

Infraestrutura
Nacional de
Computação
Distribuída

2021 Activities Report

TABLE of CONTENTS

EXECUTIVE SUMMARY **4**

1. MESSAGE FROM THE INTERNATIONAL ADVISORY COMMITTEE **5**

2. INTRODUCTION **6**

3. ABOUT THE INFRASTRUCTURE **6**

4. INFRASTRUCTURE SERVICES **8**
4.1. CLOUD COMPUTING 9
4.2. OBJECT STORAGE 9
4.3. FEDERATED CLOUD 9
4.4. HIGH PERFORMANCE COMPUTING 10
4.5. HIGH THROUGHPUT COMPUTING 10
4.6. LARGE MEMORY COMPUTING 10
4.7. ACCELERATED COMPUTING 11
4.8. FEDERATED COMPUTING 11
4.9. CONTAINERISED COMPUTING 11
4.10. DISTRIBUTED READ-ONLY FILE SYSTEM 12
4.11. DATA REPOSITORIES 12
4.12. DATA PROTECTION 12
4.13. SCIENTIFIC PORTALS AND GATEWAYS 12
4.14. VALUE-ADDED SERVICES 12
4.15. INTEGRATION OF SERVICES AND APPLICATIONS 13
4.16. RESOURCE MANAGEMENT 13
4.17. SUPPORT AND TRAINING 13

5. INFRASTRUCTURE MANAGEMENT AND OPERATIONS **13**

6. INTERNATIONAL COOPERATION **14**

7. EUROPEAN OPEN SCIENCE CLOUD **14**

8. FIGHTING COVID-19 ..... **15**

9. HIGH PERFORMANCE COMPUTING ACTIVITIES **15**

10. USAGE METRICS **16**

11. PLANS FOR 2022 ..... **19**

12. USERS **19**

13. PUBLICATIONS **22**

EXECUTIVE SUMMARY

In 2021, INCD continued the execution of the contract established with Portuguese national funding agency for science, research and technology (FCT) in the Framework of the Portuguese roadmap of research infrastructures of strategic interest (RNIE). The contract started in 2017 and covers the infrastructure development and implementation activities. This contract was extended until October 2022 under the mitigation measures for the COVID-19 pandemic. The budget was also reprogrammed, aimed at redirecting the funding previously allocated for construction, to be used for the acquisition of computing and data storage equipment to strengthen the INCD centres in the north, centre and Lisbon regions. In this context, an international public tender was prepared to procure equipment for this upgrade.

The pandemic continued to hamper mobility, communication, availability of human resources and access to the goods necessary for the execution of projects and normal infrastructure operations. Respecting the official directives, both the staff and the collaborators continued to work remotely using videoconference and collaborative tools. Still, as in the previous year, INCD managed to develop a substantial set of activities and maintain its operation in an adverse context.

Fulfilling its mission, the infrastructure continued to support a wide range of scientific users from multiple research domains. In this regard, INCD supported the first edition of the call for advanced computing projects organised by FCT. Under this call and in the context of the National Advanced Computing Network (RNCA), INCD received an allocation of more than 50 computing projects to which processing time, data storage and support were provisioned. A protocol for the formal adhesion of INCD to RNCA as operational centre was negotiated. Another protocol for the housing of a new cloud computing facility in the north region was also signed with FCT.

The international collaborations continued with the INCD participation in EGI, IBERGRID and WLCG, operating services federated in these infrastructures. INCD also continued to participate in the European project EOSC-Synergy, whose objective is the harmonisation and integration of computing and data resources in the European Open Science Cloud (EOSC). Also, within the scope of the EOSC initiative, two new European projects started in 2021, namely EGI-ACE and C-Scale. Through them, INCD intends to expand its range of activities and collaborations supporting applications and thematic services in areas such as; hearth observation, artificial intelligence, biodiversity and coastal engineering. A project proposal to Horizon Europe was also prepared, aiming at the participation in the provisioning of capacity for image processing applications.

Finally, INCD applied to the FCT call for institutional scientific employment (CEEC) and was awarded with a contract for a PhD researcher (assistant researcher). In December 2021, the management bodies of the INCD Association were renewed, starting a new cycle in the life of the organisation.

1. Message from the International Advisory Committee

The Advisory Committee (AC) is impressed by the large number of computing projects supported, reflected in a large number of publications and presentations in conferences, serving as a basis as well for a PhDs. and Master thesis, but also leading to patents. INCD is commendable for their dedication and service to the scientific community in Portugal, including links to major European initiatives, and standing out in the comparison with similar infrastructures in Spain and Italy. Much more so taking into account the small effort in human resources allocated to the infrastructure support and operation.

The key added value of INCD resides in supporting scientific excellence and scholarship by providing state-of-the-art computing tools and know-how. Especially for High Performance Computing, what delivers added value is the know-how about using/adapting Computing facilities according to multiple tasks or scientific domains. The AC believes that the exploitation of this know-how is one of the main sources for expressing the added value of INCD in the framework of the RNCA in Portugal.

Interesting drivers for innovation are the beyond-the-state of-the-art IT services provided by INCD to areas such as coastal studies or bioengineering. Support for scientific creativity and new ideas often requires experimental IT services, which have in turn large potential to increase the competitiveness of Portuguese research teams. Strengthening the weight of these services in the future evolution of the infrastructure would maximise the innovation potential of INCD.

Teaching and training is a point that could be flagged for further exploration. Exploring new collaboration opportunities with universities, as a means to identify and potentially recruit talents, and additional visibility. Offering online courses based on the current training catalog could be a starting point which requires only a reasonable investment. Given the expertise gained by the INCD members in several fields, it might also be worthwhile to offer some of these courses to an international audience, perhaps through a fee-based enrollment, exploiting the numerous links INCD has got.

As a suggestion for future evolution a fruitful link with the public sector and/or industry needs could be identified. If INCD wants to strengthen its sustainability, special attention to promoting innovation also outside research user communities needs to be paid. Addressing industrial partners or the public sector in a way that shows that INCD is able to listen to their requirements, understand and recognize their needs, being so identified as an innovative player in areas beyond scientific research, would nicely complement the currently ongoing activities.

Isabel Campos (CSIC)

Danilo Piparo (CERN)

Davide Salomoni (INFN)

2. INTRODUCTION

Infraestrutura Nacional de Computação Distribuída (INCD) is a digital infrastructure within the Portuguese roadmap of research infrastructures of strategic interest (RNIE) of the Portuguese Foundation for Science and Technology (FCT). INCD provides state-of-the-art advanced computing and data-oriented services to the national scientific and academic community. INCD supports research across all scientific and technological domains, enabling researchers to effectively participate in projects and related activities. 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, IBERGRID, WLCG and EOSC.

The INCD association (*Associação INCD*) was created in 2015 with the objectives of 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 and LIP).

In 2021, INCD delivered computing and data services to the research community that were provided through its operational centres in Minho and Lisbon. The infrastructure supported the existing user base and further extended it, namely through more than 50 new computational projects approved within the scope of the 1st call for advanced computing projects (CPCA) coordinated by FCT. In total, INCD provided in 2021 more than 33,000,000 processing hours supporting projects in multiple scientific domains such as: biodiversity, life sciences, physics, material sciences, civil engineering, information technology and environment among others.

3. ABOUT THE INFRASTRUCTURE

INCD has an holistic approach to the requirements and provisioning of Information Technology (IT) services for modern research (Fig 1). This is reflected both in the infrastructure architecture, and in the provided services. At the core of this approach is the research data which can be produced, stored, managed, accessed and processed through multiple services. 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 facilities 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. 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 2).

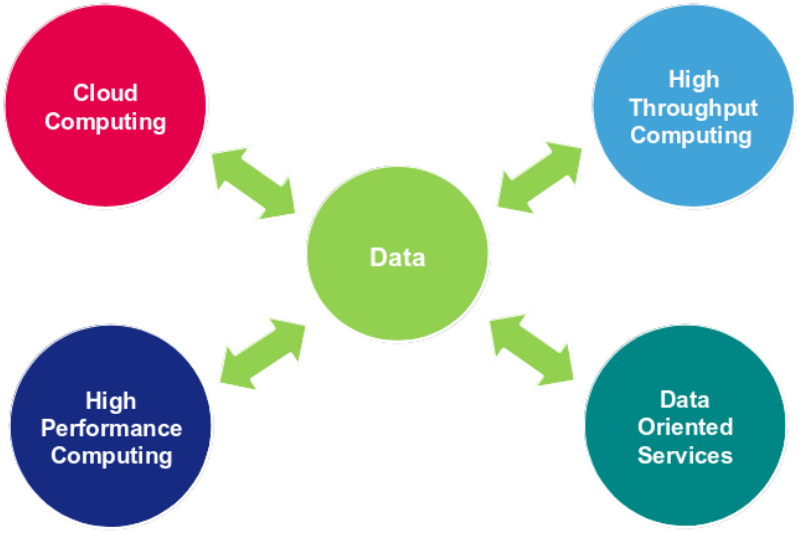

Figure 1: INCD approach to IT services delivery.

