring Intel processors. Both clusters are equipped with Infiniband networks. The storage system used in *Cirrus-A* and *Cirrus-B* is a Lustre file system optimised for parallel workloads provided by the INCD file storage service. The availability of *Cirrus-B* continued to be severely affected by power and cooling limitations and in the end of 2022 the site began to be decommissioned. At the end of 2022 the *Cirrus-A* cluster in Lisbon was upgraded with additional computing nodes. While in the north the deployment of the new *Cirrus-D* cluster began in Vila Real. Overall, in 2022 the service had a capacity of approximately 3264 CPU cores which were only partially available due to power restrictions in the Riba-de-Ave centre. The new capacity in Lisbon and Vila Real will provide a total of about 5000 CPUs.

8.2. PRIMARY DATA SERVICES

The primary services encompass the main data storage services namely Cloud Storage, File Storage and Tape Storage, upon which other secondary data services are provided.

Cloud Storage

The INCD cloud storage service provides access to object and block storage. The service is oriented to provide robust scalable storage for cloud applications. The storage service is closely related to the INCD cloud computing service and is based on the Ceph[16] data storage system. The block storage provides volumes for the cloud virtual machines, while the object storage enables data storage as objects therefore providing higher horizontal scalability than conventional file-systems. The object storage component of the service can also be used independently from the cloud computing service. Through its application programming interface (API), that includes support for S3 and SWIFT, the object storage can be easily and safely accessed remotely. In 2022, the cloud storage service supported by the INCD centre in Lisbon provided more than 1326 Terabytes*month. A new deployment in the northern region is expected to become operational in 2023. In 2022 the service had a total capacity of approximately 400 Terabytes including the Ceph triple redundancy. The new site in Vila Real will add 1 Petabyte of Ceph storage.

[15] Message passing Interface (MPI) standards: https://www.mpi-forum.org/
[16] Ceph distributed storage system: https://ceph.com/en/

File Storage

The file storage service provides access to POSIX[17] read-write file systems mainly based on Lustre and is mainly used in conjunction with the HPC and HTC services. In special cases the service can also be provided using other solutions such as NFS. The service can be also used independently from the HPC and HTC services via secondary services such as the federated storage. The service is meant to support applications that rely on conventional file systems and is especially suited for storage and processing of large files. The file storage service provides the data storage backbone for the HPC and HTC services. In 2022, the service was supported by the INCD centres in Lisbon and Riba-de-Ave. In Lisbon INCD has a file storage capacity of 2 Petabytes, while the file storage capacity at Riba-de-Ave was 600 Terabytes. The new site in Vila Real will have a total capacity of 1.2 Petabytes.

Tape Storage

Contrary to other services in this catalogue the tape storage service is a service internal to INCD that is not directly accessible to end-users. This service provides the backbone for other secondary services such as data protection and long-term storage, providing reliable yet cost-effective storage capacity for infrequently accessed data using LTO tape libraries. In 2022 the service was provided by a tape library at the LIP data centre in Lisbon. A second installation with a capacity of up to 20 Petabytes will become available in Coimbra in 2023.

8.3. PRIMARY KNOWLEDGE SERVICES

The primary knowledge services encompass software development, managed services and support together with documentation. These are services that leverage the INCD experience and competences. They are meant to support the exploitation of the computing and data services, but can also be used separately.

Software Development

Development of software to expand the INCD offering such as new tools and services, or co-development of specific software in partnership with user communities. The service includes both development of new services and software as well as porting of software to be used at INCD. The service is often provided in the framework of projects joining INCD with user communities or as part of the support provided to new projects and user communities.

[17] Posix specification: https://pubs.opengroup.org/onlinepubs/9699919799.2018edition/

Managed Services

This service is oriented to the management of virtual or physical resources integrated in INCD. The virtual resources can be virtual machines, containers or other types of resources that can be instantiated using the INCD services, and whose management can be fully or partially delegated to INCD. The physical resources can include private hardware that is housed at INCD under agreed conditions that by default include being integrated and shared via the INCD services. The resource management allows the users to benefit from the INCD capabilities, scalability and connectivity. Examples of this service in 2022 include the delivery of the managed Lustre installation for the Bob supercomputer, the management of hardware integrated in the INCD cloud for the GBIF[18] biodiversity national node, the management of virtual machines (VM) for several user communities and the management of the Portuguese Tier-2 in the Worldwide LHC Computing Grid.

Support and Documentation

This service aims at supporting the usage of the INCD services through documentation and support. Most of the documentation is provided online[19] and is continuously improved and enlarged based on the perceived user difficulties. Direct support is provided through the INCD helpdesk[20] via email, complemented with remote conferencing.

8.4. SECONDARY SERVICES

The secondary services include a wide range of service offerings that are built upon the primary computing, data and knowledge services complementing them with additional capabilities.

Large memory computing

The large memory computing service is tailored for computational tasks with large memory requirements. The service takes advantage of the HPC, HTC and cloud services, and provides access to a set of compute nodes with larger RAM capacity that can be accessed through batch partitions associated with the HPC and HTC services or via the cloud service. The maximum RAM capacity is currently limited to 512GB in Lisbon and 1TB in Vila Real. This service targets multithreaded shared memory applications with large memory requirements such as genome data processing and other *big data* applications.

[18] Global Biodiversity Information Facility (GBIF) Portuguese node at INCD: https://dados.gbif.pt/
[19] INCD wiki: https://wiki.incd.pt/
[20] INCD helpdesk contacts: https://wiki.incd.pt/books/user-support/page/helpdesk

Accelerated computing

The accelerated computing service provides access to compute nodes equipped with specialised hardware e.g. GPUs. The service is suitable for machine learning, artificial intelligence applications and other GPU enabled applications. The accelerated computing service is supported via the *Cirrus-A* cluster (HPC and HTC) and *Stratus* cloud in Lisbon. The range of supported GPUs includes NVIDIA V100, NVIDIA T4 and NVIDIA A100 for production and older NVIDIA K40 mainly for development and educational purposes. In 2022 the service continued having a very high demand in particular for machine learning applications. Besides the GPU capacity the service was backed by 384 AMD Epyc CPUs and 1 Terabyte of RAM. The service was upgraded with A100 GPUs at the end of 2022. The service provided more than 71,290 GPU computing hours.

Federated cloud computing

Access to the EGI and IBERGRID federated cloud computing infrastructures, interconnecting cloud services and data at international level. The INCD cloud service[21] is federated into the EGI and IBERGRID international infrastructures. Through the federated cloud service, INCD provides cloud capacity from its own cloud service (*Stratus*) and assists users in gaining access to additional cloud capacity integrated in the EGI and IBERGRID federations. The service is mainly oriented at supporting international research activities that benefit from the access to shared computing resources at international level for added capacity and resiliency. In 2022 the service provided 5,328,120 hours of computing time.

Federated HTC and HPC

Access to the EGI, IBERGRID and WLCG distributed computing infrastructures, interconnecting computing clusters at international level. The INCD main computing services HTC and HPC are federated in the EGI and IBERGRID international infrastructures. Through the federated computing service, INCD can provide HTC and HPC capacity from its own computing services and assist users into accessing additional capacity integrated in the EGI federation. The service is mainly oriented at supporting research activities that benefit from the access to shared computing at international level. In 2022 the federated HTC and HPC service was delivered by the *Cirrus-A* cluster in Lisbon. The service provided 14,775,900 hours of federated computing time. A second installation of the service is expected to become available in 2024 exploiting capacity from the *Cirrus-D* cluster at the Vila Real centre.

[21] INCD Openstack cloud service: https://stratus.ncg.ingrid.pt/

Containerised computing

The containerised computing service provides support for execution and orchestration of Linux containers for services and applications. The service enables portability, reproducibility and preservation of applications with their computing environments. The service is meant to support execution of simple or complex containerised services and applications. This service relies on the HPC, HTC and cloud services enabling execution of Linux containers using different types of container execution runtimes. Some of the supported tools include udocker[22], Docker[23], Singularity/Aptainer[24] and orchestrators like Docker Swarm and Kubernetes[25] among others.

Scientific portals and gateways

This service supports the deployment, operation and access to scientific gateways and portals. These are community oriented services delivered on top of the INCD cloud and/or in combination with other INCD data or compute services. Examples of such services include R-Studio, Jupyter notebooks, Galaxy portals and domain specific solutions for simulation and data analysis.

Value-added services

Provisioning of a wide range of generic services mainly delivered through the INCD cloud that target specific yet common requirements of the research and academic community both at the organisation and team level. Examples of such services include Sync & Share services, databases, agenda & meeting organisation, web servers, load balancers, proxies, among others. The range of services is updated according to the demand.

Data repositories

Following the activities already ongoing with the Portuguese Foundation for Science and Technology, INCD continued collaborating in the deployment and evaluation of a catchall data repository tailored to the Portuguese research community. The data repositories service is oriented to support open science requirements concerning open access to research data by supporting digital data repositories for specific communities. In addition, INCD worked with specific communities in the framework of the European Open Science Cloud (EOSC) to support their FAIR (Findable Accessible Interoperable and Reusable) data requirements. The service is based on the Dataverse open source

[22] udocker a container execution tool developed with INCD support: https://github.com/indigo-dc/udocker
[23] docker: https://www.docker.com/
[24] Singularity/Apptainer: https://apptainer.org/
[25] kubernetes: https://kubernetes.io/

research data repository software. This service is being further developed to be delivered as a pilot activity.

Long-term storage

This service is aimed at long-term data storage of infrequently accessed data. The service is mainly delivered using tape library based storage, but can also be provided via on-line data storage depending on the nature, size and data access patterns. This service is supported by INCD through the LIP data centre in Lisbon. An expansion of the service is expected to become available in Coimbra in 2023.

Data protection

The data protection service is aimed at data backups to protect against data loss and support data recovery. The service is delivered using tape library based storage. This service is supported by INCD through the LIP data centre in Lisbon. An expansion of the service is expected to become available in Coimbra in 2023.

Distributed read-only filesystem

The distributed read-only file system service is meant to share immutable files across the INCD centres regardless of their geographic location. The service can be used to make user specific software environments available across the INCD infrastructure. The service is based on the CernVM-FS (CVMFS)[26], a scalable POSIX read-only file system. The service is mainly meant for sharing of software and smaller immutable files in a reliable way, enabling an homogeneous computing environment across the INCD centres. The service features a stratum 0 and 1 in Lisbon and stratum 2 at the other centres. In 2022, the service had a maximum capacity of 2 Terabytes of storage.

Federated file storage

The federated storage service enables remote access to the INCD File Storage service. Is based on several middleware services that provide high performance secure access to the Lustre file system. The middleware services include StoRM[27] and XRootD[28], through which multiple data transfer protocols are supported including gridftp, WebDAV and XRootD. The federated file storage service is integrated with the EGI, IBERGRID and WLCG international infrastructures. In 2022 the service was supported

[26] CernVM-FS file system: https://cernvm.cern.ch/fs/
[27] STOrage Resource Manager (StoRM): https://italiangrid.github.io/storm/
[28] XRootD project: https://xrootd.slac.stanford.edu/

by the INCD operations centre in Lisbon with a capacity of about 1.3 Petabyte of storage.

Integration of software and services

The integration of software and services is a support service aimed at facilitating the integration of generic, thematic or community specific software to take advantage of the INCD services. This is a human resources intensive service that is subjected to the availability of experts that work in co-development with the users providing guidance and accelerating the process of software integration. This service is oriented to both cloud services to be hosted at INCD and integration of HTC and HPC applications. This service also includes the integration at the federation level in order to take advantage of international infrastructures and initiatives like EGI, IBERGRID and EOSC to provide higher capacity, scalability and enable sharing of software, data and computing resources.

Software quality assurance

With this service, INCD aims to support software development and the adoption of software quality best practices. The service builds upon the SQAaaS[29] platform developed by IBERGRID in the EOSC-Synergy[30] project to enable on-demand creation of CI/CD pipelines making quality verification and validation easily accessible to researchers and software developers. Besides the SQAaaS other services such as CI/CD and software repositories are also provided.

Training and consultancy

Complementing the core support and documentation activities, INCD also provides different types of training, either generic such as induction and assistance for new users or specific to address advanced usage topics or targeting specific communities. Consultancy and technology transfer are also part of these activities.

9. INFRASTRUCTURE MANAGEMENT AND OPERATIONS

The infrastructure management and operations is split mainly across the centres in Lisbon and Minho. The teams in these centres have been previously focused on the local services and projects associated with their centres. In order to improve efficiency and redundancy the internal processes were revised and the teams are now working and collaborating more tightly in the development and management of the infrastructure, participation in projects and user support.

[29] SQAaaS platform: https://sqaaas.eosc-synergy.eu/
[30] EOSC-Synergy project: https://www.eosc-synergy.eu/

The improvement of the infrastructure has been a continuous effort and in 2022 included both multiple software updates and also hardware upgrades. In this context, the oldest computing and storage equipment was replaced by newer equipment. The old equipment was either retired when obsolete, placed on reserve as spare or in certain cases reused to support less demanding services.

Several software improvements were introduced. A transition from CentOS to AlmaLinux and in certain cases Ubuntu has started inline with the upcoming RHEL 7 end-of-life. All new equipment and upgrades are now targeting AlmaLinux[31]. The internal virtualization and containerization platforms that support the infrastructure management as well as other highly critical services continued to be improved. A new solution for the helpdesk was selected and is being implemented using the Zammad[32] platform.