The main INCD services (cloud, HPC, HTC and data oriented) sit immediately above the housing and network layers. The main services can be used either directly by the end-users or indirectly through other higher level services. The higher level services are meant to provide additional capabilities tailored to specific needs. 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. Transversal to all layers of the architecture are activities such as security, training, interoperability, support, collaboration, research and innovation.

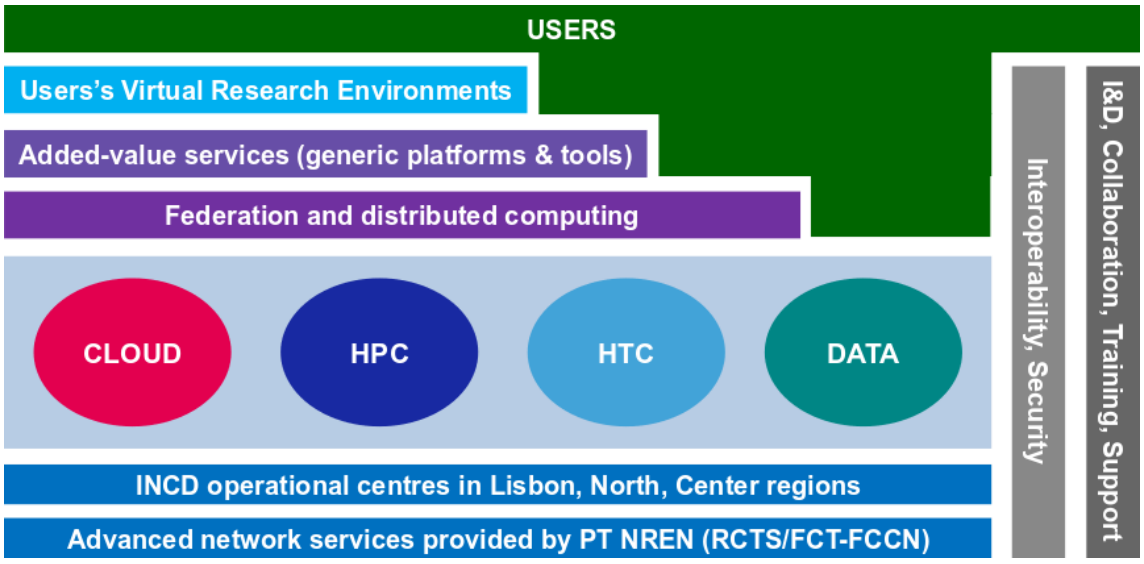

Figure 2: INCD high level architecture.

4. INFRASTRUCTURE SERVICES

The INCD service catalogue includes both the main services already mentioned (cloud, HPC, HTC and data oriented) as well as the most relevant high level services. The virtual research environments are grouped under Scientific Portals and Gateways while other services are grouped under Value-Added Services. The catalogue is continuously improved according to the technology evolution and user requirements. The catalogue of services provided in 2021 is summarised in Table 1 and further described in the subsections.

INCD Services Portfolio
Cloud Computing (CLOUD)
Federated Cloud
Object Storage
High Performance Computing (HPC)
High Throughput Computing (HTC)
Large Memory Computing
Accelerated Computing
Federated Computing
Containerised Computing
Distributed Read-only File system
Data Repositories
Data Protection
Scientific Portals and Gateways
Value-Added Services
Integration of Services and Applications
Resource Management
Documentation, Support and consultancy

Table 1: INCD services catalogue

4.1. CLOUD COMPUTING

The INCD cloud computing service (named *Stratus*) is an infrastructure as a service (IaaS) cloud that provides access to virtual computing resources on-demand. In addition, Platform-as-a-service (PaaS) and Software-as-a-Service (SaaS) can also be supported using the IaaS cloud as the basis. The cloud service is built-on the Openstack cloud management framework leveraging its most important components, to provide a resilient set-up. The cloud computing service is complemented by a Ceph based data storage system, providing robust block storage from which virtual data volumes can be delivered. The cloud computing service is currently provided by the INCD node in Lisbon. In 2021, the process of upgrading the Openstack and Ceph based cloud service has started. A parallel test environment was set-up and used to evaluate the upgrade of the Lisbon installation. The planning of the second Openstack installation in the northern region whose deployment is expected to start in 2022 has begun. With this second installation INCD aims at providing additional capacity and increased resiliency. The monitoring of the cloud service and the collection of accounting was also improved. The service has seen a steady increase of usage since mid-2020 and is being currently used by 63 projects. In 2021 the cloud computing service delivered 8,523,308 hours of processing time.

4.2. OBJECT STORAGE

The INCD object storage service provides access to cloud based object storage using interoperable cloud APIs for large scale highly reliable data storage. The service is closely related to the INCD cloud computing service. It is based on the same Ceph data storage system that provides block storage to the INCD cloud, however the object storage service can also be used independently from the cloud computing service. With the object storage service data can be stored and retrieved as objects, therefore providing higher horizontal scalability than other storage solutions such as conventional file-systems. Through its application programming interface (API), that includes support for S3 and SWIFT, the service can be easily and safely accessed remotely. The object storage service is provided by the INCD node in Lisbon. The planning of a second deployment in the northern region has also started in 2021.

4.3. FEDERATED CLOUD

Access to the EGI and IBERGRID federated cloud computing infrastructures, interconnecting cloud services and data at international level. The INCD cloud and object storage services are federated into the EGI and IBERGRID international infrastructures. The federated cloud service adheres to the EGI infrastructure monitoring, both the underlying cloud computing service and its federated access have yielded in 2021 close to 100% availability and reliability. 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 and data resources at international level for added capacity, data sharing or higher resiliency.

4.4. HIGH PERFORMANCE COMPUTING

The High Performance Computing (HPC) service is composed of two computing clusters equipped with low latency interconnects, located in Minho and Lisbon. The Lisbon cluster (named *Cirrus-A*) features computing nodes equipped with AMD Epyc processors interconnected via Infiniband. In 2021, the *Cirrus-A* cluster delivered 19,315,837 hours of processing time. The cluster in Minho (named *Cirrus-B*) corresponds to a partition of the Bob supercomputer operated under agreement with the Portuguese Foundation for Science and Technology (FCT). The storage system used in *Cirrus-A* and *Cirrus-B* is a Lustre file system optimised for parallel workloads. The *Cirrus-B* cluster features compute nodes equipped with Intel Xeon processors that are also interconnected via Infiniband. In 2021, this cluster delivered 5,483,969 hours of processing time. The batch system of *Cirrus-B* is Slurm, while in *Cirrus-A* the batch system completed in 2021 a phased migration from SoGE to Slurm. The availability of *Cirrus-B* has been severely affected by power and cooling limitations at the commercial datacenter that under contract with FCT houses the BOB supercomputer. These limitations affected a wide range of users. Several users had to be moved from *Cirrus-B* to *Cirrus-A* and the execution of several computing projects had to be extended until the end of 2021 to enable their completion.

4.5. HIGH THROUGHPUT COMPUTING

The High Throughput Computing (HTC) service is based on a partition of the *Cirrus-A* cluster in Lisbon. The 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 computing processes need to communicate with low latency while executing, the HTC computing processes are individual tasks that can be executed separately. For higher efficiency, the HTC and HPC services share the same Slurm batch system. The HTC partition is composed of heterogeneous nodes both Intel Xeon and AMD Epyc interconnected via a high performance Ethernet network. The service also relies on the Lustre file-system for data storage, although in this case the Lustre file-system is optimised for non-parallel workloads.

4.6. LARGE MEMORY COMPUTING

The large memory computing service is tailored for computational tasks with large memory requirements. The service is set-up to take 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 and

currently is only supported in Lisbon. Planning for higher memory capacity nodes has started and is expected to be made available in 2022. This service targets multithreaded shared memory applications with large memory requirements such as genome data processing and other *big data* applications.

4.7. 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 and Stratus cloud in Lisbon. The range of supported GPUs includes NVIDIA V100, NVIDIA T4 for production and older NVIDIA K40 mainly for development and educational purposes. In 2021 the service had a very high demand in particular for machine learning applications. Planning for an upgrade to take place in 2022 has started.

4.8. FEDERATED COMPUTING

Access to the EGI, IBERGRID and WLCG distributed computing infrastructures, interconnecting computing clusters and data 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 HTC and HPC services in Lisbon (Cirrus-A) and assist users into accessing additional capacity integrated in the EGI federation. The service is mainly oriented at supporting international research activities that benefit from the access to shared computing and data resources at international level. The upgrade of the middleware for federated computing previously initiated in 2020 was finalised in 2021. This included new ARC-CE computing elements and XRootD storage elements integrated with the EGI, IBERGRID and WLCG infrastructures. The Lustre data storage system served by the StoRM middleware, and now also through XRootD, remains the main file system based storage solution supporting the federated computing service.

4.9. 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, Docker, Singularity and orchestrators like Docker Swarm and Kubernetes among others.

4.10. DISTRIBUTED READ-ONLY FILE SYSTEM

The distributed read-only file system service is meant to share immutable files across the INCD sites regardless of their geographic location. The service is based on the CernVM-FS (CVMFS), 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 homogeneous computing environments across INCD sites and therefore facilitating the combined use of the infrastructure services.

4.11. DATA REPOSITORIES

In 2021, INCD started a new activity with the Portuguese Foundation for Science and Technology for 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 research data repository software. This service is currently under development and is being delivered as a pilot activity as part of the R&I towards new services.

4.12. DATA PROTECTION

The data protection service is aimed at data protection, long-term data storage, storage of critical data and disaster recovery. 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 access patterns of the data. This service is supported by the INCD and LIP datacenters in Lisbon. An expansion of the tape based storage capacity was planned and is expected to take place in 2022 and 2023.

4.13. 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 service 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.

4.14. 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 and meeting organisation support services, web servers,

load balancers, proxies, among others. INCD is increasing the range of these services according to the demand.

4.15. INTEGRATION OF SERVICES AND APPLICATIONS

The integration of services and applications 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 both to cloud services aimed to be hosted at INCD for a long term, and also to the integration of HTC and HPC applications. This service also includes integration at the federation level in order to take advantage of international infrastructures and initiatives (EGI, IBERGRID and EOSC) to provide higher capacity, scalability and sharing of resources.

4.16. RESOURCE MANAGEMENT

The resource management 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 IT service management capabilities, experience and scalability of INCD.

4.17. SUPPORT AND TRAINING

This service aims at supporting the usage of the INCD services through documentation, training, consultancy and via the helpdesk. Most of the documentation is provided online via the INCD wiki and is continuously improved and enlarged based on the perceived user difficulties. In addition INCD produces training materials and organises training events and/or seminars either regularly or upon request. Direct support is provided through the INCD helpdesk via email, complemented with private video-conferences with the users to address specific issues. Consultancy and technology transfer are also part of the support and training activities.

5. INFRASTRUCTURE MANAGEMENT AND OPERATIONS

The COVID-19 pandemic continued to limit the activities due to the difficulties arising from human resources limitations as well as from the recommendations of the health authorities and the restrictions legally imposed. Equipment purchase processes were

also affected by the breakdown of logistic networks and the shortage of semiconductor and ICT equipment. INCD continued to adopt remote work, favouring the use of videoconferencing tools and collaborative work. Despite the challenges, INCD managed to maintain a high operational level and develop the activities described in this report.

Several improvements were introduced at the level of the internal infrastructure services and operations. The internal virtualization platforms based on KVM aimed at supporting the infrastructure management and highly critical services were improved. The deployment of a new Kubernetes cluster started to better support the internal services already relying on Linux containers. Among them the deployment of a new ELK based monitoring system with higher scalability on Kubernetes also started. In Lisbon, the power distribution was improved with new hardware having remote monitoring capabilities. The fault monitoring system was also revised. An evaluation of new helpdesk software solutions started aiming at identifying suitable alternatives to streamline the user support activities.

6. INTERNATIONAL COOPERATION

The participation of INCD as a provider in the international digital infrastructures IBERGRID and EGI is an essential part 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 2021, INCD delivered more than 13,500,000 computing hours supporting research projects and communities of national interest in the scope of the IBERGRID and EGI federations.

7. EUROPEAN OPEN SCIENCE CLOUD

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 (https://opencoasts.ncg.ingrid.pt/). This thematic service developed by LNEC in collaboration with LIP and INCD is now part of the EOSC services portfólio and was of the first services to be onboarded into the EOSC.

Also in the EOSC scope, INCD continued its participation in the European project EOSC-Synergy, whose objective is the harmonisation of policies, development of state-of-the-

art tools to foster service integration through quality, and the integration into the EOSC of computing services, data repositories and thematic services. The EOSC-Synergy project joins 20 partners from 10 countries, including INCD and its associates LIP, LNEC and FCT. In the context, INCD provides support for the integration and operation of the Water monitoRing SentInel Cloud (WorSiCA) thematic service (https://worsica.lnec.pt) which is being developed by LNEC, aiming at integration in the EOSC in 2022.

Two new EOSC related projects started in 2021 (EGI-ACE and C-Scale). In EGI-ACE, the objective is to provide 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 the scope of the IBERGRID and EGI activities. INCD houses the Portuguese GBIF node and is collaborating in supporting the implementation of an Iberian combined portal for biodiversity. In C-Scale, the objective is the integration of earth observation services exploring data from Copernicus.

8. FIGHTING COVID-19

As part of the fight against the SARS-CoV-2 pandemic, the INCD has been supporting the National Institute of Health Doutor Ricardo Jorge (INSA) since March 2020 by providing cloud computing resources supporting the validation of the platform used in the "Study of the genetic diversity of the novel coronavirus SARS-CoV-2".

Within the context of the FCT advanced computing projects supported by INCD, one of the projects conducted by researchers from UCIBIO used the INCD accelerated computing service to perform the screening of compounds for treatment of SARS-CoV-2 infections. This research enable the selection of a short list of candidate substances that was later confirmed in laboratory resulting in two patentes:

- EP21306547 / BNT231376EP00 - Vincent Parissi, Sérgio F. Sousa, D. Lapaillere, O. Delelis, L. Meertens, S. Gallois-Montbrun, S. Routier - Pharmaceutical composition, its use as a drug and new compounds, especially for treating SARS-CoV-2 infection (Indole derivaties), 04 November 2021
- EP21306521 / BNT231394EP00 - Vincent Parissi, Sérgio F. Sousa, D. Lapaillere, O. Delelis, L. Meertens, S. Gallois-Montbrun, M. Teulade-Fichou, R. Lartia, G. Bordeau - Pharmaceutical composition, its use as a drug and new compounds, especially for treating SARS-CoV-2 infection (triphenylamine derivatives), 29 October 2021

9. HIGH PERFORMANCE COMPUTING ACTIVITIES

Within the scope of the national advanced computing network (RNCA), 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, through which FCT grants computing time for research projects. Namely, INCD participated in the first CPCA as an operational centre supporting a wide range of computing projects. INCD also participated in the preparation of the second CPCA call

and in the technical evaluation of projects whose execution is meant to take place in 2022.

A formal protocol to join the RNCA was prepared in 2021 and finally 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 to be agreed annually. Also included in this protocol, is the collaboration between FCT and INCD towards the piloting of a catchall data repository for research data.

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 is also supplied by INCD.

INCD is supporting the activities of the Portuguese National High Performance Computing Competence Centre (NCC) in the framework of the EuroCC project. In this regard, INCD is collaborating with the LIP and FCT associates that are partners in the EuroCC project to support the dissemination, training and engagement of new users in the public and private sector. INCD is providing the housing to support the Portuguese NCC web presence.

10.Usage metrics

Figure 1 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. Overall in 2021 more than 33,000,000 hours of processing time were delivered.

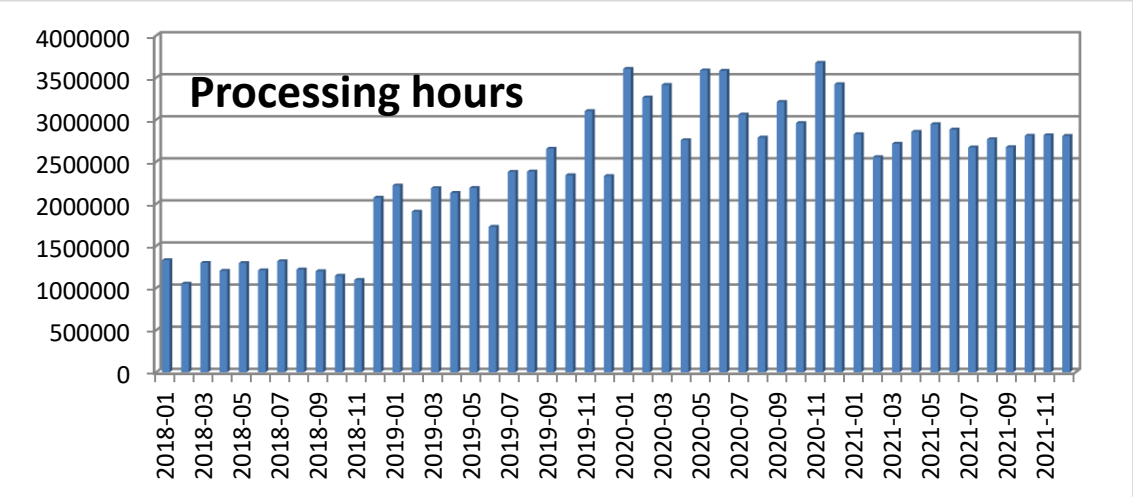

Figure 1: combined usage of all INCD services from January of 2018 to December of 2021.

Figure 2 shows the usage of the batch services at the two INCD centres in Lisbon and Minho since January of 2019. The figure includes both HPC and HTC usage. The effect of the gradual migration of the Lisbon batch scheduler from SoGE to Slurm can be observed.