The migration of part of the Bob supercomputer from Riba-de-Ave to Lisbon started in 2022 and finished in the beginning of 2023, the installation of the network and Lustre storage was performed by the Lisbon team, while the migration of the INCD hardware from Riba-de-Ave to Vila Real was performed by the Minho team. The mini-Bob partition assigned to INCD in Lisbon was also fully reinstalled. The HPC capacity in Lisbon was also further upgraded with new compute and storage hardware acquired through the last international public tender. The HTC partition of the Lisbon cluster was upgraded with hardware from the ATLAS experiment donated by CERN. The software environment both for HPC and HTC applications has been rebuilt and optimised for AlmaLinux. The new HPC and HTC cluster in Vila Real started to be deployed and the commissioning is pending improvements in the data centre energy and cooling infrastructure that are ongoing. In Coimbra a complete reorganisation of the local infrastructure including network and services is also ongoing in parallel with the implementation of the services for the new tape based storage.

10.FEDERATION ACTIVITIES IN EGI, IBERGRID AND WLCG

The participation of INCD as a provider in the international digital infrastructures IBERGRID (ibergrid.eu) and EGI (egi.eu) continued as a key aspect of the INCD strategy to support international projects and research communities. The three main computing services provided by INCD (cloud, HTC and HPC) are integrated in IBERGRID, and through the Iberian infrastructure they are also integrated in the wider EGI federation, therefore enabling the sharing of compute and data resources to support international research. The high energy physics collaborations, such as the ATLAS and CMS experiments at the CERN Large Hadron Collider (LHC), are good examples of research communities supported through this approach. Other examples include: the Portuguese node of the Global Biodiversity Information Facility (GBIF), the astroparticles experiment SNO+, or the eNMR.eu virtual organisation, among others. In 2022, INCD delivered more than 14,775,900 HTC/HPC federated computing hours and 5,328,120 federated cloud computing hours supporting research projects and

[31]AlmaLinux: https://almalinux.org/
[32] Zammad: https://zammad.org/

communities of national interest in the scope of the IBERGRID and EGI federations. The federation in IBERGRID and EGI of the new computing and storage services to be made available in Vila Real is also being prepared.

INCD provides the computing and data storage capacity for the Portuguese Tier-2 facility that supports the national participation in the ATLAS[33] and CMS[34] experiments at the CERN LHC. The Tier-2 is operated under the MoU for the Collaboration in the Deployment and Exploitation of the Worldwide LHC Computing Grid (WLCG) signed by the Portuguese government. Under this MoU, Portugal contributes to its share of the LHC computing costs through the delivery of computing and data capacity to the CERN experiments, supporting both global simulation and data processing for the experiments, and data analysis by Portuguese researchers. The WLCG is the world's largest thematic distributed computing infrastructure. The WLCG sits on top of the computing and storage capacity delivered by the computing facilities such as the Portuguese Tier-2 that are federated in either EGI (European Grid Infrastructure), OSG (Open Science Grid), or NeIC (Nordic e-Infrastructure Collaboration). In 2022, the Tier-2 storage capacity was slightly increased with hardware supported by a project under the FCT-CERN cooperation agreement. In 2022, the WLCG Tier-2 consumed 165,631,870 HEPSCORE23 normalised computing hours fulfilling the yearly pledged capacity. However, the Tier-2 capacity is largely below the necessity and the participation in the upcoming High Luminosity LHC with its huge computing and data requirements will be unfeasible without major upgrades.

INCD is now hosting the EGI software repositories[35] for the Unified Middleware Distribution (UMD), Cloud Middleware Distribution (CMD) and Certification Authorities for the International Grid Trust Federation (IGTF). These repositories support the distribution at global level of all middleware for the EGI federation and related digital infrastructures including the Worldwide LHC Computing Grid. This activity is conducted in the context of a tender for the EGI software management awarded to IBERGRID. In this context INCD also participated in the development of new repositories in partnership with LIP. The new repositories are part of a complete reorganisation of the EGI software management and will enter into production in 2023.

Also in the scope of the IBERGRID collaboration, INCD contributed to the organisation of the 11th edition of the IBERGRID conference. The IBERGRID 2022 conference took place in the University of Algarve in October 2022 and was focused on topics related with the development, integration, quality and adoption of services, applications and digital twins to support cutting-edge research. The event also counted with several parallel events including the first EOSC tripartite event in the Iberian region joining researchers, national funding authorities and the European Commission, a meeting of the LifeWatch ESFRI, and the final All-Hands meeting of the EOSC-Synergy project.

[33] ATLAS Experiment at CERN: https://atlas.cern/
[34] CMS Experiment at CERN: https://cms.cern/
[35] EGI middleware repositories at INCD: https://dev-repository.a.incd.pt/software-distributions/

11.EUROPEAN OPEN SCIENCE CLOUD and EUROPEAN PROJECTS

Bridging with the IBERGRID and EGI activities, INCD participated in several activities related to the European Open Science Cloud (EOSC), both through participation in projects and by supporting thematic services in the framework of EOSC. Among others INCD is supporting in EOSC the coastal modelling service OPENCoastS[36] and water detection service WorSiCa[37]. These thematic services developed by LNEC in collaboration with LIP and INCD are now part of the EOSC services portfólio.

Also in the EOSC scope, INCD participated in the European project EOSC-Synergy that finished in October 2022. The project's main activities included development of state-of-the-art tools for the quality assurance of software and services, development of new thematic services, and integration of computing services and data repositories in EOSC. The EOSC-Synergy project joined 20 partners from 10 countries, including INCD and its associates LIP, LNEC and FCT. In this context, INCD provided cloud capacity and support for the development, integration and operation of the Water monitoRing SentInel Cloud (WorSiCA) thematic service and for the Software Quality Assurance as a Service platform (SQAaaS) that was developed in the project by LIP, IFCA/CSIC and UPV. The project final evaluation was very successful with the developments and achievements being praised[38] by the evaluators particularly the quality assurance part. The core partners of the consortium, including INCD, have submitted a follow-up project.

The participation in the two EOSC projects EGI-ACE[39] and C-Scale[40] started in 2021 and continued in 2022. In EGI-ACE, the work was focused on providing cloud computing services to support applications in biodiversity, coastal modelling and machine learning. The project also includes the federation of the GBIF national nodes from Portugal and Spain. In C-Scale, the work was focused on the integration of earth observation services exploring data from Copernicus using the EGI infrastructure. INCD supported the integration and hosting of two earth observation cloud services and worked in the caching of satellite images. These projects will finish in 2023.

The participation in the iMagine project started in September 2022. The project will provide a selection of image datasets, AI-empowered high-performance image analysis tools, and best practices for scientific image analysis. These services and materials will enable better processing and analysis for imaging marine and freshwater data. The project builds on the European Open Science Cloud (EOSC) and aims to deliver an AI model development, training, and deployment for AI-based applications applied to marine and freshwater science.

Also in the context of the EOSC activities, INCD teamed with Google to apply to an European procurement opened in the context of the EOSC-Future[41] project for the distribution of commercial cloud services to European researchers, aimed at bridging

[36] OPENCoastS: https://opencoasts.ncg.ingrid.pt/
[37] WorSiCa: http://worsica.lnec.pt/
[38] EOSC -Synergy final review: https://www.incd.pt/index.php?p=noticias/detalhes&id=29
[39] EGI-ACE: https://www.egi.eu/project/egi-ace/
[40] C-Scale: https://c-scale.eu/
[41] EOSC-Future: https://eoscfuture.eu/

the gap between commercial service providers and researchers through the EOSC ecosystem. The procurement was open to the commercial cloud providers of the OCRE[42] framework teaming up with digital service aggregators (e.g. non-profit entities, NRENs, RIs and e-Infrastructures, HPC centres, etc.) that act as the distributors of the awarded capacity. Applications were evaluated on their ability to craft an action plan for a distribution mechanism of state-of-the-art digital services, to be made available and distributed through EOSC in a sustainable and cost-effective way. The proposal from INCD with Google was submitted in December 2022 and was awarded at European level with OCRE credits receiving half a million Euro. INCD proposed the usage of Google cloud in conjunction with its own cloud service enabling the INCD cloud to burst into Google for higher capacity and additional capabilities.

12.RNCA AND HIGH PERFORMANCE COMPUTING ACTIVITIES

Within the scope of the national advanced computing network (RNCA)[43], INCD together with its partners, continued to participate in activities aimed at establishing and developing the RNCA network (https://www.fccn.pt/computacao/rnca/). In this context INCD participated in the support to the FCT calls for advanced computing projects (CPCA), through which FCT grants computing time for research projects. Namely, INCD participated in the second CPCA as an operations centre supporting 20 computing projects in several scientific domains for a total allocation of 4,760,744 hours including HPC, cloud and GPU computing. INCD also participated in the preparation of the third CPCA call and also in the technical evaluation of projects whose execution is meant to take place in 2023. In addition INCD supported 2 projects from the calls for research in data science and artificial intelligence applied to public administration (DSAIPA). The number of hours committed in 2022 was limited due to the restrictions in the Riba-de-Ave data centre.

A formal protocol to join RNCA was signed in January of 2022. Under this protocol INCD has the responsibility of supporting research activities of strategic interest related with CERN and high energy physics while simultaneously supporting research projects in the context of FCT calls. In return, FCT will contribute to the operational costs of INCD under conditions that are agreed annually. The yearly conditions for 2023 were also agreed and updated in December 2022.

Under the agreement to support the BOB supercomputer in Minho, INCD has been managing the complete storage system that serves both the INCD and MACC partitions of the BOB supercomputer. Part of the hardware that supports the storage system was also supplied by INCD. The migration of a subset of the BOB supercomputer from Riba de Ave to Lisbon started in December 2022 and finished already in the beginning of 2023. Shortly after, the Riba-de-Ave site was decommissioned. The INCD storage and network equipment from Riba-de-Ave was moved to the new INCD centre in Vila Real

[42] Open Clouds for Research Environments (OCRE): https://www.ocre-project.eu/
[43] Portuguese Advanced Computing Network (RNCA): https://rnca.fccn.pt/

to reinforce the new equipment delivered in December 2022 as part of the public tender previously described in section 4.

INCD continued supporting the activities of the Portuguese National High Performance Computing Competence Center (NCC) in the framework of the EuroCC[44] project. In this regard, INCD collaborated with the LIP and FCT associates that are partners in the EuroCC project to support the dissemination, training and engagement of new users. INCD is also providing the housing to support the Portuguese NCC web presence.

13.OPEN SCIENCE AND RESEARCH DATA

In the context of the EOSC-Synergy project, INCD experimented with data repository technologies aiming at supporting new thematic services in EOSC. In cooperation with FCT-FCCN and LIP, this initial work is being applied to build a pilot catchall data repository based on the Harvard Dataverse open source software aiming at making research data openly available according to the open science values and FAIR principles. In 2022, this activity was significantly developed and became part of a collaboration protocol with FCT-FCCN. INCD is housing development and piloting instances of the data repository for FCT-FCCN, and is assisting in the adaptation and deployment of the software to the national requirements. Experimentation with user communities is expected to start in the summer of 2023.

In the C-Scale project, INCD is developing a cache service based on the OpenEO software to serve Copernicus satellite images for multiple earth observation applications that are being integrated in the project. This activity has promoted collaboration with other organisations in the country, among these is a potential participation in the European partnership for the agriculture of data. INCD has been following this initiative that aims to support sustainable agriculture in Europe as well as policy monitoring and implementation by using the possibilities that digital technologies in combination with environmental observation and other data offer. In this context, INCD has been pursuing the concept of a data lake for agriculture related data. For 2023, within the context of the CPCA calls several entities related to the partnership have submitted a first project to explore the sharing of data and services using the INCD cloud.

With the acquisition and installation of additional tape based storage in December 2022, a new activity to implement tape based storage as a service has started. The objective is to make the tape storage directly available to the users aimed at the storage of infrequently accessed data. This activity aims at providing scalable storage with high capacity and lower operational and investment costs.

[44] Portuguese EuroCC site hosted at the INCD cloud: https://eurocc.fccn.pt/en

14.USAGE METRICS

Overall in 2022 more than 43,854,961 hours of processing time were delivered across all INCD services. The figure 3 shows the combined usage in processing hours of the INCD infrastructure since January of 2018. The usage includes the high performance computing, high throughput computing and cloud computing services.

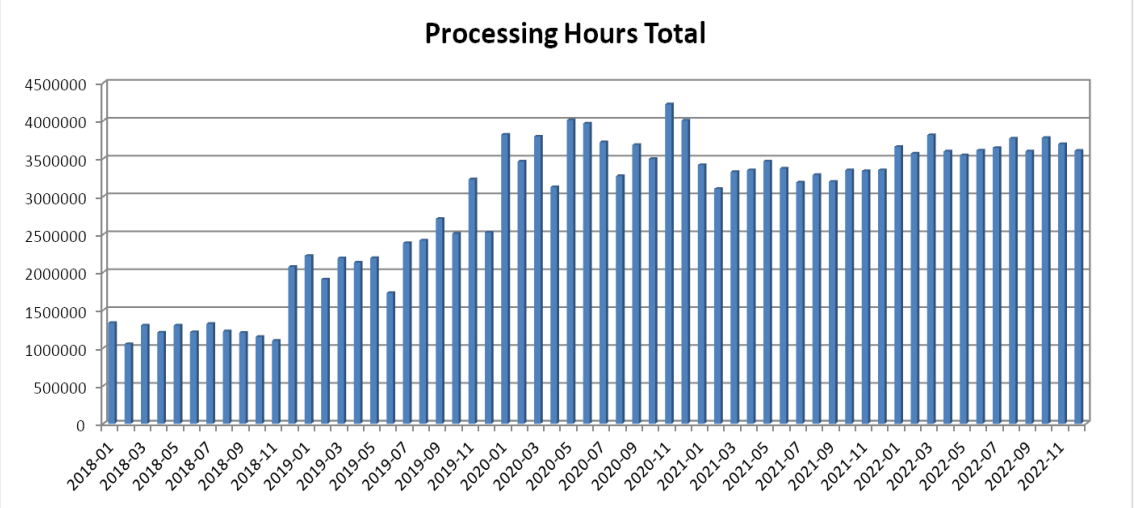

Figure 3: combined usage of all INCD services from January of 2018 to December of 2022.