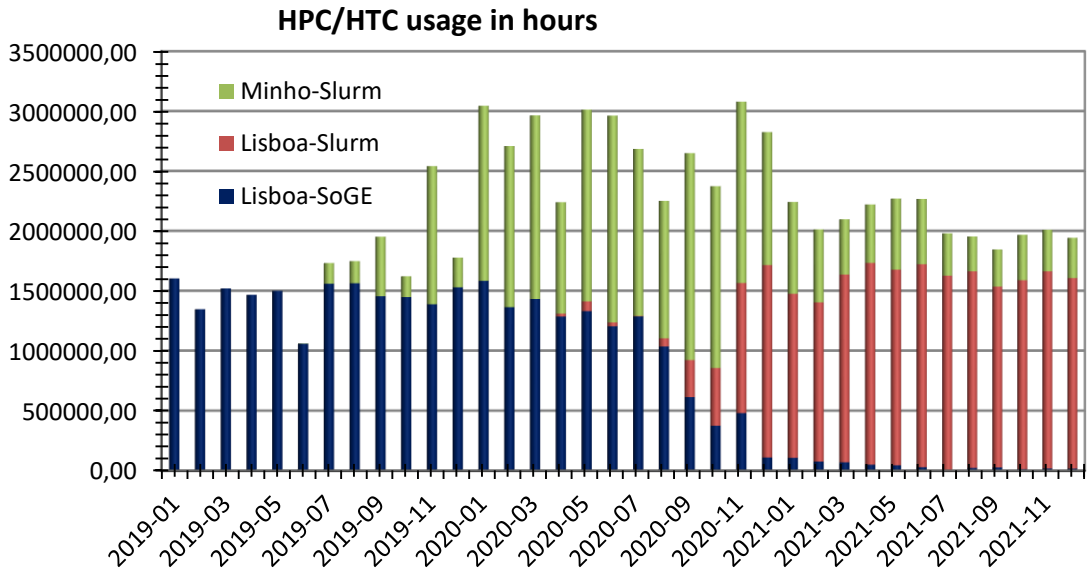

Figure 2: usage of both HPC and HTC batch services from January of 2019 to December of 2021.

Although the delivered capacity in Lisbon improved, datacentre limitations in Minho resulted in a large reduction of the HPC capacity in 2021, particularly when compared with 2020. The reduction of HTC/HPC capacity was caused by power and cooling limitations imposed at the Minho Riba-de-Ave commercial datacentre 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, most of the INCD computing capacity at the site had to be powered down, affecting the INCD users considerably and having a very negative impact in terms of usage. The capacity is currently restricted to about one fourth.

Figure 3 shows the usage of the INCD cloud computing service provided by the Lisbon centre since January of 2017. An increase in usage is observable from mid-2020. In December 2021 there were 60 projects registered in the cloud service.

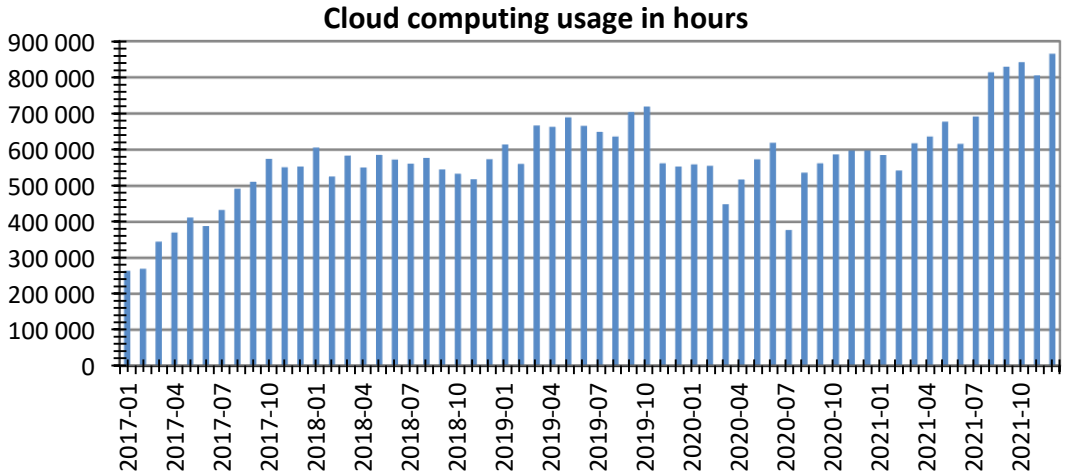

Figure 3: usage of the INCD cloud computing service from January 2017 to December of 2021.

In 2021, INCD supported 62 organisations, infrastructures and research units from multiple domains and geographic areas in the country. Section 11 contains the list of the supported entities. INCD supported 50 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. Besides these projects INCD continued to support its established user base. In this context INCD continued to support the Portuguese participation in the ATLAS and CMS experiments at the CERN LHC. The Portuguese Tier-2 in the Worldwide LHC Computing Grid (WLCG) has delivered 100% of its pledged capacity for 2021 executing 486.779 processing jobs and delivering 111,525,785 HEP-Spec-06 normalised processing hours.

One of the best measures of the relevance and impact of INCD is in the research that is made possible through the usage of the INCD services. Figure 4 shows the evolution of the number of publications published or approved for publication that benefited from the usage of the INCD services. This figure includes papers in peer review journals, papers in proceedings, conference posters, books, PhD thesis and MSc thesis. The actual list is provided in the last section.

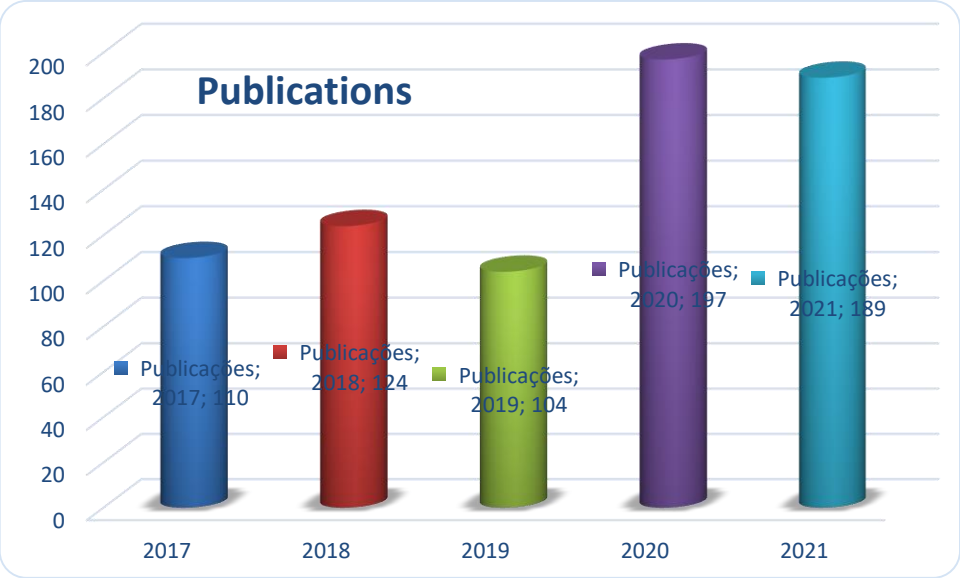

Figure 4: publications that benefited from INCD from 2017 to 2021.

Besides the publications INCD also made possible two patentes on compounds for treatment of SARS-CoV-2, and enabled the creation of two datasets with research data that were published according to the FAIR data principles.

11.Plans for 2022

Science and innovation are increasingly compute, data and network intensive. The conventional approaches towards scientific computing focused on a single paradigm and closed services are insufficient to address the diversity and collaborative nature of modern research.

From supporting data simulations and data processing, to facilitating data analysis, data sharing and enabling thematic services, INCD works closely with the researchers to address their requirements. Through its holistic approach and comprehensive catalogue of computing and data oriented services, backed by international collaboration and federated services, INCD aims to continue enabling flagship research and innovation across all scientific and technological domains at national and international level, while developing knowledge and capabilities in the country.

12.Users

Table 1 provides a list of 62 organisations, infrastructures and research units that used services provided by INCD in 2021.

Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação (ARDITI)

Biomolecular SIMulations Research Group (BioSIM)

Business Research Unit (BRU) / ISCTE

Research Center for Biosciences & Health Technologies (CBIOS) / U.Lusofona

Concepção e Desenvolvimento de Sistemas de Informação (CDSI) / ISCTE

Centro de Estudos de Doenças Crónicas (CEDOC)

Centro de Engenharia e Tecnologia Naval e Oceânica (CENTEC)

Center for Astrophysics and Gravitation (CENTRA)

Centro de Ciências do Mar e do Ambiente (MARE)

Centro de Ecologia Evolução e Alterações Ambientais (cE3c)

Centro de Física do Porto (CFP)

Centro de Investigação e Desenvolvimento em Matemática e Aplicações (CIMA)

Centro de Investigação em Sistemas Electromecatrónicos (CISE)

Centro de Física da Universidade de Coimbra (CFISUC)

Centro de Física Teórica de Partículas (CFTP)

Fundação Champalimaud

Instituto de Materiais de Aveiro (CICECO)

Centro de Neurociências e Biologia Celular (CNBC)

Departamento de Engenharia Informática / FEUP / U.Porto

Departamento de Engenharia Informática / UC

Departamento de Biologia / U.Minho

Departamento de Física / U.Coimbra

Departamento de Informática / U.Coimbra

Faculdade de Ciências / U.Porto

Faculdade de Farmácia / U.Lisboa

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)

Instituto de Biologia Experimental e Tecnológica (IBET)

Instituto Dom Luiz (IDL)

Instituto Gulbenkian de Ciência (IGC)

Instituto de Geografia e Ordenamento do Território (IGOT)

Instituto de Medicina Molecular (IMM)

Instituto de Ciência e Inovação em Engenharia (INEGI)

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

Instituto de Engenharia de Sistemas e Computadores, Tecnologia e Ciência (INESC-TEC)

Instituto Nacional de Saúde Doutor Ricardo Jorge (INSA)

Instituto de Ciências Sociais da Universidade de Lisboa (ICS)

Instituto de Saúde Ambiental (ISAMB)

Instituto de Telecomunicações (IT)

Instituto de Plasmas e Fusão Nuclear (IPFN)

Instituto Superior de Agronomia (ISA)

Instituto Superior de Educação e Ciências (ISEC)

Instituto Superior de Engenharia de Lisboa (ISEL)

Instituto Universitário de Ciências Psicológicas, Sociais e da Vida (ISPA)

Instituto Superior Técnico (IST)

Instituto de Tecnologia Química e Biológica António Xavier (ITQB)

Computer Science and Engineering Research Centre (LASIGE)

Laboratório de Instrumentação e Física Experimental de Partículas (LIP)
Laboratório Nacional de Engenharia Civil (LNEC)
Nova School of Business and Economics (Nova SBE)
Research Center for Risks and Sustainability in Construction (RISCO)
Sociedade Portuguesa de Botânica (SPBOTANICA)
Universidade Aberta (U.Aberta)
Universidade do Algarve (UALG)
Applied Molecular Biosciences Unit (UCIBIO)
Portuguese node of the Global Biodiversity Network (GBIF)
Portuguese Coastal Monitoring Network (CoastNET)
Portuguese Biological Data Network (BIODATA.PT)
National Facility for Genome Sequencing and Analysis (GenomePortugal)

Table 1: organisations, infrastructures and research units that used INCD provided services in 2021.

13.Publications

PhD Thesis produced with the support of INCD in 2021

- GONÇALVES, C. (2019-present). Coleoid venoms: Predicting cephalotoxin function and biotechnological applications from ecological and evolutionary traits. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: Ongoing. (January 2019). FCT grant ref. SFRH/BD/144914/2019.
- MARTINS, C. (2017-present). Carcinogenic toxicants and emerging pollutants. A comprehensive case-study on toxicant interactions in vivo and in vitro: from Molecular Toxicology to Environmental Risk Assessment. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: Ongoing. (September 2017). FCT grant ref. SFRH/BD/120030/2016.
- RODRIGO, A.P.C. (2021). The biotechnological value of a novel potent marine biotoxin from the polychaete worm Eulalia viridis: chemical and toxicological evaluation. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica, 246 pp. Status: Approved. Classification: N/A. FCT grant ref. SFRH/BD/109462/2015.
- Henrique Silva Fernandes Título: Computational studies addressed to PLP-Dependent enzymes Programa Doutoral em Química, FCUP/FEUP, Univ Porto Concluída em Julho de 2021.

- Carla Sílvia Silva Teixeira Título: Computational studies addressed to multifunctional enzyme complexes Programa Doutoral em Química, FCUP/FEUP, Univ Porto Concluída em Julho de 2021.
- Cátia Sofia dos Santos Pereira Novel insights on the interaction of lactoferrin with proton pumping ATPases towards understanding its antifungal and anticancer activities Programa Doutoral em Biologia Molecular e Ambiental Molecular (PDBMA), Univ Minho Concluída em Setembro de 2021.
- Inês Raquel Carvalho Leonardo 2020.08210.BD Tecnologias Agrárias e Alimentares Portugal Universidade Nova de Lisboa.
- Tiago Vale, Search for heavy fermions with LHC data, Universidade do Minho, MAP-Fis.
- Ana Peixoto, Search for new interactions in the top quark sector, Universidade do Minho, MAP-Fis.
- Emanuel Gouveia, Probing the CP nature of the Higgs couplings to top quarks at the Run 2 of the LHC, Universidade do Minho, MAP-Fis.
- Artur Amorim de Sousa, Holography, QCD and Regge Theory, Universidade do Porto, MAP-Fis.
- Paulo Brás, New physics phenomenology and data processing tools for the LZ experiment, Doutoramento em Física, FCTUC.

MSc Thesis produced with the support of INCD in 2021

- CABRAL, I. (2020-present). A computational approach to identify target receptors of marine toxins in the human proteome: Potential biotechnological applications. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: submitted.
- SANTOS, M.L. (2021). A transcriptomic approach to the metabolism of porphyrin-like pigments in a marine Polychaeta (Eulalia sp.). M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. 43 pp. + Appendix. Final status: Approved. Classification: 18 (0-20).
- GROU, M. (2021). A molecular and pathophysiological approach to tissue regeneration in the planarian model. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica, 40 pp. + Annexes. Final status: Approved. Classification: 19 (0-20).
- PIMPÃO, A. (2021). Novel developments on the association of the AHR-CYP1A1 axis and arterial hypertension related to obstructive sleep apnea. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica (in collaboration with NOVA Medical School), Universidade Nova de Lisboa, Monte de Caparica, 77 pp. + Annexes. Final status: Approved. Classification: 19 (0-20).
- Mestrado Informação e Sistemas Empresariais, Univ. Aberta/IST da dissertação intitulada "Feature Selection using LAID and its Implementation on High-Performance Computing Systems" de Paulo Morgado, orientado por L. Cavique e defendido em novembro 2021.
- Mestrado Bolonha em Bioengenharia e Nanossistemas, IST/LISBOA "Empowering Antibiotic Polymers Design through Coarse Grained Molecular Dynamics" Gabriel Nascimento Serafim.
- P. Xavier and N. Galambaa) Effect of urea on the hydration and aggregation of hydrophobic and amphiphilic solute models: Implications to protein aggregation J. Chem. Phys. 155, 144501 (2021); https://doi.org/10.1063/5.006470.
- Manghnani, K. (2021) Extraction and Visualization of Fake News Indicators (Tese de mestrado) - Instituto Superior Técnico, Universidade de Lisboa. Lisboa, Portugal.

- Mariana Luz, Projecto de mestrado com o titulo: "Assessing the Prevalence of Transcription Readthrough in healthy tissues through computational approaches", Mestrado em Genetica Molecular e Biomedicina, FCT-NOVA.
- Valerio Fiori, Projecto de mestrado com o titulo: "Finding Biomarkers of Metastatic Potential in Colorectal Cancer", Mestrado em Bioinformatica e Biologia Computacional, FCUL.
- B. Oliveira, "High-Pressure He/H2/O2 Mixtures Combustion on the ESTHER Driver: Experiment and Modeling", Ms.C. Thesis, Eng. Aeroespacial, Instituto Superior Técnico, Universidade de Lisboa.
- Ricardo Silva (2021), Atomic structure calculations in lanthanide ions relevant to kilonovae,FCUL.
- André Cordeiro, Towards the space-time picture of a QCD parton shower, IST.
- Filipa Baltazar (2021), A Monte Carlo based study of the FLASH effect in radiotherapy with protons, IST.
- Miguel Martins, Measurement of the features of muon number distribution using MARTA engineering array, IST.
- Alexandra Fernandes, Measurement of the features of muon number distribution using MARTA engineering array, mestrado em Astronomia e Astrofisica da universidade do Porto.
- Pedro Costa, Detection of astrophysical neutrinos with a gamma-ray observatory, IST.
- Laura Peres, A novel energy reconstruction for high-energy gamma-ray wide field of view observatories, IST.
- Eduardo Ferreira, From light-front wave functions to parton distribution functions, IST MEFT.
- Nuno Fernandes, Development of GPU-Accelerated Trigger Algorithms for the ATLAS Experiment at the LHC, Mestrado em Engenharia Física Tecnológica IST.
- Maria Faria, Investigating the flavour anomalies through the rare beauty decay B0→K∗0μ+μ−, IST MEFT.
- Beatriz Pinheiro Pereira, Radiation damage of the optical components of the ATLAS TileCal calorimeter at the High-Luminosity LHC, IST MEFT.

Publications produced with the support of INCD in 2021

- MODELING THE IMPACTS OF HARBOR DREDGING AND DISPOSAL ON COASTAL WATER-LEVELS AND RUN-UP WITH XBEACH, Coastal Dynamics Conference, 28 June-2 July 2021.
- Pereira, C., Maranha, J. R. e Cardoso R. (2021). A general mathematical framework for modelling soil-water retention behaviour. 3rd Pan-American Conference on Unsaturated Soils, Rio de Janeiro, Brazil (aceite para publicação).
- CRAVO A., ROSA A., RODRIGUES M. (2020). Effects of climate change and anthropogenic pressures in the water quality of the Ria Formosa (Portugal). XX Seminário Ibérico de Química Marina - SIQUIMAR 2020, 1 pp.
- Mendes, Lourenço S.; Lara, Javier L.; Viseu, Maria T. 2021. "Is the Volume-of-Fluid Method Coupled with a Sub-Grid Bubble Equation Efficient for Simulating Local and Continuum Aeration?" Water 13, no. 11: 1535.
- Balduíno César Mateus,Mateus Mendes,José Torres Farinha and António Marques Cardoso "Anticipating Future Behavior of an Industrial Press Using LSTM Networks" Appl. Sci. 2021, 11(13), 6101; https://doi.org/10.3390/app11136101.
- Paolillo, A., Sinval, J., Silva, S. A., & Scuderi, V. E. (2021). The relationship between inclusion climate and voice behaviors beyond social exchange obligation: The role of psychological needs satisfaction. Sustainability, 13(18), 1-19. https://doi.org/10.3390/su131810252.