The figure 4 shows the usage of the main INCD services since January of 2017 per centre and service. The figure shows the batch services supporting HPC and HTC both in Riba-de-Ave and Lisbon, and the cloud computing service also in Lisbon.

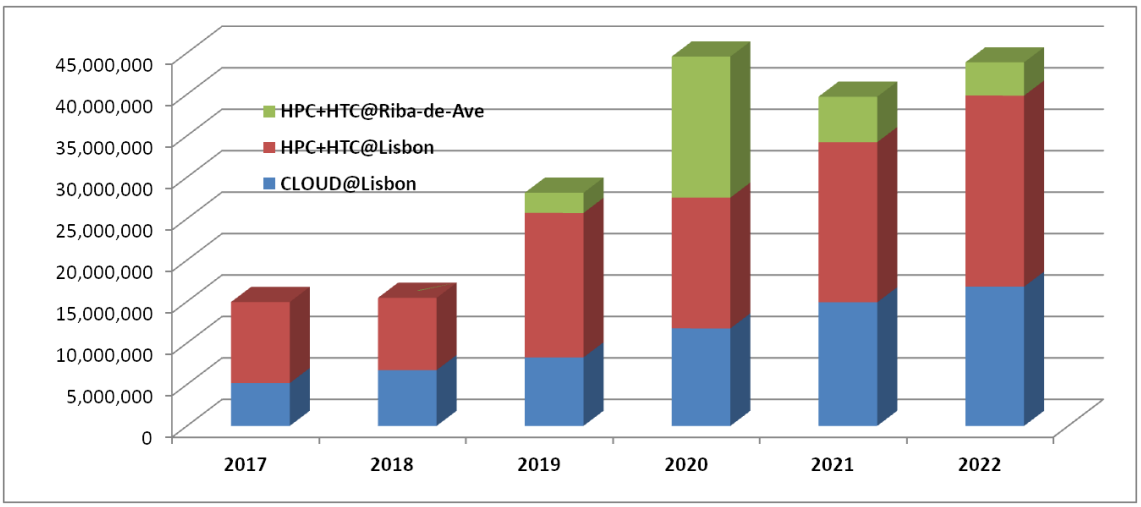

Figure 4: usage in hours of both HPC and HTC batch services from January of 2017 to December of 2022.

In comparison with 2021, the HPC and HTC capacity delivered by the Lisbon centre was 23,053,625 hours corresponding to a small increase. The upgrades performed in Lisbon during the year were mainly replacement of old equipment or installation of new equipment performed close to the end of the year, therefore these improvements had a small impact in terms of additional capacity. The operations necessary to install the new equipment and move part of the Bob supercomputer to Lisbon had a small negative impact in the capacity delivered in the last months of the year. In Riba-de-Ave the capacity delivered decreased to 4,008,595 hours, resulting from power and cooling limitations at the commercial data centre contracted by FCT to house the Bob supercomputer. INCD is operating part of the capacity of this machine in partnership with FCT and MACC. INCD is unrelated to these issues and has taken all possible measures to minimise the impact. Unfortunately, 75% of the INCD computing capacity at the site had to be powered down with a very negative impact in terms of capacity and usage. Overall the HPC and HTC services supported 65 projects from 32 research units and organisations. The services were exploited to the fullest available capacity.

Following the trend of the previous years the cloud computing service in Lisbon had an increase of the usage of 12% and is now completely saturated. The figure 5 shows the usage of the INCD cloud computing service provided by the Lisbon centre since January of 2017. In 2022 the service was used by 49 projects from 28 research units and organisations that consumed a total of 16,793,741 vCPU hours.

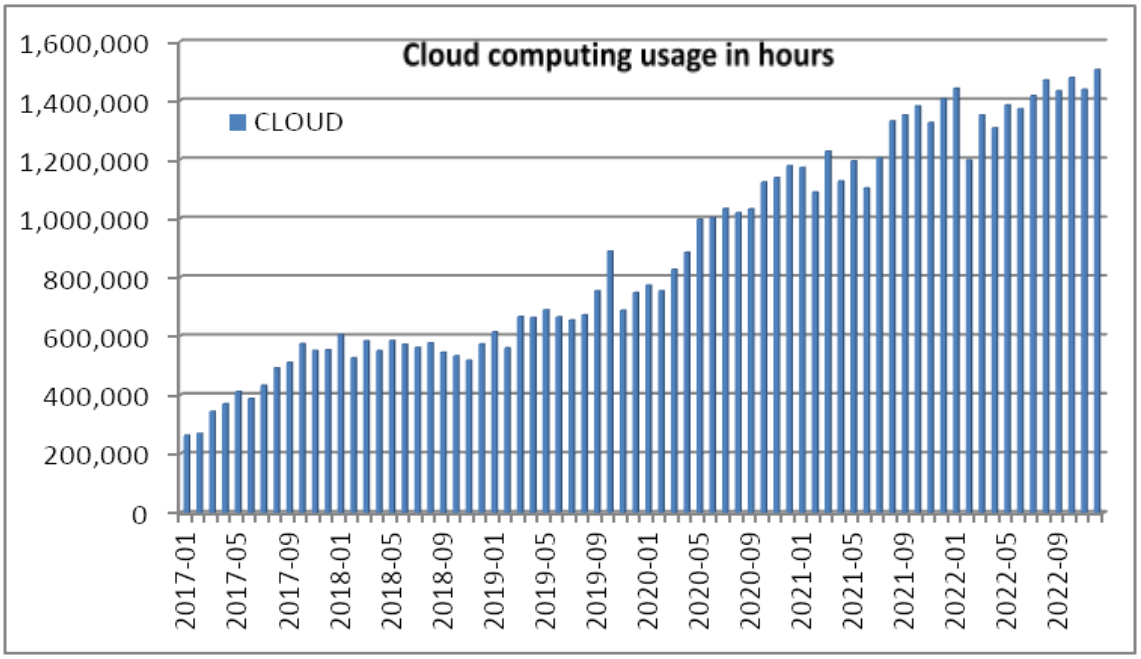

Figure 5: usage of the INCD cloud computing service from January 2017 to December of 2022.

In 2022, INCD supported a wide range of usage from infrastructures, research units and departments of universities from multiple domains and geographic areas in the country. Section 15 contains the list of the supported entities. INCD supported 20 computing projects from the FCT calls for advanced computing projects and 2 projects from the calls for projects on artificial intelligence in the public administration. INCD continued to support the Portuguese participation in CERN related experiments such as the ATLAS and CMS experiments at the CERN LHC. The Portuguese Tier-2 in the Worldwide LHC Computing Grid (WLCG) has fulfilled its pledged capacity for 2022 executing 471.068 processing jobs and delivering 165,631,870 HEPSCORE23[45] normalised hours. Table 2 shows the usage of the INCD primary computing services in 2022.

Services	Hours	Percentage
Cloud	16,793,741	38 %
HPC	8,948,082	21 %
HTC	18,113,138	41 %
Total	43,854,961	100 %

Table 2: summary of the services usage in 2022.

15.USERS

The table 3 shows the number of projects supported by INCD per year between 2017 and 2022. Due to the power and cooling limitations in Riba-de-Ave the number of processing hours committed to the second CPCA had to be limited, consequently the number of supported projects was also impacted. The figure 6 shows the split of the projects supported in 2022 per research field.

Projects supported yearly	2017	2018	2019	2020	2021	2022
Number of projects	61	57	65	122	123	114

Table 3: Projects supported yearly by INCD

[45] HEPScore23 (HS23) benchmark: https://w3.hepix.org/benchmarking.html

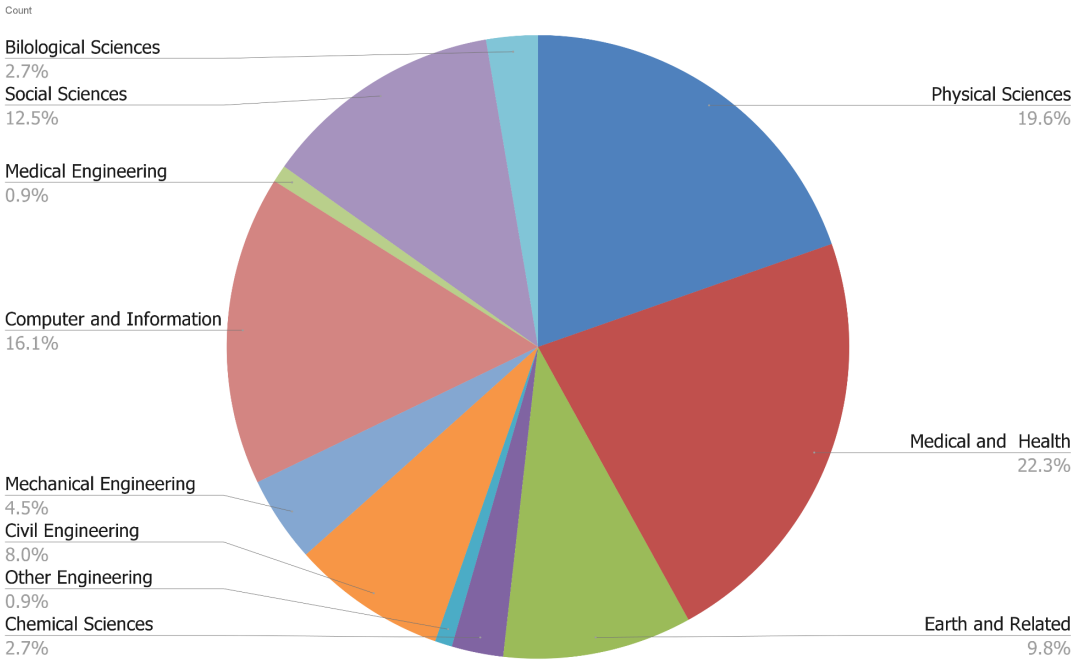

Figure 6: projects per field of research in 2022.

The table 4 provides a list of organisations, centres, infrastructures and research units of the INCD users in 2022.

Biomolecular SIMulations Research Group (BioSIM) / UCIBIO
Business Research Unit (BRU) / ISCTE
Concepção e Desenvolvimento de Sistemas de Informação (CDSI) / ISCTE
Centro de Estudos de Doenças Crónicas (CEDOC) / UNL
Centro de Engenharia e Tecnologia Naval e Oceânica (CENTEC) / U.Lisboa
Centro de Ecologia Evolução e Alterações Ambientais (cE3c) / U.Lisboa
Centro de Ecologia Funcional (CEF) / U.C
Centro de Física do Porto (CFP)
Centro de Investigação em Biomedicina (CBMR) / UALG
Centro Interdisciplinar de Investigação Marinha e Ambiental (CIIMAR) / U.Porto

Fundação Champalimaud

Instituto de Biossistemas e Ciências Integrativas (BioISI) / U.Lisboa

Centro de Neurociências e Biologia Celular (CNBC) / U.Coimbra

Departamento de Informática / FCUL / U.Lisboa

Departamento de Informática / FCT-UNL

Departamento de Engenharia Civil / U.Aveiro

Departamento de Física / IST / U.Lisboa

Departamento de Física / FCUL / U.Lisboa

Departamento de Física / U.Minho

Departamento de Engenharia Informática / U.Coimbra

Departamento de Informática / U.Porto

Departamento de Química / U.Aveiro

Faculdade de Ciências Sociais e Humanas / UNL

Faculdade de Letras / U.Porto

Faculdade de Medicina / U.Lisboa

Fundação para a Ciência e a Tecnologia - Unidade FCCN (FCT-FCCN)

Nova School of Science and Technology (FCT/UNL)

Institute for Bioengineering and Biosciences (IBB) / U.Lisboa

Instituto de Biologia Experimental e Tecnológica (IBET/ITQB)

Instituto de Geografia e Ordenamento do Território (IGOT) / U.Lisboa

Instituto de Ciência e Inovação em Engenharia (INEGI)

Instituto de Engenharia de Sistemas e Computadores - Investigação e Desenvolvimento (INESC-ID)

Instituto Nacional de Saúde Doutor Ricardo Jorge (INSA)

Instituto de Ciências Sociais da Universidade de Lisboa (ICS) / U.Lisboa
Instituto de Saúde Ambiental (ISAMB) / U.Lisboa
Instituto Tecnologico e Nuclear (ITN) / U.Lisboa
Instituto de Plasmas e Fusão Nuclear (IPFN) / U.Lisboa
Instituto Superior de Agronomia (ISA)
Instituto Superior de Engenharia de Coimbra (ISEC)
Instituto Superior de Engenharia de Lisboa (ISEL)
Instituto Universitário de Ciências Psicológicas, Sociais e da Vida (ISPA)
Júnior Empresas do Instituto Superior Técnico (JUNITEC)
Computer Science and Engineering Research Centre (LASIGE) / U.Lisboa
Laboratório de Instrumentação e Física Experimental de Partículas (LIP)
Laboratório Nacional de Engenharia Civil (LNEC)
Nova School of Business and Economics (Nova SBE) / UNL
Rede de Química e Tecnologia (REQUIMTE) / UCIBIO
Sociedade Portuguesa de Botânica (SPBOTANICA)
Universidade Aberta (U.Aberta)
Applied Molecular Biosciences Unit / UCIBIO
Portuguese node of the Global Biodiversity Network (GBIF)
Portuguese Coastal Monitoring Network (CoastNET)
Portuguese Biological Data Network (BIODATA.PT)

Table 4: organisations, infrastructures and research units that used INCD provided services in 2022.