- Balduino Mateus, Mateus Mendes, José Torres Farinha, António Marques Cardoso, Data Analysis for Predictive Maintenance Using Time Series and Deep Learning Models – A Case Study in a Pulp Paper Industry, in Proceedings of the TEPEN 2021 & IncoME-VI, Oct 20-23, 2021, Tianjin, China.
- João Rodrigues, José Torres Farinha, António Marques Cardoso1 and Mateus Mendes, Prediction of Sensor Values in Paper Pulp Industry Using Neural Networks, Proceedings of the TEPEN 2021 & IncoME-VI, Oct 20-23, 2021, Tianjin, China.
- Pais, P., Oliveira, J., Almeida, V., Yilmaz, M., Monteiro, P.T., Teixeira, M.C. "Transcriptome-wide differences between Saccharomyces cerevisiae and Saccharomyces cerevisiae var. boulardii: clues on host survival and probiotic activity based on promoter sequence variability". Genomics, 113(2): 530-539, 2021.
- Mendes S, et al. (2021) Genomic data and multi-species demographic modelling uncover past hybridization between currently allopatric freshwater species. HEREDITY https://doi.org/10.1038/s41437-021-00466-1.
- Clemente F, et al. (2021) The genomic history of the Aegean palatial civilizations CELL 184: P2565-2586.e21 https://doi.org/10.1016/j.cell.2021.03.039.
- Palma JHN, 2017, CliPick – Climate change web picker. A tool bridging daily climate needs in process based modelling in forestry and agriculture, Forest Systems [S.l.], v. 26, n. 1, p. eRC01, may 2017. ISSN 2171-9845. https://doi.org/10.5424/fs/2017261-10251.
- SANTOS, M.L., D'AMBROSIO, M., RODRIGO, A.P., PAROLA, A.J. & COSTA, P.M. (2021). A transcriptomic approach to the metabolism of tetrapyrrolic photosensitizers in a marine annelid. Molecules 26, 3924. (doi: 10.3390/molecules26133924).
- RODRIGO, A.P., GROSSO, A.R., BAPTISTA, P.V., FERNANDES, A.R., & COSTA, P.M. (2021). A transcriptomic approach to the recruitment of venom proteins in a marine annelid. Toxins 13, 97 (doi: 10.3390/toxins13020097).
- RODRIGO, A.P., MENDES, V.M., MANADAS, B., GROSSO, A.R., ALVES DE MATOS, A.P., BAPTISTA, P.V., COSTA, P.M., FERNANDES, A.R. (2021). Specific antiproliferative properties of proteinaceous toxin secretions from the marine annelid Eulalia sp. onto ovarian cancer cells. Marine Drugs 19, 31 (doi: 10.3390/md19010031).
- Assessing the effects of PMM2 variants on protein stability Quelhas, D., Carneiro, J., Lopes-Marques, M., Jaeken, J., Martins, E., Rocha, J.F., Teixeira Carla, S.S., Ferreira, C.R., Sousa, S.F., Azevedo, L. (2021) Molecular Genetics and Metabolism, 134 (4), pp. 344-352. DOI: 10.1016/j.ymgme.2021.11.002.
- In silico identification of possible inhibitors for protein kinase B (PknB) of mycobacterium tuberculosis Vieira, T.F., Martins, F.G., Moreira, J.P., Barbosa, T., Sousa, S.F. (2021) Molecules, 26 (20), art. no. 6162.
- Structure and thermodynamics of empty clathrate hydrates below the freezing point of water† Fernando J. A. L. Cruz [OBJ] *a and José P. B. Motaa Phys. Chem. Chem. Phys., 2021,23, 16033-16043 https://doi.org/10.1039/D1CP00893E.
- The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain Santos-Pereira, C., Rocha, J.F., Fernandes, H.S., Rodrigues, L.R., Côrte-Real, M., Sousa, S.F. (2021) International Journal of Biological Macromolecules, 186, pp. 54-70. DOI: 10.1016/j.ijbiomac.2021.06.200.
- Compensatory epistasis explored by molecular dynamics simulations Serrano, C., Teixeira, C.S.S., Cooper, D.N., Carneiro, J., Lopes-Marques, M., Stenson, P.D., Amorim, A., Prata, M.J., Sousa, S.F., Azevedo, L. (2021) Human Genetics, 140 (9), pp. 1329-1342. DOI: 10.1007/s00439-021-02307-x.
- The complete catalytic mechanism of xanthine oxidase: A computational study Ribeiro, P.M.G., Fernandes, H.S., Maia, L.B., Sousa, S.F., Moura, J.J.G., Cerqueira, N.M.F.S.A. (2021) Inorganic Chemistry Frontiers, 8 (2), pp. 405-416. DOI: 10.1039/d0qi01029d.

- The Catalytic Mechanism of Pdx2 Glutaminase Driven by a Cys-His-Glu Triad: A Computational Study Pina, A.F., Sousa, S.F., Cerqueira, N.M.F.S.A. (2021) ChemBioChem, DOI: 10.1002/cbic.202100555.
- New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach Fernandes, H.S., Sousa, S.F., Cerqueira, N.M.F.S.A. (2021) Molecular Diversity DOI: 10.1007/s11030-021-10259-7.
- Identification of new potential inhibitors of quorum sensing through a specialised multi-level computational approach Martins, F.G., Melo, A., Sousa, S.F. (2021) Molecules, 26 (9), art. no. 2600 DOI: 10.3390/molecules26092600.
- Morgado P., L. Cavique (2021), Seleção de atributos usando LAID e sua implementação em sistemas de computação de alto desempenho, Revista de Ciências da Computação n.16, pp. 93-112.
- Finding new physics without learning about it: anomaly detection as a tool for searches at colliders M. Crispim Romao, N. F. Castro, R. Pedro EPJC 81 (2021) 27 Jrn-Dir 2021-01-15 10.1140/epjc/s10052-020-08807-w.
- Light Higgs searches in t(t)over-bar phi production at the LHC Duarte Azevedo, Rodrigo Capucha, Emanuel Gouveia, Antonio Onofre, Rui Santos J. High Energy Phys. 4 (2021) 77 Jrn-Dir 2021-04-09 10.1007/JHEP04(2021)077.
- Measurement of the associated production of a Higgs boson decaying into b-quarks with a vector boson at high transverse momentum in pp collisions at \sqrt(s)=13TeV with the ATLAS detector ATLAS Collaboration (2927 authors) Phys. Lett. B 816 (2021) 136204 Jrn-Dir 2021-04-27 10.1016/j.physletb.2021.136204.
- A continuous integration and web framework in support of the ATLAS Publication Process Juan Pedro Araque Espinosa, Gabriel Baldi Levcovitz, Riccardo-Maria Bianchi, Ian Brock, Tancredi Carli, Nuno Filipe Castro, Alessandra Ciocio, Maurizio Colautti, Ana Carolina Da Silva Menezes, Gabriel De Oliveira da Fonseca, Leandro Domingues Macedo Alves, Andreas Hoecker, Bruno Lange Ramos, Gabriela Lemos Lúcidi Pinhão, Carmen Maidantchik, Fairouz Malek, Robert McPherson, Gianluca Picco, Marcelo Teixeira Dos Santos JINST 16 (2021) T05006 Jrn-Dir 2021-05-11 10.1088/1748-0221/16/05/T05006.
- Configuration and performance of the ATLAS b-jet triggers in Run 2 ATLAS Collaboration Eur. Phys. J. C 81 (2021) 1087 Jrn-Dir 2021-12-01 10.1140/epjc/s10052-021-09775-5.
- Constraining the energy spectrum of neutral pions in ultra-high-energy proton-air interactions Lorenzo Cazon, Ruben Conceição, Miguel Alexandre Martins, and Felix Riehn Phys. Rev. D 103, 022001 Jrn-Dir 2021-01-08 10.1103/PhysRevD.103.022001.
- Measurement of the Fluctuations in the Number of Muons in Extensive Air Showers with the Pierre Auger Observatory Pierre Auger Collaboration (360 authors) Phys. Rev. Lett. 126 (2021) 152002 Jrn-Dir 2021-04-16 10.1103/PhysRevLett.126.152002.
- Timing performance of a multi-pad PICOSEC-Micromegas detector prototype M. Gallinaro et al. Nucl. Instrum. Methods Phys. Res. Sect. A-Accel. Spectrom. Dect. Assoc. Equip. 993 (2021) 165076 Jrn-Dir 2021-03-21 10.1016/j.nima.2021.165076.
- Modeling the timing characteristics of the PICOSEC Micromegas detector J. Bortfeldt et al. (41 authors) Nucl. Instrum. Methods Phys. Res. Sect. A-Accel. Spectrom. Dect. Assoc. Equip. 993 (2021) 165049 Jrn-Dir 2021-03-21 10.1016/j.nima.2021.165049.
- Measurement of the CP-violating phase phi(s) in the B-s(0) -> J/psi phi(1020) -> mu(+)mu-K+K- channel in proton-proton collisions at root s=13 TeV CMS Collaboration (2307 authors) Phys. Lett. B 816 (2021) 136188 Jrn-Dir 2021-05-10 10.1016/j.physletb.2021.136188.
- Vector Boson Scattering Processes: Status and Prospects M. Gallinaro et al. arXiv:2106.01393 Jrn-Dir 2021-06-02.

- Test beam characterization of sensor prototypes for the CMS Barrel MIP Timing Detector CMS MTD Collaboration (199 authors) J. Instrum. 16 (2021) P07023 Jrn-Dir 2021-07-01 10.1088/1748-0221/16/07/P07023.
- Test beam characterization of sensor prototypes for the CMS Barrel MIP Timing Detector D. Bastos, M. Gallinaro, T. Niknejad, J.C. Silva, J. Varela, et al. JINST 16 (2021) P07023 Jrn-Dir 2021-07-15.
- Observation of B0s mesons and measurement of the B0s/B+ yield ratio in PbPb collisions at 5.02 TeV CMS Collaboration arXiv:2109.01908 Jrn-Dir 2021-09-04.
- Advances in Multi-Variate Analysis Methods for New Physics Searches at the Large Hadron Collider M. Gallinaro, G. Strong, J. Varela, et al. Rev.Phys. 7 (2021) 100063 Jrn-Dir 2021-11-06.
- Improving sensitivity to low-mass dark matter in LUX using a novel electrode background mitigation technique D. S. Akerib et al. Phys. Rev. D 104, 012011 Jrn-Dir 2021-07-19 https://doi.org/10.1103/PhysRevD.104.012011.
- Projected sensitivity of the LUX-ZEPLIN experiment to the two neutrino and neutrinoless double beta decays in Xe-134 D. S. Akerib et al. Phys. Rev. C 104 (2021) 065501 Jrn-Dir 2021-12-10 https://doi.org/10.1103/PhysRevC.104.065501.
- Simulation of 125 I Auger emission spectrum with new atomic parameters from MCDHF calculations J.M. Sampaio, J. Ekman, B.P.E. Tee, R. du Rietz, B.Q. Lee, M.S. Pires, P. Jönsson, T. Kibédi , M. Vos , A.E. Stuchbery, and J.P. Marques J. Quant. Spectr. Rad. Tranf. 227, 107964 (2022) Jrn-Dir 2021-10-12 10.1016/j.jqsrt.2021.107964.
- Optical readout studies of the Thick-COBRA gaseous detector F. Garcia, F.M. Brunbauer, M. Lisowskac, H. Müller, E. Oliveri, D. Pfeiffer, L. Ropelewski, J. Samarati, F. Sauli, L. Scharenber, A.L.M. Silva, M. van Stenis, R. Veenhof and J.F.C.A. Veloso JINST 16 (2021) T01001 Jrn-Dir 2021-01-07 10.1088/1748-0221/16/01/T01001.
- Operation of a novel large area, high gain, single stage gaseous electron multiplier F.D. Amaro, R. Roque, N.V. Duarte, A. Cortez, and J.A. Mir Journal of Instrumentation 16 (2021) P01033 Jrn-Dir 2021-01-27 10.1088/1748-0221/16/01/P01033.
- Forecasting contrasting coastal and estuarine hydrodynamics with OPENCoastS A. Oliveira, A.B. Fortunato, M. Rodrigues, A. Azevedo, J. Rogeiro, S. Bernardo, Laura Lavaud, Xavier Bertin, Alphonse Nahon, Gonçalo de Jesus, Miguel Rocha, P. Lopes Anabela Oliveira, André B. Fortunato, Marta Rodrigues, Alberto Azevedo, João Rogeiro, Samuel Bernardo, Laura Lavaud, Xavier Bertin, Alphonse Nahon, Gonçalo de Jesus, Miguel Rocha, Pedro Lopes, Forecasting contrasting coastal and estuarine hydrodynamics with OPENCoastS, Environmental Modelling & Software, Volume 143, 2021 Jrn-Dir 2021-06-13 10.1016/j.envsoft.2021.105132.
- New methods to reconstruct Xmax and the energy of gamma-ray air showers with high accuracy in large wide-field observatories R. Conceição, L. Peres, M. Pimenta, B. Tomé Eur. Phys. J. C 81, 80 (2021) Jrn-Dir 2021-01-25 10.1140/epjc/s10052-021-08883-6.
- Muon identification in a compact single-layered water Cherenkov detector and gamma/hadron discrimination using Machine Learning techniques R. Conceição, B. S. González, A. Guillén, M. Pimenta and B. Tomé Eur. Phys. J. C 81, 542 (2021) Jrn-Dir 2021-05-13 10.1140/epjc/s10052-021-09312-4.
- The SNO+ Experiment, M.R. Anderson et al. (SNO+ Collaboration) JINST 16 P08059 (2021) Jrn-Dir 2021-08-25 10.1088/1748-0221/16/08/P08059.
- Optical calibration of the SNO+ detector in the water phase with deployed sources M.R. Anderson et al. (SNO+ Collaboration) JINST 16 P10021 Jrn-Dir 2021-10-19 10.1088/1748-0221/16/10/P10021.
- Quark Mass Function from an OGE-type Interaction in Minkowski Space E. P. Biernat, F. Gross, M. T. Peña, A. Stadler, S. Leitão Acta Phys. Polon. Supp. 14 (2021) 9 Jrn-Dir 2021-01-01 10.5506/AphysPolBSupp.14.9.

- Fundamental Parameters Related to Selenium Kα and Kβ Emission X-Ray Spectra Mauro Guerra, Jorge M. Sampaio, Gonçalo R. Vília, César A. Godinho, Daniel Pinheiro, Pedro Amaro, José P. Marques, Jorge Machado, Paul Indelicato, Fernando Parente, José Paulo Santos Atoms 9,8 (2021) Jrn-Dir 2021-01-22 10.3390/atoms 9010008.
- Peeling graphite layer by layer reveals the charge exchange dynamics of ions inside a solid Anna Niggas, Sascha Creutzburg, Janine Schwestka, Benjamin Wöckinger, Pedro L. Grande, Bernhard C. Bayer, José P. Marques, Friedrich Aumayr, Robert Bennett, Richard A. Wilhelm Communications Physics 4, 1801 (2021). Jrn-Dir 2021-08-12 10.1038/s42005-021-00686-1.
- NeuLAND: The high-resolution neutron time-of-flight spectrometer for R3B at FAIR K. Boretzky, I. Gasparic, M. Heil, et al. Nucl. Instr. and Methods A 1014, 165071 (2021) Jrn-Dir 2021-10-21 10.1016/j.nima.2021.165701 The large COMPASS polarized solid ammonia target for Drell–Yan measurements with a pion beam V. Andrieux, C. Pires, C. Quintans et al NIM A 1025 (2022) 166069 Jrn-Dir 2021-12-10 https://doi.org/10.1016/j.nima.2021.166069.
- Constraining the energy spectrum of neutral pions in ultra-high-energy proton-air interactions Lorenzo Cazon, Ruben Conceição, Miguel Alexandre Martins, and Felix Riehn Phys. Rev. D 103, 022001 Jrn-Dir 2021-01-08 10.1103/PhysRevD.103.022001.
- Running in the ALPs M. Chala, G. Guedes, M. Ramos and J. Santiago Eur. Phys. J. C (2021) 81: 181 Jrn-Dir 2021-02-23 10.1140/epjc/s10052-021-08968-2.
- Use of a Generalized Energy Mover's Distance in the Search for Rare Phenomena at Colliders M. Crispim Romao, N.F. Castro , J.G. Milhano, R. Pedro, T. Vale Eur. Phys. J. C 81, 192 (2021) Jrn-Dir 2021-02-26 10.1140/epjc/s10052-021-08891-6.
- New leptons with exotic decays: collider limits and dark matter complementarity Guilherme Guedes, José Santiago arXiv:2107.03429 Jrn-Dir 2021-07-09.
- Deep Learning for the Classification of Quenched Jets L. Apolinário, N. F. Castro, M. Crispim Romão, J. G. Milhano, R. Pedro, F. C. R. Peres JHEP11 (2021) 219 Jrn-Dir 2021-11-29 10.1007/JHEP11(2021)219.
- Finding new physics without learning about it: anomaly detection as a tool for searches at colliders M. Crispim Romao, N. F. Castro, R. Pedro EPJC 81 (2021) 27 Jrn-Dir 2021-01-15 10.1140/epjc/s10052-020-08807-w.
- Use of a Generalized Energy Mover's Distance in the Search for Rare Phenomena at Colliders M. Crispim Romao, N.F. Castro , J.G. Milhano, R. Pedro, T. Vale Eur. Phys. J. C 81, 192 (2021) Jrn-Dir 2021-02-26 10.1140/epjc/s10052-021-08891-6.
- Deep Learning for the Classification of Quenched Jets L. Apolinário, N. F. Castro, M. Crispim Romão, J. G. Milhano, R. Pedro, F. C. R. Peres JHEP11 (2021) 219 Jrn-Dir 2021-11-29 10.1007/JHEP11(2021)219.
- 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 Jrn-Dir 2022-01-14 DOI: 10.1126/sciadv.abm4234.
- The LHC Olympics 2020 a community challenge for anomaly detection in high energy physics, G. Kasieczka et al, ROPP Vol 84, No. 12, p124201, 10.1088/1361-6633/ac36b9.
- Average minijet rapidity ratios in Mueller Navelet jets, N. B. de Leon, G. Chachamis and A. Sabio Vera, Eur. Phys. J. C 81, no.11, 1019 (2021), 10.1140/epjc/s10052-021-09967-z.
- Polarimetry With a Multilayer CdTe Prototype for Soft Gamma-Ray Astrophysics, M. Moita, R. M. Curado da Silva, J. M. Maia, E. Caroli, E. Virgilli, N. Auricchio, J. B. Stephen, F. Frontera, S. del Sordo, IEEE Trans. Nucl. Sci. 68 (2021) 2655-2660, 10.1109/TNS.2021.3110472.