16.PUBLICATIONS AND OTHER RESULTS

As a measure of the relevance and impact of INCD the figure 7 shows the evolution of the number of scientific results already published or approved for publication that

benefited from the usage of the INCD services in 2022. Early in 2023 the criteria used to classify the publications was revised by INCD and applied uniformly to all previous recorded results since 2017. This effort also included identification of publications with acknowledgements to INCD but not reported, which usually happens when the research is published after the INCD yearly campaign to collect the results. The figures 7 and 8 contain the sum of all results including publications with peer review, publications in conference proceedings, conference posters, books, PhD thesis, MSc thesis, patents and published datasets. The breakdown of the results is shown on figure 8. The number of peer reviewed publications in 2022 was the highest since 2017 (126 in 2022 against 97 in 2020). The actual list of publications is provided in the appendix I. The same list can be obtained from the INCD wiki[46].

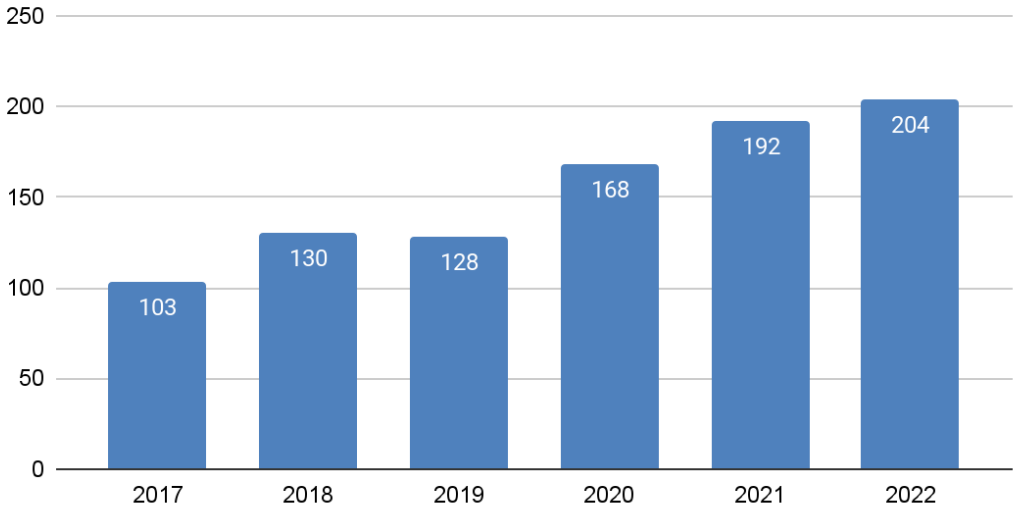

Figure 7: results made possible by using INCD from 2017 to 2022.

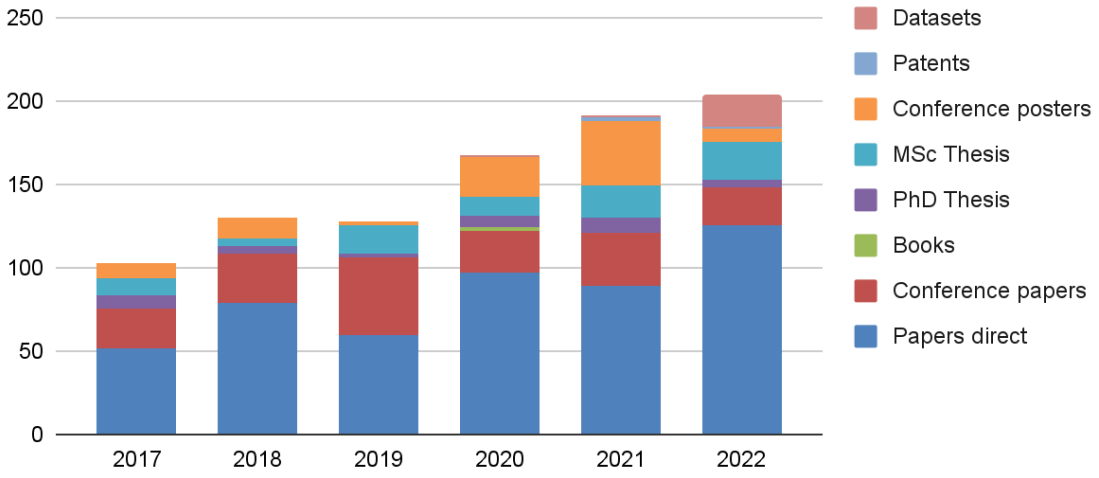

Figure 8: results per type from 2017 to 2022

[46] INCD wiki scientific publications section: https://wiki.incd.pt/books/scientific-publications

The results also include one patent in the area of area of biochemistry and biomedicine, namely in the area of biocatalysis and biopolymers, obtained by researchers from the Universities of Coimbra and Aveiro :

> *Alexandra T.P. Carvalho, Beatriz C. Almeida, Pedro R. Figueiredo, Daniel F.A.R. Dourado, Stephanie Paul, Derek J. Quinn, Thomas S. Moody, Andreia F. Sousa, and Armando J.D. Silvestre. Novel Variants of Hyperthermophilic Carboxylesterase for Polymer Synthesis (PCT/IB2022/051111) 2022.*

Besides the publications, the results of 2022 also include 19 curated datasets. Regarding support to thesis 5 PhD and 23 MSc thesis were produced in 2022 by the supported projects. In addition to these, INCD provided support to 34 PhD thesis that are ongoing and 38 MSc thesis that are also ongoing. The table 4 shows the complete set of results since 2017.

	2017	2018	2019	2020	2021	2022
Papers direct	52	79	59	97	89	126
Conference papers	24	30	47	25	32	22
Books	0	0	0	2	0	0
PhD Thesis	8	4	3	7	9	5
MSc Thesis	10	5	17	12	19	23
Conference posters	9	12	2	24	39	8
Patents					2	1
Datasets				1	2	19

Table 4: results per type from 2017 to 2022

ANNEX I - PUBLICATIONS AND OTHER RESULTS

Patents produced with the support of INCD in 2022

- Alexandra T.P. Carvalho, Beatriz C. Almeida, Pedro R. Figueiredo, Daniel F.A.R. Dourado, Stephanie Paul, Derek J. Quinn, Thomas S. Moody, Andreia F. Sousa, and Armando J.D. Silvestre. Novel Variants of Hyperthermophilic Carboxylesterase for Polymer Synthesis (PCT/IB2022/051111) 2022.

Publications produced with the support of INCD in 2022

- Santos, João Xavier, et al. "A Role for Gene-Environment Interactions in Autism Spectrum Disorder Is Supported by Variants in Genes Regulating the Effects of Exposure to Xenobiotics." Frontiers in Neuroscience 16 (2022). 10.3389/fnins.2022.862315
- Magalhães, Rita P., et al. "Identification of novel candidates for inhibition of LasR, a quorum-sensing receptor of multidrug resistant Pseudomonas aeruginosa, through a specialized multi-level in silico approach." Molecular Systems Design & Engineering 7.5 (2022): 434-446. https://doi.org/10.1039/D2ME00009A
- Burke, Anthony J., Carla SS Teixeira, and Sergio F. Sousa. "Transformation of a Chiral Glycolic Acid to an Isoaurone: Stereochemical Assignment of a Benzilic Acid Rearrangment Product." Asian Journal of Organic Chemistry 11.4 (2022): e202100692. https://doi.org/10.1002/ajoc.202100692
- Lapaillerie, Delphine, et al. "Selection of Bis-Indolyl Pyridines and Triphenylamines as New Inhibitors of SARS-CoV-2 Cellular Entry by Modulating the Spike Protein/ACE2 Interfaces." Antimicrobial Agents and Chemotherapy 66.8 (2022): e00083-22. https://doi.org/10.1128/aac.00083-22
- Araškov, Jovana B., et al. "Zn (II) complexes with thiazolyl–hydrazones: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity." CrystEngComm 24.29 (2022): 5194-5214. https://doi.org/10.1039/D2CE00443G
- Keller-Costa, Tina, et al. "Evidence for cross-feeding, metabolic specialization, and niche partitioning in the octocoral holobiont." (2022). https://doi.org/10.21203/rs.3.rs-1630933/v1
- Nogueira, Paulo Jorge, et al. "Multimorbidity profile of COVID-19 deaths in Portugal during 2020." Journal of clinical medicine 11.7 (2022): 1898. https://doi.org/10.3390/jcm11071898
- Silva, Sandra Godinho, et al. "Insights into the antimicrobial activities and metabolomes of Aquimarina (Flavobacteriaceae, Bacteroidetes) species from the rare marine biosphere." Marine Drugs 20.7 (2022): 423. https://doi.org/10.3390/md20070423
- Fernandes, Henrique S., et al. "A Molecular Mechanics Energy Partitioning Software for Biomolecular Systems." Molecules 27.17 (2022): 5524. https://doi.org/10.3390/molecules27175524
- Vieira, Tatiana F., et al. "Drug Repurposing Targeting Pseudomonas aeruginosa MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations." Antibiotics 11.2 (2022): 185. https://doi.org/10.3390/antibiotics11020185

- Rocha, Juliana F., Sérgio F. Sousa, and Nuno MF Sousa A. Cerqueira. "Computational Studies Devoted to the Catalytic Mechanism of Threonine Aldolase, a Critical Enzyme in the Pharmaceutical Industry to Synthesize β-Hydroxy-α-amino Acids." ACS Catalysis 12.9 (2022): 4990-4999. https://doi.org/10.1021/acscatal.1c05567
- Pereira, Ana Cláudia, et al. "Identification of novel aptamers targeting cathepsin B-overexpressing prostate cancer cells." Molecular Systems Design & Engineering (2022). https://doi.org/10.1039/D2ME00022A
- Rodrigues, João Antunes, et al. "Automatic Risk Assessment for an Industrial Asset Using Unsupervised and Supervised Learning." Energies 15.24 (2022): 9387. https://doi.org/10.3390/en15249387
- Silva, Sara, et al. "Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface." Molecules 27.9 (2022): 2734. https://doi.org/10.3390/molecules27092734
- Pires, Rita Costa, et al. "Transcriptome Analysis in Cork Oak Using Laser Microdissection and RNA-Seq." Biology and Life Sciences Forum. Vol. 11. No. 1. MDPI, 2021. https://doi.org/10.3390/IECPS2021-11914
- Vilela, Joana, et al. "Biomedical knowledge graph embeddings for personalized medicine: Predicting disease-gene associations." Expert Systems (2022): e13181. https://doi.org/10.1111/exsy.13181
- Caled, D., Carvalho, P., Silva, M.J. (2022). MINT - Mainstream and Independent News Text Corpus. In: , et al. Computational Processing of the Portuguese Language. PROPOR 2022. Lecture Notes in Computer Science(), vol 13208. Springer, Cham. https://doi.org/10.1007/978-3-030-98305-5_3
- Silva, Margarida, et al. "A glimpse at an early stage of microbe domestication revealed in the variable genome of Torulaspora delbrueckii, an emergent industrial yeast." Molecular Ecology (2022). https://doi.org/10.1111/mec.16428
- Vieira, Tatiana F., et al. "Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach." Molecular Systems Design & Engineering 7.10 (2022): 1294-1306. https://doi.org/10.1039/D2ME00088A
- Catumba, Guilherme TR, Orlando Oliveira, and Paulo J. Silva. "Another look at the Landau gauge three-gluon vertex." EPJ Web of Conferences. Vol. 258. EDP Sciences, 2022. https://doi.org/10.1051/epjconf/202225802008
- Comparison of Different Features and Neural Networks for Predicting Industrial Paper Press Condition; João Antunes Rodrigues, José Torres Farinha, Mateus Mendes, Ricardo J. G. Mateus, António J. Marques Cardoso. https://doi.org/10.3390/en15176308
- Antunes Rodrigues J, Torres Farinha J, Mendes M, Mateus R, Marques Cardoso A. Short and long forecast to implement predictive maintenance in a pulp industry. Eksploatacja i Niezawodnosc – Maintenance and Reliability 2022; 24 (1): 33–41 http://dx.doi.org/10.17531/ein.2022.1.5
- Isidro, J., Borges, V., Pinto, M. et al. Phylogenomic characterization and signs of microevolution in the 2022 multi-country outbreak of monkeypox virus. Nat Med 28, 1569–1572 (2022). https://doi.org/10.1038/s41591-022-01907-y
- Adriana M. Saur, Jorge Sinval, Cristina M. Del-Ben, Rosângela F. L. Batista8, Antônio A. M. Da Silva, Marco A. Barbieri, Heloisa Bettiol The Postpartum Bonding Questionnaire: validity evidence from the Brazilian version; Journal of Child and Family Studies (https://doi.org/10.1007/s10826-022-02406-x)
- João A.Marques da Silva, Miguel Vieira de Carvalho, Rui P.Cardoso Coelho, Igor A.Rodrigues Lopes, Francisco M.Andrade Pires; On the representativeness of polycrystalline models

with transformation induced plasticity; Finite Elements in Analysis and Design (https://doi.org/10.1016/j.finel.2022.103875)

- Aggregation of a Parkinson's Disease-Related Peptide: When Does Urea Weaken Hydrophobic Interactions? N. Galamba* Cite this: ACS Chem. Neurosci. 2022, 13, 12, 1769–1781 Publication Date:May 26, 2022 https://doi.org/10.1021/acschemneuro.2c00169
- Gadelho, J., Guedes Soares, C., Barajas, G., & Lara, J. L. (2022). CFD analysis of the PTO damping on the performance of an onshore dual chamber OWC. In C. Guedes Soares & T. A. Santos, Trends in Maritime Technology and Engineering Volume 2 (1st ed., pp. 381–389). CRC Press. https://doi.org/10.1201/9781003320289-40
- Gadelho, J., & Guedes Soares, C., (2022). Pneumatic performance improvement of an onshore dual chamber OWC using a CFD model. In Trends in Renewable Energies Offshore (Guedes Soares C., (Ed.)). https://doi.org/10.1201/9781003360773-36
- Non-B DNA conformations analysis through molecular dynamics simulations - ScienceDirect André F. Pina, Sérgio F. Sousa, Luísa Azevedo, João Carneiro, Non-B DNA conformations analysis through molecular dynamics simulations, Biochimica et Biophysica Acta (BBA) - General Subjects, Volume 1866, Issue 12, 2022, 130252, ISSN 0304-4165, https://doi.org/10.1016/j.bbagen.2022.130252.
- Comparison Study on Wild and Cultivated Opuntia sp.: Chemical, Taxonomic, and Antioxidant Evaluations (mdpi.com) Boudjouan F, Zeghbib W, Carneiro J, Silva R, Morais J, Vasconcelos V, Lopes G. Comparison Study on Wild and Cultivated Opuntia sp.: Chemical, Taxonomic, and Antioxidant Evaluations. Agriculture. 2022; 12(11):1755. https://doi.org/10.3390/agriculture12111755
- Bendall EE, Bagley R, Linnen CR, Sousa VC (2022) Faster-haplodiploid evolution under divergence-with-gene-flow: Simulations and empirical data from pine-feeding hymenopterans. Molecular Ecology, 31, 2348–2366. https://doi.org/10.1111/mec.16410
- João Carvalho, Hernan Morales, Rui Faria, Roger Butlin, Vitor Sousa (2022) Integrating Pool-seq uncertainties into demographic inference. Authorea. December 05, 2022. DOI: 10.22541/au.167023671.11036754/v1
- Pedro R. Figueiredo, Ricardo D. González, and Alexandra T.P. Carvalho. Insights into the Degradation of Polymer-Drug Conjugates by an Overexpressed Enzyme in Cancer Cells, J. Med. Chem. 2023, doi.org/10.1021/acs.jmedchem.2c01781.
- Beatriz C. Almeida, Pedro R. Figueiredo, Daniel F.A.R. Dourado, Stephanie Paul, Derek Quinn, Thomas S. Moody, Andreia F. Sousa, Armando J.D. Silvestre, and Alexandra T.P. Carvalho. Org. Process Res. Dev. 2022. doi.org/10.1021/acs.oprd.1c00480.
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2022) A drug discovery approach based on comparative transcriptomics between two toxin-secreting marine annelids: Glycera alba and Hediste diversicolor. Mol Omics, 18(8), 731-744. doi: 10.1039/D2MO00138A
- RODRIGO, A.P., LOPES, A., PEREIRA, R., ANJO, S.I., MANADAS, B., GROSSO, A.R., BAPTISTA, P.V., FERNANDES, A.R., COSTA, P.M. (2022) Endogenous Fluorescent Proteins in the Mucus of an Intertidal Polychaeta: Clues for Biotechnology. Mar Drugs, 20(4), 224. doi: 10.3390/md20040224
- Carvalho Leonardo, I., Barreto Crespo, M. T., Capelo, J., & Bustos Gaspar, F. (2022). The complete plastome of Echium plantagineum L. (Boraginaceae), the first chloroplast genome belonging to the Echium genus. Mitochondrial DNA Part B, 7(6), 1154–1156. https://doi.org/10.1080/23802359.2022.2087559
- Carvalho Leonardo, I., Barreto Crespo, M. T., Capelo, J., & Bustos Gaspar, F. (2022). The complete plastome of Nonea vesicaria (L.) Rchb. (Boraginaceae), the first chloroplast

genome belonging to the Nonea genus. Mitochondrial DNA Part B, 7(7), 1302–1304. https://doi.org/10.1080/23802359.2022.2095233

- Leonardo, I. C., Barreto Crespo, M. T., & Gaspar, F. B. (2022). Unveiling the complete genome sequence of Alicyclobacillus acidoterrestris DSM 3922T, a taint-producing strain. G3 Genes|Genomes|Genetics, jkac225. https://doi.org/10.1093/g3journal/jkac225
- Non-B DNA conformations analysis through molecular dynamics simulations Pina A.F., Sousa S.F., Azevedo L., and Carneiro J.Biochimica et Biophysica Acta - General Subjects 1866 (12) (2022) Article | DOI: 10.1016/j.bbagen.2022.130252
- Liposomal Formulations Loaded with a Eugenol Derivative for Application as Insecticides: Encapsulation Studies and In Silico Identification of Protein Targets Fernandes M.J.G., Pereira R.B., Rodrigues A.R.O., Vieira T.F., Fortes A.G., Pereira D.M., Sousa S.F., Goncalves M.S.T., and Castanheira E.M.S. Nanomaterials 12 (20) (2022) Article | DOI: 10.3390/nano12203583
- A Molecular Mechanics Energy Partitioning Software for Biomolecular Systems Fernandes H.S., Cerqueira N.M.F.S.A., Sousa S.F., and Melo A.Molecules 27 (17) (2022) Article | DOI: 10.3390/molecules27175524
- Selection of Bis-Indolyl Pyridines and Triphenylamines as New Inhibitors of SARS-CoV-2 Cellular Entry by Modulating the Spike Protein/ACE2 Interfaces Lapaillerie D., Charlier C., Guyonnet-Duperat V., Murigneux E., Fernandes H.S., Martins F.G., Magalhães R.P., Vieira T.F., Richetta C., Subra F., Lebourgeois S., Charpentier C., Descamps D., Visseaux B., Weigel P., Favereaux A., Beauvineau C., Buron F., Teulade-Fichou M.-P., Routier S., Gallois-Montbrun S., Meertens L., Delelis O., Sousa S.F.,and Parissi V. Antimicrobial Agents and Chemotherapy 66 (8) (2022) Article | DOI: 10.1128/aac.00083-22
- Synthesis, computational and nanoencapsulation studies on eugenol-derived insecticides Coelho C.M.M., Pereira R.B., Vieira T.F., Teixeira C.M., Fernandes M.J.G., Rodrigues A.R.O., Pereira D.M., Sousa S.F.,Gil Fortes A., Castanheira E.M.S., and T. Goncalves M.S. New Journal of Chemistry 46 (30) pp.14375-14387 (2022) Article | DOI: 10.1039/d2nj01893d
- Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach Vieira T.F., Magalhães R.P., Cerqueira N.M.F.S.A., Simoes M., and Sousa S.F. Molecular Systems Design and Engineering (2022) Article | DOI: 10.1039/d2me00088a
- Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters Markovic S.B., Maciejewska N., Olszewski M., Visnjevac A., Puerta A., Padron J.M., Novakovic I., Kojic S., Fernandes H.S., Sousa S.F., Ramotowska S., Chylewska A., Makowski M., Todorovic T.R., and Filipovic N.R. European Journal of Medicinal Chemistry 238 (2022) Article | DOI: 10.1016/j.ejmech.2022.114449
- New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach Fernandes H.S., Sousa S.F., and Cerqueira N.M.F.S.A. Molecular Diversity 26 (3) pp.1373-1381 (2022) Article | DOI: 10.1007/s11030-021-10259-7
- Computational Studies Devoted to the Catalytic Mechanism of Threonine Aldolase, a Critical Enzyme in the Pharmaceutical Industry to Synthesize β-Hydroxy-α-amino Acids Rocha J.F., Sousa S.F., and Cerqueira N.M.F.S.A. ACS Catalysis 12 (9) pp.4990-4999 (2022) Article | DOI: 10.1021/acscatal.1c05567
- The Catalytic Mechanism of Pdx2 Glutaminase Driven by a Cys-His-Glu Triad: A Computational Study Pina A.F., Sousa S.F., and Cerqueira N.M.F.S.A. ChemBioChem 23 (9) (2022) (IF 3.461, Q1)Article | DOI: 10.1002/cbic.202100555
- Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface Silva S., Marto J., Goncalves L.M., Fernandes H.S., Sousa S.F., Almeida A.J., and Vale N. Molecules 27 (9) (2022) Article | DOI: 10.3390/molecules27092734

- The critical role of Asp206 stabilizing residues on the catalytic mechanism of the Ideonella sakaiensis PETase Magalhães R.P., Fernandes H.S., and Sousa S.F. Catalysis Science and Technology 12 (11) pp.3474-3483 (2022) Article | DOI: 10.1039/d1cy02271g
- Transformation of a Chiral Glycolic Acid to an Isoaurone: Stereochemical Assignment of a Benzilic Acid Rearrangment Product Burke A.J., Teixeira C.S.S., and Sousa S.F.Asian Journal of Organic Chemistry 11 (4) (2022) Article | DOI: 10.1002/ajoc.202100692
- Identification of novel aptamers targeting cathepsin B-overexpressing prostate cancer cells Pereira A.C., Pina A.F., Sousa D., Ferreira D., Santos-Pereira C., Rodrigues J.L., Melo L.D.R., Sales G., Sousa S.F., and Rodrigues L.R. Molecular Systems Design and Engineering 7 (6) pp.637-650 (2022) Article | DOI: 10.1039/d2me00022a
- Identification of novel candidates for inhibition of LasR, a quorum-sensing receptor of multidrug resistant Pseudomonas aeruginosa, through a specialized multi-level in silico approach Magalhães R.P., Vieira T.F., Melo A., and Sousa S.F. Molecular Systems Design and Engineering 7 (5) pp.434-446 (2022) Article | DOI: 10.1039/d2me00009a
- Drug Repurposing Targeting Pseudomonas aeruginosa MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations Vieira T.F., Magalhães R.P., Simões M., and Sousa S.F. Antibiotics 11 (2) (2022) (IF 5.22) Article | DOI: 10.3390/antibiotics11020185
- Zn(II) complexes with thiazolyl-hydrazones: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity Araskov J.B., Visnjevac A., Popovic J., Blagojevic V., Fernandes H.S., Sousa S.F., Novakovic I., Padron J.M., Hollo B.B., Monge M., Rodriguez-Castillo M., Lopez-De-Luzuriaga J.M., Filipovic N.R., and Todorovic T.R. CrystEngComm (2022) Article | DOI: 10.1039/d2ce00443g
- Biguino, B., Olmedo, E., Ferreira, A., Zacarias, N., Lamas, L., Favareto, L., Palma, C., Borges, C., Teles-Machado, A., Dias, J., Castellanos, P. & Brito, A.C. 2022. Evaluation of SMOS L4 Sea Surface Salinity product in the Western Iberian Coast. Remote Sensing, 14. 423. https://www.mdpi.com/2072-4292/14/2/423
- Cereja, R., Brotas, V., Nunes, S., Rodrigues, M., Cruz, J.P. & Brito, A.C. 2022. Tidal influence on water quality indicators in a temperate mesotidal estuary (Tagus estuary, Portugal). Ecological Indicators, 136. 108715. https://www.sciencedirect.com/science/article/pii/S1470160X22001868
- Santos, C., Cabral, S., Carvalho, F., Sousa, P., Goulding, T., Ramajal, J. Silva, G., Brito, A.C., Costa, J.L. & Chainho, P. 2022. Spatial and temporal variations of cockle (Cerastoderma spp.) populations in two Portuguese estuarine systems with low directed fishing pressure. Frontiers in Marine Science 9. 699622. https://www.frontiersin.org/articles/10.3389/fmars.2022.699622/full
- Silva, A.F., Costa, B.H..; Costa, J.L., Pereira, E., Marques, J.P., Castro, J.J., Lino, P.G., Candeias-Mendes, A., Pousão-Ferreira, P., Sousa, I., Bentes L., Gonçalves, J.M.S., Almeida, P.R. & Quintella, B.R. 2022. Movements of Hatchery-Reared Dusky Groupers Released in a Northeast Atlantic Coastal Marine Protected Area. Journal of Marine Sciences and Engineering, 94. 10. https://www.mdpi.com/2077-1312/10/7/904
- On the conformal spin dependence of the perturbative QCD vacuum singularity G. Chachamis and A. Sabio Vera JHEP 07 (2022) 109 https://doi.org/10.1007/JHEP07(2022)109
- A parametric approach for the identification of single-charged isotopes with AMS-02 E. Bueno, F. Barão, M. Vecchi NIMA A 1031 (2022) 166564 10.1016/j.nima.2022.166564
- Iterative-Bayesian unfolding of cosmic-ray isotope fluxes measured by AMS-02 E. Bueno, F. Barão, M. Vecchi NIMA A 1046 (2023) 167695 10.1016/j.nima.2022.167695

- Search for pair-production of vector-like quarks in pp collision events at s√=13 TeV with at least one leptonically decaying Z boson and a third-generation quark with the ATLAS detector N. Castro, T. Vale et al. (ATLAS Collaboration) PLB, arXiv:2210.15413
- Upgrade of the ATLAS Tile Calorimeter high voltage system A. Gomes, J. S. Augusto, F. Cuim, G. Evans, R. Fernandez, L. Gurriana, R. Marques, F. Martins, C. Pereira (ATLAS Tile Calorimeter Group) J. Instrum. 17 (2022) C01061 10.1088/1748-0221/17/01/C01061
- Measurement of Higgs boson decay into b-quarks in associated production with a top-quark pair in pp collisions at root s=13 TeV with the ATLAS detector ATLAS Collaboration (2917 authors) J. High Energy Phys. 6 (2022) 097 10.1007/JHEP06(2022)097
- The Muon Puzzle in cosmic-ray induced air showers and its connection to the Large Hadron Collider Johannes Albrecht, Lorenzo Cazon, Hans Dembinski, Anatoli Fedynitch, Karl-Heinz Kampert, Tanguy Pierog, Wolfgang Rhode, Dennis Soldin, Bernhard Spaan, Ralf Ulrich, Michael Unger Astrophys. Space Sci. 367 (2022) 27 10.1007/s10509-022-04054-5
- Arrival Directions of Cosmic Rays above 32 EeV from Phase One of the Pierre Auger Observatory Pierre Auger Collaboration (373 authors) Astrophys. J. 935 (2022) 170 10.3847/1538-4357/ac7d4e
- A Catalog of the Highest-Energy Cosmic Rays recorded during Phase I of Operation of the Pierre Auger Observatory The Pierre Auger Collaboration Astrophysical Journal Supplement 264 (2023) 2, 50
- Search for nonresonant Higgs boson pair production in final state with two bottom quarks and two tau leptons in proton-proton collisions at 13 TeV CMS Collaboration arXiv.2206.09401 https://doi.org/10.48550/arXiv.2206.09401
- Vector Boson Scattering Processes: Status and Prospects M. Gallinaro et al. Rev.Phys. 8 (2022) 100071
- Observation of Bs0 mesons and measurement of the Bs0/B+ yield ratio in PbPb collisions at 5.02 TeV CMS Collaboration (2328 authors) Phys. Lett. B 829 (2022) 137062 10.1016/j.physletb.2022.137062
- A portrait of the Higgs boson by the CMS experiment ten years after the discovery CMS collaboration Nature 607 (2022) 7917, 60-68 10.1038/s41586-022-04892-x
- Search for high-mass exclusive gammagamma-> WW and gammagamma-> ZZ production in proton-proton collisions at sqrt(s) = 13 TeV CMS and TOTEM Collaborations arXiv:2211.16320
- Proton reconstruction with the CMS-TOTEM Precision Proton Spectrometer CMS and TOTEM Collaborations arXiv:2210.0585
- A machine learning-based methodology for pulse classification in dual-phase xenon time projection chambers P. Bras, F. Neves, A. Lindote, A. Cottle, R. Cabrita, E. Lopez Asamar, G. Pereira, C. Silva, V. Solovov, M.I. Lopes Eur. Phys. J. C 82 (2022) 553 10.1140/epjc/s10052-022-10502-x
- Radiation as a Tool against Neurodegeneration-A Potential Treatment for Amyloidosis in the Central Nervous System Coelho CM, Pereira L, Teubig P, Santos P, Mendes F, Viñals S, Galaviz D, Herrera F 10.3390/ijms232012265
- Determination of Ionizing Threshold of Trimethylamine Ions with a High Resolution RGA Mass Spectrometer A.M.F. Trindade, J. Escada, M. Rajado Silva, F.I.G.M. Borges, F.P. Santos 10.1088/1748-0221/17/02/P02031
- Dual-Polarity Ion Drift Chamber: A new system to measure the mobility of positive and negative ions D.J.G. Marques, A.F.V. Cortez, M.A.G. Santos, F.P. Santos, A.P. Marques, J. Escada, C.A.N. Conde, F.I.G.M. Borges NIMA 1029 (2022) 166416 10.1016/j.nima.2022.166416

- Dual-Polarity Ion Drift Chamber: Experimental results with Xe–S mixtures A. Marques, D. Marques, N. Duarte, J. Teles, A. Cortez, A. Trindade, J. Escada, F. Santos, F. Borges Nucl. Inst. Met. A, Volume 1045, 1 January 2023, 167575 https://doi.org/10.1016/j.nima.2022.167575
- A new experimental system for electron transverse diffusion measurements A. Trindade, J. Escada, J. Maia, R. Curado da Silva, F. Borges, A. Marques, F. Santos Nucl. Inst. Met. A, Volume 1045, 1 January 2023, 167603 https://doi.org/10.1016/j.nima.2022.167603
- Improving count rate capability of timing RPCs by increasing the detector working temperature A. Blanco et al. NIMA 1045, 2023 10.1016/j.nima.2022.167652
- All-sky Medium Energy Gamma-ray Observatory eXplorer mission concept Regina Caputo, Marco Ajello, Carolyn A. Kierans, Jeremy S. Perkins, Judith L. Racusin, Luca Baldini, Matthew G. Baring, Elisabetta Bissaldi, Eric Burns, Nicholas Cannady, Eric Charles, Rui M. Curado da Silva, Ke Fang, Henrike Fleischhack, Chris Fryer, Yasushi Fukazawa, J. Eric Grove, Dieter Hartmann, Eric J. Howell, Manoj Jadhav, Christopher M. Karwin, Daniel Kocevski, Naoko Kurahashi, Luca Latronico, Tiffany R. Lewis, Richard Leys, Amy Lien, Lea Marcotulli, Israel Martinez-Castellanos, Mario Nicola Mazziotta, Julie McEnery, Jessica Metcalfe, Kohta Murase, Michela Negro, Lucas Parker, Bernard Phlips, Chanda Prescod-Weinstein, Soebur Razzaque, Peter S. Shawhan, Yong Sheng, Tom A. Shutt, Daniel Shy, Clio Sleator, Amanda L. Steinhebel, Nicolas Striebig, Yusuke Suda, Donggeun Tak, Hiro Tajima, Janeth Valverde, Tonia M. Venters, Zorawar Wadiasingh, Richard S. Woolf, Eric A. Wulf, Haocheng Zhang, Andreas Zoglauer Journal of Astronomical Telescopes, Instruments, and Systems, Vol. 8, Issue 4, 044003 (October 2022). https://doi.org/10.1117/1.JATIS.8.4.044003
- Upgrade of the ATLAS Tile Calorimeter high voltage system A. Gomes, J. S. Augusto, F. Cuim, G. Evans, R. Fernandez, L. Gurriana, R. Marques, F. Martins, C. Pereira (ATLAS Tile Calorimeter Group) J. Instrum. 17 (2022) C01061 10.1088/1748-0221/17/01/C01061
- Concept of a fast neutron detector based on 10B-RPCs A. Morozov, L.M.S. Margato, A. Blanco and D. Galaviz A. Morozov et al 2022 JINST 17 P02016 10.1088/1748-0221/17/02/P02016
- Techniques for TPC Calibration: application to liquid Ar-TPCs J. Maneira for the DUNE Collaboration Particles 2022, 5(1), 74-83
- Improved search for invisible modes of nucleon decay in water with the SNO+ detector SNO+ Collaboration Phys. Rev. D 105, 112012 (2022) 10.1103/PhysRevD.105.112012
- Going to the light front with contour deformations Gernot Eichmann, Eduardo Ferreira, Alfred Stadler (selected for Editor's Choice) Phys.Rev.D 105 (2022) 3, 034009 https://doi.org/10.1103/PhysRevD.105.034009
- Theory introduction to baryon spectroscopy, Gernot Eichmann Few-Body Systems volume 63, Article number: 57 (2022) https://doi.org/10.1007/s00601-022-01756-y
- Isotopic cross sections of fragmentation residues produced by light projectiles on carbon near 400A MeV J. M. Boillos, D. Cortina-Gil, J. Benlliure, et al. (R3B collaboration) Phys. Rev. C 105, 014611 (2022) 10.1103/PhysRevC.105.014611
- Structure Calculations in Nd III and U III Relevant for Kilonovae Modelling Ricardo F. Silva, Jorge M. Sampaio, Pedro Amaro, Andreas Flörs, Gabriel Martínez-Pinedo, and José P. Marques Atoms2022,10,18 10.3390/atoms10010018
- Structure of single KL0–, double KL1–, and triple KL2−ionization in Mg, Al, and Si targets induced by photons, and their absorption spectra Y. Ménesguen, M.-C. Lépy, Y. Ito, M. Yamashita, S. Fukushima, T. Tochio, M. Polasik, K. Slabkowska,L. Syrockif, P. Indelicatog, J. P. Gomilsekh, J. P. Marques, J.M.Sampaio, J. Machado, P. Amaro, M. Guerra, J. P. Santos, and F. Parente Rad. Phys. Chem. 194, 110048 (2022) 10.1016/j.radphyschem.2022.110048

- Unveiling the two-proton halo character of 17Ne: Exclusive measurement of quasi-free proton-knockout reactions C. Lehr, F. Wamers, F.Aksouh, et al. Phys. Lett. B 827, 136957 (2022) 10.1016/j.physletb.2022.136957
- Experimental and theoretical approaches for determining the K-shell fluorescence yield of carbon Philipp Hönicke, Rainer Unterumsberger, Nils Wauschkuhn, Burkhard Beckhoff, Markus Krämer, Paul Indelicato, Jorge Sampaio, José Pires Marques, Mauro Guerra, Fernando Parente, and José Paulo Santos Rad. Phys. Chem. 202, 110501 (2023) 10.1016/j.radphyschem.2022.110501
- L-shell fluorescence yield for heavy elements with 80≤Z≤96 K. Meddouh, S. Daoudi, A. Kahoul, J.M. Sampaio, J.P. Marques, F. Parente, N. Kup Aylikci, V. Aylikci, Y. Kasri, A. Hamidani Rad. Phys. Chem. 202, 110481 (2023) 10.1016/j.radphyschem.2022.110481
- K- and L-shell theoretical fluorescence yields for the Fe isonuclear sequence Daniel Pinheiro, André Fernandes, César Godinho, Jorge Machado, Filipe Grilo, Luís Sustelo, Jorge M. Sampaio, Pedro Amaro, Roberta G. Leitão, José P. Marques, Fernando Parente, Paul Indelicato, Miguel de Avillez, José Paulo Santos, Mauro Guerra Rad. Phys. Chem. 203, 110594 (2023) 10.1016/j.radphyschem.2022.110594
- Semi-empirical and empirical calculation of Kβ/Kα intensity ratios for Low-Z Elements A. Hamidani, A. Kahoul, S. Daoudi, J.M. Sampaio, J.P. Marques, F. Parente, K. Meddouh, N. Kup Aylikci, V. Aylikci, Y. Kasri At. Nucl. Data Tables 149, 101549 (2023) 10.1016/j.adt.2022.101549
- Independently Optimized Orbital Sets in GRASP – The Case of Hyperfine Structure in Li I Y. Li, P. Jönsson, M. Godefroid, G. Gaigalas, J. Bieron, J. P. Marques, P. Indelicato, and C. Chen Atoms 2023, 11, 4 10.3390/atoms11010004
- Design of beam optics for RF-separated kaon and antiproton beams in the M2 beam line of the CERN North Area A. Gerbershagen et al. (14 authors) NIM A 1048 (2023) 168004 https://doi.org/10.1016/j.nima.2022.168004
- An experiment for electron-hadron scattering at the LHC K.D. J. André et al Eur.Phys.J.C 82 (2022) 1, 40 10.1140/epjc/s10052-021-09967-z
- A template method to measure the t(t)over-bar polarisation J. A. Aguilar-Saavedra, M. C. N. Fiolhais, P. Martin-Ramiro, J. M. Moreno, A. Onofre Eur. Phys. J. C 82 (2022) 134 10.1140/epjc/s10052-022-10063-z
- Impact of jet-production data on the next-to-next-to-leading-order determination of HERAPDF2.0 parton distributions H1 Collaboration / ZEUS Collaboration (234 authors) Eur. Phys. J. C 82 (2022) 243 10.1140/epjc/s10052-022-10083-9
- Jets and Jet Substructure at Future Colliders Johan Bonilla et al. (27 authors) Front. Physics 10 (2022) 897719 10.3389/fphy.2022.897719
- On the conformal spin dependence of the perturbative QCD vacuum singularity G. Chachamis and A. Sabio Vera JHEP 07 (2022) 109 https://doi.org/10.1007/JHEP07(2022)109
- On the polarization of the non-prompt contribution to inclusive J/psi production in pp collisions Pietro Faccioli, Carlos Lourenco J. High Energy Phys. 10 (2022) 010 10.1007/JHEP10(2022)010
- NNLO interpolation grids for jet production at the LHC D. Britzger, A. Gehrmann-De Ridder, T. Gehrmann, E. W. N. Glover, C. Gwenlan, A. Huss, J. Pires, K. Rabbertz, D. Savoiu, M. R. Sutton, J. Stark Eur.Phys.J.C 82 (2022) 10, 930 10.1140/epjc/s10052-022-10880-2
- Improved background subtraction and a fresh look at jet sub-structure in JEWEL J. G. Milhano and K. Zapp Eur. Phys. J. C82 (2022) no.11, 1010 10.1140/epjc/s10052-022-10954-1

- Multiparticle production in proton-nucleus collisions beyond eikonal accuracy P. Agostini, T. Altinoluk, N. Armesto, F. Dominguez and J. G. Milhano Eur. Phys. J. C82 (2022) no.11, 1001 10.1140/epjc/s10052-022-10962-1
- Flavour-Changing Neutral Scalar Interactions of the Top Quark, Nuno Castro, Kirill Skovpen Universe 2022, 8, 609 10.3390/universe8110609
- Heavy quarks and jets as probes of the QGP Liliana Apolinário, Michael Winn, Yen-Jie Lee Prog.Part.Nucl.Phys. 127 (2022) 103990 10.1016/j.ppnp.2022.103990
- Concept of a fast neutron detector based on 10B-RPCs A. Morozov, L.M.S. Margato, A. Blanco and D. Galaviz A. Morozov et al 2022 JINST 17 P02016 10.1088/1748-0221/17/02/P02016
- Improving count rate capability of timing RPCs by increasing the detector working temperature A. Blanco et al. NIMA 1045, 2023 10.1016/j.nima.2022.167652
- SND@LHC: The Scattering and Neutrino Detector at the LHC SND@LHC Colaboration To be published in JINST (arXiv:2210.02784)
- The SHiP experiment at the proposed CERN SPS Beam Dump Facility SHiP Collaboration Eur.Phys.J.C 82 (2022) 5, 486 https://doi.org/10.1140/epjc/s10052-022-10346-5
- Search for pair-production of vector-like quarks in pp collision events at s√=13 TeV with at least one leptonically decaying Z boson and a third-generation quark with the ATLAS detector N. Castro, T. Vale et al. (ATLAS Collaboration) PLB, arXiv:2210.15413
- Fitting a Collider in a Quantum Computer: Tackling the Challenges of Quantum Machine Learning for Big Datasets Miguel Caçador Peixoto, Nuno Filipe Castro, Miguel Crispim Romão, Maria Gabriela Jordão Oliveira, Inês Ochoa arXiv:2211.03233 10.48550/arXiv.2211.03233
- A source of very energetic oxygen located in Jupiter's inner radiation belts Elias Roussos,Christina Cohen, Peter Kollmann, Marco Pinto, Norbert Krupp, Patricia Gonçalves, Konstantinos Dialynas Space Advances, Vol 8, Issue 2 DOI: 10.1126/sciadv.abm4234
- Validation of dMEREM, the Detailed Mars Energetic Radiation Environment Model, with RAD Data from the Surface of Mars Patricia Goncalves, Luisa Arruda, Marco Pinto Front. Astron. Space Sci. 9 (2022) 833144 10.3389/fspas.2022.833144
- Pioneering evaluation of GaN transistors in geostationary satellites Hugo Mostardinha, Diogo Matos, Nuno Borges Carvalho, Jorge Sampaio, Marco Pinto, Patricia Gonçalves, Tiago Sousa, Paul Kurpas, Joachim Wuerfl, Andrew Barnes, François Garat & Christian Poivey Sci Rep 12, 12886 (2022) https://doi.org/10.1038/s41598-022-17179-y
- The BepiColombo Environment Radiation Monitor, BERM Marco Pinto, Beatriz Sanchez-Cano, Richard Moissl, Johannes Benkhoff, Carlota Cardoso, Patrícia Gonçalves, Pedro Assis, Rami Vainio, Philipp Oleynik, Arto Lehtolainen, Manuel Grande & Arlindo Marques Space Sci. Rev. 218 (2022) 54 10.1007/s11214-022-00922-2
- Tackling the muon identification in water Cherenkov detectors problem for the future Southern Wide-field Gamma-ray Observatory by means of Machine Learning B.S. González, R. Conceição, M. Pimenta, B. Tomé, A. Guillén Neural Computing & Applications 34, pages 5715–5728 (2022) https://doi.org/10.1007/s00521-021-06730-z
- P_{\gamma h}^{\alpha} A new variable for γ/h discrimination in large gamma-ray ground arrays R. Conceição, B.S. González, M. Pimenta, B. Tomé Phys.Lett.B 827 (2022) 136969 10.1016/j.physletb.2022.136969
- The relation between optical and γ-ray emission in BL Lac sources G La Mura, J Becerra Gonzalez, G Chiaro, S Ciroi, J Otero-Santos Monthly Notices of the Royal Astronomical Society, Volume 515, Issue 4, October 2022, Pages 4810–4827 10.1093/mnras/stac2041
- The Mercedes water Cherenkov detector P. Assis, A. Bakalová, U. Barres de Almeida, P. Brogueira, R. Conceição, A. De Angelis, L. Gibilisco, B. S. González, A. Guillén, G. La Mura, L.

M. D. Mendes, L. F. Mendes, M. Pimenta, R. C. Shellard, B. Tomé, J. Vícha Eur.Phys.J.C 82 (2022) 10, 899 10.1140/epjc/s10052-022-10857-1

- Gamma/hadron discrimination at high energies through the azimuthal fluctuations of the particle distributions at ground R. Conceição, L. Gibilisco, M. Pimenta, B. Tomé JCAP 10 (2022) 086 https://doi.org/10.1088/1475-7516/2022/10/086
- Evaluation of the potential of a gamma-ray observatory to detect astrophysical neutrinos through inclined showers Jaime Alvarez-Muñiz, Ruben Conceição, Pedro J. Costa, Mário Pimenta, Bernardo Tomé Phys.Rev.D 106 (2022) 10, 102001 10.1103/PhysRevD.106.102001

Publications in conference proceedings produced with the support of INCD in 2022

- Title: Distal edge determination for a multi-slat prompt-gamma camera: Irradiation with a 200-MeV proton beam, date: 2022-02-11, Authors: H. Simões, A. Morozov, J. Silva, J. Teodoro, P. Crespo
- Title: Understanding COVID-19 pandemic trajectories: why changes in online behavior matter for now-casting, date: 2022-02-10, Authors: Sara Mesquita, Lília Perfeito, João Loureiro and Joana Gonçalves-Sá, Conference: NetSciX 2022 - International School and Conference on Network Science Porto, Portugal
- Title: Sensitivity to neutrinoless double beta decay of 136Xe with a third generation TPC dark matter experiment, date: 2022-06-01, Authors: A. Lindote and I. Olcina, Conference: Neutrino 2022, Seoul, Korea (virtual)
- Title: Neutrino physics with the LUX-ZEPLIN Detector, date: 2022-05-31, Authors: Paulo Brás (on behalf of LZ Collaboration), Neutrino 2022 Seul,Coreia (virtual)
- Title: Deciphering Jet Quenching Effects with Novel Reclustering Tool, date: 2022-04-06, Authors: Liliana Apolinario, Pablo Rodriguez, Korinna Zapp, Conference: Quark Matter 2022 Krakow, Poland (remote)
- Title: Timing RPC for thermal neutron detection with 3D position sensitivity, date: 2022-09-26, Conference: XVI Workshop on Resistive Plate Chambers and Related Detectors CERN, 26–30 Sept 2022
- Title: Advances Towards a Large-Area, Ultra-Low-Gas-Consumption RPC Detector, date: 2022-05-22, Conference: PM2021 - 15th Pisa Meeting on Advanced Detectors - Edition 2022 May 22-28, 2022, La Biodola - Isola d'Elba (Italy)
- Title: Improving count rate capability of timing RPCs by increasing the detector working temperature, date: 2022-05-22, Conference: PM2021 - 15th Pisa Meeting on Advanced Detectors - Edition 2022 May 22-28, 2022, La Biodola - Isola d'Elba (Italy)
- Title: Large Field CdTe Monitor for Astrophysics and TGF Science on board the Space Rider, date: 2022-11-07, Authors: R. M. Curado Da Silva, J. M. Maia, J. Sousa, P. Póvoa, J. Mingacho, G. Falcão, J. Gonçalves, G. Salgado, M. Moita, Conference: IEEE Nuclear Science Symposium Milano, Italy
- Title: Dual-Polarity Ion Drift Chamber: Experimental results with Xe-SF6 mixtures, date: 2022-05-22
- Title: Between even and odd: probing the CP-nature of the Higgs-Top Yukawa coupling, date: 2022-07-08, conference: International Conference on High Energy Physics (ICHEP 2022) Bologna, Italy
- Title: The microevolution of information on social media, date: 2022-10-20, Authors: Lília Perfeito and Joana Gonçalves-Sá, Conference: CCS 2022 - Conference on Complex Systems Palma de Maiorca, Spain

- Title: Flu or Not: A computational approach to respiratory-disease surveillance before and after COVID-19, date: 2022-10-20, Authors: Eleonora Tulumello, Sara Mesquita, Lilia Perfeito, Irma Varela-Lasheras and Joana Gonçalves-Sá, Conference: CCS 2022 - Conference on Complex Systems Palma de Maiorca, Spain
- Title: Flu or Not: A computational approach to respiratory-disease before and after COVID-19, date: 2022-11-09, Authors: Irma Varela-Lasheras, Sara Mesquita, Eleonora Tulumello,Lília Perfeito, and Joana Gonçalves-Sá, Conference: EPH - 15th European Public Health Conference 2022 Berlin, Germany
- Title: Flu or Not: A computational approach to respiratory-disease before and after COVID-19, date: 2022-11-09, Authors: Irma Varela-Lasheras, Sara Mesquita, Eleonora Tulumello,Lília Perfeito, and Joana Gonçalves-Sá, conference: [3C] Cells, Computers & Clinics Oeiras, Portugal
- Title: Proton Multi-Beam FLASH Radiotherapy: Combining FLASH and IMPT, date: 2022-11-30, Authors: Joana Leitão, João Seco, Patrícia Gonçalves, Conference: Flash Radiotherapy and Particle Therapy 2022 Barcelona
- Title: Monte Carlo Modeling of Inter-Track Radical Reactions for FLASH, date: 2022-11-30, Authors: Miguel Molina, Yujie Chi, T. Zhang, Patrícia Gonçalves and João Seco, Conference: Flash Radiotherapy and Particle Therapy 2022 Barcelona
- Title: Simulation of a multi-slat prompt-gamma camera for proton beam distal edge determination during pelvic irradiation, date: 2022-11-05, Authors: J. Silva, H. Simões, A. Morozov, J. Teodoro, P. Crespo, Conference: IEEE Nucl. Sci. Symp. & Med. Imag. Conf. (NSS/MIC) Milano, Italymulti-slat
- Title: Simulation of proton range monitoring in an anthropomorphic phantom using a multi-slat prompt-gamma camera, date: 2022-11-05, Authors: J. Teodoro, H. Simões, A. Morozov, J. Silva, P. Crespo, Conference: IEEE Nucl. Sci. Symp. & Med. Imag. Conf. (NSS/MIC) Milano, Italy
- Title: Positron emission tomography for proton range verification in proton radiation therapy, date: 2022-11-05, Authors: S.P. Tavernier, R. Bugalho, F. Caramelo, J.P. Cesar, P.Crespo, J.C. Da Silva, L. Ferramacho, N. Ferreira, P. Gonçalves, D.Grosshans, B. Jesus, K.Klein, K. Lang, C. Layden, C. Leong, W. Matava,A. Mozorov, F. Poenisch, M. Proga, N. Sahoo, J. Seco, H. Simões, R.Silva, M. Silveira, J. Varela, Conference: IEEE Nucl. Sci. Symp. & Med. Imag. Conf. (NSS/MIC) Nov. 5 - 12, Milano, Italy

Conference posters produced with the support of INCD in 2022

- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2022). Bioprospecting marine environments for unravelling novel drugs: Transcriptomics and interactome-directed analyses of two toxin-secreting Polychaeta. 1st Egas Moniz One Health Symposium.
- NUNES, M., MOUTINHO CABRAL, I., GONÇALVES, C., MISSIONÁRIO, M., FERNANDES, J.F., TRAVESSO, M., MADEIRA, D., COSTA P.M., MADEIRA, C. (2022). Transcriptome profiling of the common goby Pomatoschistus microps exposed to seasonal warming reveals gene downregulation as an energy-saving mechanism to cope with thermal stress. 1st Egas Moniz One Health Symposium.
- MARTINS, C., MOUTINHO CABRAL, I., CARVALHO, L.M., DE OLIVEIRA GALVÃO, M.F., SAÚDE, M.L., DREIJ, K., COSTA P.M. (2022). Molecular mechanisms behind the effects from

interaction of carcinogens and emerging pollutants: in vivo and in vitro perspective. XVIth International Congress of Toxicology.

- GONÇALVES, C., COSTA, P.M. (2022). Unravelling cephalopod venom glands through histological and transcriptomic approaches. Encontro Ciência'22.
- Barbosa, A.J.M.; Arianna Nurrito; Ana Margarida Dias; Soares, Cátia; Lychko, Iana; Roque, ACA. "Modeling studies of reflectin de novo peptide assembly". Paper presented in 15th National Physical Chemistry Meeting (15ENQF) and 4th Computational Chemistry Symposium, 2023.
- Carlos Costa; Barbosa, A.J.M.; Ana Margarida Dias; Roque, ACA. "Affinity reagents towards the SARS-CoV-2 spike protein". Paper presented in BPP2022 Biopartitioning & Purification Conference, 2022.
- GONÇALVES, C., GROSSO, A.R., COSTA, P.M. (2022). Advances on the venom glands of Cephalopoda: Targets for the prospecting of novel bioactives. UCIBIO Scientific Advisory Board Meeting.

PhD Thesis produced with the support of INCD in 2022

- On the measurement and interpretation of the fluxes of galactic cosmic-ray nuclei Eduardo Bueno (https://doi.org/10.33612/diss.253636377)
- Guilherme Guedes A global approach to physics beyond the Standard Model (https://hdl.handle.net/10481/76867)
- Ana Sofia Inácio Measurement of the 130 Te Two-Neutrino Double Beta Decay Half-life with the SNO+ Experiment
- Maria Ramos The interplay between collider and astrophysical probes of non-minimal composite Higgs models (https://digibug.ugr.es/bitstream/handle/10481/72877/95029%281%29.pdf)
- Correia, M.J. 2022. Tools for the management and conservation of the European eel (Anguilla anguilla): An application to Santo André lagoon. Faculdade de Ciências, Universidade de Lisboa, 203 pp. Submitted in May 2022.

PhD Thesis ongoing with the support of INCD in 2022

- Susana Santos Study of the ttH production and Higgs couplings to Top quarks in the ATLAS experiment
- Miguel Orcinha Estudo da modulação Solar no fluxo de raios cósmicos com dados da experiência AMS
- The effects of proton therapy on protein self-organization: potential benefits for neurodegenerative disorders Carina Coelho (UL/FCUL)
- Adaptive dose reconstruction with online in-vivo range verification in particle therapy Mariana Brás (UL/IST)
- Developing Multi-Beam FLASH with Proton Beams Joana Leitão (UL/IST)
- Radiation Damage of Optical Components in Scintillator Detectors: from the ATLAS/LHC Tile Calorimeter to Future Experiments Beatriz Pinheiro Pereira (UL/IST)
- Radiation Damage of the TileCal Optics components at the High Luminosity LHC phase Rudnei Machado (UL/IST)

- Raios Cósmicos: desenvolvimento de módulos de divulgação através design participativo Luís Afonso
- Reaching for PeVatrons with the future Southern Wide-field Gamma-ray Observatory Lucio Gibilisco (UL/IST)
- Development of microdosimetric detectors for radiobiology in hadron therapy facilities Cristiana Rodrigues (UL/FCUL)
- Accelerating the ATLAS Trigger system with Graphical Processing Units Nuno Fernandes (UL/IST)
- Measurement of Collider Neutrinos with the SND@LHC Experiment Guilherme Soares (UL/IST)
- Disentangling and Quantifying Jet-Quenching With Generative Deep Learning João Arruda Gonçalves (UL/IST)
- Enhanced Searches with the Pierre Auger Observatory in the Era of Multi-messenger Astrophysics Alexandra Fernandes (U.Minho)
- Measurements of Short Range Correlations on Exotic Nuclei at R3B using TRPCs Manuel Xarepe (UL/FCUL)
- Jetography in Heavy Ion Collisions André Cordeiro (UL/IST)
- AutoBSM: Validating Beyond the Standard Model Physics with Machine Learning Fernando Souza (U.Minho)
- Study of lepton universality in top quarks pairs events Giacomo Da Molin (UL/IST)
- Multi-messenger physics with the Pierre Auger Observatory and SWGO Pedro Costa (UL/IST)
- The Partonic Structure of Hadrons Eduardo Ferreira (UL/IST)
- Formal and phenomenological studies in the high energy limit of QCD Dario Vaccaro (UL/IST)
- Characterization of liquid argon detectors for next generation neutrino physics Wallison Campanelli (UL/FCUL)
- Differential tracking on disinformation websites and its impact on search engine results Íris Damião (UL/IST)
- Probing CP couplings in ttX production at the Run3 of the LHC Esteban Chalbaud (U.Coimbra, IDPASC PT-CERN Call 2022/1)
- Beatriz C. Almeida, Ricardo S.V. Pires, Kristala L.J. Prather, and Alexandra T.P. Carvalho. The role of zing in transcription factor allosteric regulation.
- Ricardo D. González, Warispreet Singh, Lino Ferreira, and Alexandra T.P. Carvalho. Enzymatic synthesis of RNA-peptide conjugates as potential therapeutics for COVID-19.
- Inês Carvalho Leonardo (2020.08210.BD)
- 2021.07128.BD - Fábio Martins - Rational Development of Nanomedicines for Cardiovascular Diseases.
- 2020.09087.BD - Rita Magalhães - In Silico Optimization of Biocatalysts for Plastic Biodegradation.
- SFRH/BD/147276/2019 - Susana Maria da Fonseca Fernandes - Development of biocidal formulations for effective biofouling control.
- SFRH/BD/136594/2018 - André Figueiredo Pina - Innovative approach to fight tuberculosis and malaria targeting the extraordinary PLP synthase macromolecular complex.
- SFRH/BD/137844/2018 - Claudia Tatiana Freitas Vieira - New Drugs Against Biofilm Formation and Development: a Computational and Experimental Approach.
- SFRH/BD/136746/2018 - Juliana Ferreira Rocha - Rational development of new biocatalysts for the production of Parkinson Disease Drugs.

- Cereja, R. (2023). Phytoplankton in estuarine waters: assessment of temporal and spatial variability. Doutoramento Earthsystems, Faculdade de Ciências, Universidade de Lisboa.

MSc Thesis produced with the support of INCD in 2022

- João Antunes Particle reconstruction in large liquid scintillator detectors using charge and time signal modelization - the SNO+ neutrino physics experiment (UL/IST)
- Daniel Neacsu Dark matter searches at the LHC in models with extended scalar sectors
- Lígia Lopes Lecionar através de métodos não convencionais: uma investigação sobre a abordagem lúdica no ensino
- Fátima Alcaso Design and optimisation of a xenon TPC with SiPM readout for neutrinoless double beta decay studies
- Rúben Inácio Exploiting Graph Neural Networks for jet identification in LHC experiments
- António Oliveira Unsupervised machine learning techniques in high energy physics
- Beatriz Artur Impact of Quark-Gluon Plasma in Extensive Air Showers (https://fenix.tecnico.ulisboa.pt/cursos/meft21/dissertacao/1972678479055537))
- Rita Silva Optimisation studies for the pion-induced Drell-Yan measurement at the AMBER experiment (UL/IST https://fenix.tecnico.ulisboa.pt/cursos/meft21/dissertacao/565303595502847)
- Henrique Neves From the Concept to Development of Astrophysics Payloads for Gamma Radiation Studies (U.Coimbra)
- Carlota Cardoso Flight data analysis of the BERM radiation monitor aboard the BepiColombo mission to Mercury (UL/IST)
- Francisco Barba Characterization of thin silicon strip detectors for nuclear experiments (UL/FCUL http://hdl.handle.net/10451/53658)
- André Torcato Heavy-baryon spectroscopy in a quark-diquark 1. approach (UL/FCUL http://hdl.handle.net/10451/51871)
- David Almeida PandeMedia: an annotated corpus of digital media for issue salience (UL/FCUL http://hdl.handle.net/10451/55576)
- Matilde Santos Caracterização e teste funcional de um micro dosímetro de fibras ópticas cintilantes (UL/FCUL http://hdl.handle.net/10451/53766)
- Nísia Fernandes Estudo da radiossensibilização de células tumorais do pâncreas com nanopartículas (http://hdl.handle.net/10451/51982)
- José Rodrigues Embedded systems for heating and machine learning in microcontrollers (U.Coimbra)
- João Lopes Looking for (de)coherence effects in the Quark-Gluon Plasma (UL/IST https://fenix.tecnico.ulisboa.pt/cursos/left21/dissertacao/565303595502771)
- Nuno Madureira Jet substructure tools to identify hadronization timescales (UL/IST https://fenix.tecnico.ulisboa.pt/cursos/meft21/dissertacao/565303595502772)
- NUNES, M. (2022). Gene networks modulating heat acclimatization in common gobies: influence of latitude and season in fish metabolism and health. M.Sc. thesis, NOVA School of Science and Technology, NOVA University of Lisbon, Monte de Caparica. Advisors: Carolina Madeira and Pedro M. Costa.
- MOUTINHO CABRAL, I. (2021). A computational approach to identify target receptors of marine toxins in the human proteome: Potential biotechnological applications. M.Sc. thesis, NOVA School of Science and Technology, NOVA University of Lisbon, Monte de Caparica. Advisors: Pedro M. Costa and Ana Rita Grosso.

- Brandão, P.R. 2022. Portuguese estuarine systems and their essential ecological role for some fish species: trends and predictions in face of global changes. Mestrado em Ecologia Marinha, Universidade de Lisboa, Faculdade de Ciências. 61 pp.
- Santos, Gil, 2022. Activity patterns and tridimensional space use of the European catfish (Silurus glanis) on Belver reservoir. Mestrado em Biologia da Conservação, Universidade de Lisboa, Faculdade de Ciências. 57 pp. http://hdl.handle.net/10451/51885
- Almeida, J. 2022. Trace Metals in the Sado Estuary and their implications on the Environmental Quality. Mestrado em Ciências do Mar, Faculdade de Ciências, Universidade de Lisboa, 103 pp. Submitted in July 2022.

MSc Thesis ongoing with the support of INCD in 2022

- Rúben Inácio Exploiting Graph Neural Networks for jet identification in LHC experiments (UL/IST)
- Carolina Felgueiras Simulations and benchmark of a fast neutron detector for nuclear astrophysics (UL/FCUL)
- Magda Duarte Development of high-resolution, three-dimensional muographies (U.Minho)
- Joana Vences Next-generation Neutrino Physics: Development of the DUNE laser-based Calibrations
- Simão Costa Quark hadronization with B mesons at the LHC (UL/IST)
- André Neves Astrofísica Multi-Mensageira com o Telescópio AMEGO da NASA (U.Coimbra)
- Francisca Santos Launching the Radiation Hard Electron Monitor aboard the ESA JUICE mission (UL/IST)
- Francisco Barreiro Geometrical aspects of jet quenching in small systems
- Manuel Mariano Sensitivity of jet sub-structure observables to jet quenching in collisions of light nuclei (UL/IST)
- Tomás Almeida Design of a phantom for radiobiology studies (UL/FCUL)
- Igor Gago Life prospection on Mars - Studing the Martian Subsurface Radiation Environment (UL/IST)
- João Pires Deep Neural Networks in Experimental Data Analyses (UL/FCUL)
- Milton Freitas Measurement of the number of muons in high occupancy MARTA stations (UL/IST)
- Lia Pereira Modelling protein amyloid structures and observing the effects of radiation using the GEANT4-DNA toolkit (UL/FCUL)
- João Jantarada Simulation of a p-process in a Supernova Explosion using the NucNet Tools framework (UL/FCUL)
- Tomás Sousa Characterization of CsI(Tl) Crystals and Implementation of tools for the CALIFA calorimeter at FAIR
- Rita Pestana Development of a standard methodology for online dose calculation in air (UL/FCUL)
- Henrique Legoinha Probing the properties of the plasma of quarks and gluons with heavy flavour (UL/IST)
- Joana Reis Implementation of quark mass effects in QCD three-jet production observables produced by hadronic decays of the Z-boson at FCC-ee collider (UL/FCUL)
- Daniel Salgueiro Design of a fiber-phantom detector for quality assurance in PT (UL/FCUL)
- Patrícia Ferreira Machine Learning for Anomaly Detection in the Atlas Trigger at the LHC (U.Coimbra)

- Sandro Saltão Optimisation of the vertical separation of multiple scatter events in the LZ detector with applications in the sensitivity to the $0\nu2\beta$ decay of Xe-136 (U.Coimbra)
- Gulherme Calé Jet jet correlations in QCD (UL/FCUL)
- Céu Neiva Advanced machine learning techniques in rare events research at the Large Hadron Collider (U.Minho)
- José Cordeiro Development of an FPGA-accelerated clustering for the ATLAS trigger system (UL/IST)
- Catarina Pereira Performance of the TileCal High Voltage Upgrade System (UL/FCUL)
- Pedro Lagarelhos Prospects for the HL-LHC of the measurement of the top quark couplings in the ttbar semileptonic channel (UL/IST)
- Ana Campos Estudo da dispersão de partículas alfa em filmes finos (UL/FCUL)
- Guilherme Crispim Pre-equilibrium of the Quark-Gluon Plasma (UL/IST)
- Miguel Lopes Integration of the HiRezBrainPET with a clinical PET/CT system - Image performance evaluation of a prototype for next-generation brain tomography (UL/IST)
- Maria Borges Beam tests of a scintillation array detector for high-resolution dosimetry (UL/IST)
- Fábio Carmo Cálculo de espetro de emissão de Auger para simulações de radioterapia sensibilizada com nanopartículas de ouro (UL/FCUL)
- Marco Leitão Disentangling QGP response using energy flow correlators (UL/IST)
- António carvalho Fast algorithms of simulation of the positron-emitting activity generation for multi-beamlet proton therapy treatment plans (U.Coimbra)
- Rúben Inácio Exploiting Graph Neural Networks for jet identification in LHC experiments (UL/IST)
- João Lopes Looking for (de)coherence effects in the Quark-Gluon Plasma (UL/IST)
- Nuno Madureira Jet substructure tools to identify hadronization timescales (UL/IST)
- Ana Filipa Fernandes (MSc in Biotechnology / FCT-NOVA)

Datasets produced with the support of INCD in 2022

- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Cysteine-rich venom protein from Glycera alba. Direct submission to GenBank – Accession OL606744
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Serine protease inhibitor Kazal-type from Glycera alba. Direct submission to GenBank – Accession OL606745
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Cysteine-rich secretory protein from Hediste diversicolor. Direct submission to GenBank – Accession OL606746
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Thyrostimulin beta-5 subunit from Hediste diversicolor. Direct submission to GenBank – Accession OL606747
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Whole-transcriptome dataset for Glycera alba. Direct submission to GEO – Accession GPL31947
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Whole-transcriptome dataset for Hediste diversicolor. Direct submission to GEO – Accession GPL31948
- GONÇALVES, C., MOUTINHO CABRAL, I., GROSSO, A.R., COSTA, P.M. Cysteine-rich venom protein from Sepia officinalis. Direct submission to GenBank - Accession number: OP198203 (under publication embargo)
- GONÇALVES, C., MOUTINHO CABRAL, I., GROSSO, A.R., COSTA, P.M. SE-cephalotoxin from Sepia officinalis. Direct submission to GenBank - Accession number: OP198204 (under publication embargo)

- GONÇALVES, C., MOUTINHO CABRAL, I., GROSSO, A.R., COSTA, P.M. Venom Insulin from Sepia officinalis. Direct submission to GenBank - Accession number: OP198205 (under publication embargo)
- GONÇALVES, C., GROSSO, A.R., COSTA, P.M. Cysteine-rich venom protein from Octopus vulgaris. Direct submission to GenBank - Accession number: OP209720 (under publication embargo)
- GONÇALVES, C., GROSSO, A.R., COSTA, P.M. Cysteine-rich venom protein (latisemin-like) from Octopus vulgaris. Direct submission to GenBank - Accession number: OP209721 (under publication embargo)
- GONÇALVES, C., GROSSO, A.R., COSTA, P.M. Chitinase from Octopus vulgaris. Direct submission to GenBank - Accession number: OP209722 (under publication embargo)
- GONÇALVES, C., GROSSO, A.R., COSTA, P.M. Hyaluronidase from Octopus vulgaris. Direct submission to GenBank - Accession number: OP209723 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Cysteine-rich venom protein from Eulalia sp. Direct submission to GenBank – Accession OP254189 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Peptidase M12A from Eulalia sp. Direct submission to GenBank – Accession OP254190 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Peptidase M12B from Eulalia sp. Direct submission to GenBank – Accession OP254191 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Peptidase M13 from Eulalia sp. Direct submission to GenBank – Accession OP254192 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Serine protease from Eulalia sp. Direct submission to GenBank – Accession OP254193 (under publication embargo)
- RODRIGO, A.P., MOUTINHO CABRAL, I., ALEXANDRE, A., COSTA, P.M. Hyaluronidase from Eulalia sp. Direct submission to GenBank – Accession OP254194 (under publication embargo)