Publications in conference proceedings produced with the support of INCD in 2021

- "Plantas ameaçadas de extinção - A Lista Vermelha da Flora Vascular de Portugal Continental", por André Carapeto (Sociedade Portuguesa de Botânica), a 20 de Janeiro de 2021, integrada nas comemorações do Dia do Município de Vila do Bispo, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Vila do Bispo.
- "A flora ameaçada no Município de Leiria", por André Carapeto (Sociedade Portuguesa de Botânica), a 25 de Fevereiro de 2021, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Leiria e o Centro de Interpretação Ambiental de Leiria.
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A study on whole-transcriptomes of two Polychaeta for discovering novel bioproducts with potential biotechnological applications. International Conference for YOUNG Marine Researchers. The Bremen Society for Natural Sciences, Berlin (Germany), September 2021.
- GONÇALVES, C., MOUTINHO CABRAL, I., RODRIGO, A.P., FONSECA,D., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A stinging issue: omics and computational tools for the bioprospecting of novel marine toxins. XII European Conference on Marine Natural Products. National University of Ireland, Galway (Ireland), August 2021.
- MOUTINHO CABRAL, I. (2021). A computational approach to identify target receptors of marine toxins in the human proteome: Potential biotechnological applications. Jornadas Intercalares das Dissertações Anuais dos Mestrados dos Departamentos de Química e Ciências da Vida 2021. NOVA School of Science and Technology, NOVA University of Lisbon, Monte de Caparica (Portugal), February 2021.
- Deciphering the interaction of lactoferrin with V-ATPase towards a deeper understanding of its mechanisms of action Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes, Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online).
- Structure-based Virtual Screening, Molecular Dynamics and Free Energy calculations for the identification of novel inhibitors against biofilm formation by C.violaceum Fábio G. Martins, André Melo, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online).
- Structure-based Virtual Screening,Molecular Dynamics and Free Energy calculations for the identification of New Quorum Sensing Inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP) May 7th 2021, Porto, Portugal.
- Specialized multi-level computational approach for the identification of novel quorum sensing inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa The 24th meeting of the International Society for Molecular Recognition, Affinity 2021 22-24 June 2021, Lisboa, Portugal (online).
- Identification of potential quorum sensing inhibitors through structure-based virtual screening, molecular dynamics, and free energy calculations Fábio G. Martins, André Melo, Sérgio F. Sousa e-Conference on Innovation in Microbial Control, October 7-8 2021, Porto, Portugal (online).
- Targeting the PQS system: Discovery of New Quorum Sensing Inhibitors for P. aeruginosa through an in silico methodology Tatiana F. Vieira, Rita P. Magalhães, Manuel Simões, Sérgio F. Sousa e-Conference on Innovation in Microbial Control October 7-8, 2021, Porto, Portugal (online).
- Machine Learning Classification Models for Identification of Ligand-Target Inhibition Pairs in Biofilm Formation in P.aeruginosa Rita P. Magalhães, Victor de la Oliva, João Carneiro,

Sérgio F. Sousa e-Conference on Innovation in Microbial Control October 7-8, 2021, Porto, Portugal (online).

- Using Biomolecular Simulations to Understand the Enzymatic Activity of Xanthine Oxidase Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira BioSeminars@UCIBIO July 21st 2021, Lisbon, Portugal (Online).
- Exploring the Nitrate and Nitrite Reductase Activity of Xanthine Oxidase – a QM/MM study Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira 12th Molybdenum and Tungsten Enzymes Conference (MoTEC 2021) September 28th to October 1st 2021, Marseille, France (Online).
- The Nitrate and Nitrite Reductase Activity of Xanthine Oxidase: a Computational Study Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira XXI SPB National Congress of Biochemistry October 14th to 16th 2021, Universidade de Évora, Évora, Portugal (Online) Note: Award Best Oral Communication.
- Developed of Inverted Virtual Screening Approaches for the Identification of Protein Targets Associated to the Biological Activity of Specific Molecules Tatiana F. Vieira, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- A multidisciplinary approach to untangle the mechanisms behind the antifungal activity of lactoferrin Cátia Santos-Pereira, María T. Andrés, Juliana F. Rocha, Henrique S. Fernandes, Susana R. Chaves, José F. Fierro, Hernâni Gerós, Stéphen Manon, Sérgio F. Sousa, Lígia R. Rodrigues, Manuela Côrte-Real 15th International Conference on Lactoferrin: Structure, Function and Applications December 6-10th 2021, Beijing, China (online).
- Multilocus DNA metabarcoding of complex mixtures containing members of the Boraginaceae family: a step further to assure food safety and quality Inês CARVALHO LEONARDO, Martijn STAATS, Marleen VOORHUIJZEN, Valerie VAN DER VORST, Bas FRONEN, Jorge CAPELO, Maria Teresa BARRETO CRESPO, Frédéric BUSTOS GASPAR November 2021 ISEKI e-conference 2021 - Food Texture, Quality, Safety and Biosecurity in the Global Bioeconomy Online (Austria).
- Multilocus DNA metabarcoding of complex mixtures containing members of the Boraginaceae family for food safety and quality assurance Inês Carvalho. Leonardo, Martijn Staats, Marleen Voorhuijzen, Valerie van der Vorst, Bas Fronen, Jorge Capelo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021.
- Two-particle Correlations in multi-Regge Kinematics, N. B. de Leon, G. Chachamis and A. S. Vera, arXiv:2112.13794 [hep-ph]; contribution to Low-x workshop 2021.
- New results on the modification of jet structure in Heavy Ion collisions, Helena Santos, on behalf of the ATLAS, ALICE and CMS Collaborations, PoS(LHCP2021)082, https://doi.org/10.22323/1.397.0082.
- Rare heavy-flavour decays, A. Boletti (on behalf of the ATLAS, CMS, and LHCb Collaborations), PoS(LHCP2021)139.
- Comparison of Voxel S-values and Monte Carlo Simulation in [177Lu]Lu-DOTA-TATE Quantification for Patient-Specific Dosimetry, Rodrigues, C., Ferreira, P., Oliveira, F. P. M., Silva, Â., Peralta, L., Costa, D. C., Eur J Nucl Med Mol Imaging, 48 (2021) S75, https://doi.org/10.1007/s00259-021-05547-1.
- Study of central exclusive production of top quark-antiquark pairs at LHC, M. Pisano, Nuovo Cimento 44C (2021) 66.
- Gamma/hadron discrimination using a small-WCD with four PMTs, R. Conceição, P. Assis, F. Assunção, A. Bakalova, U. Barres de Almeida, C. Roque Bom, J. Correia, A. De Angelis, L.O. Dias, B. Serrano González, A. Guillén, G. La Mura, N. Lourenço, P. Machado, S. Marques, L. Mendes, M. Pimenta, R. Shellard, B. Tomé and J. Vicha, Proceedings of 37th

International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 707, https://doi.org/10.22323/1.395.0707.
- Monitoring Gamma-Ray Burst VHE emission with the Southern Wide-field-of-view Gamma-ray Observatory, G. La Mura, Proceedings of 37th International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 709, https://doi.org/10.22323/1.395.0709.
- New methods to reconstruct Xmax and the energy of gamma-ray air showers with high accuracy in large wide-field observatories, R. Conceição, L. Peres, M. Pimenta and B. Tomé, Proceedings of 37th International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 711, https://doi.org/10.22323/1.395.0711.
- Search for new physics in b→sℓ+ℓ− transitions at CMS, A. Boletti, on behalf of the CMS Collaboration, PoS(ICHEP2020)365.
- The ATLAS Hardware Track Trigger performance studies for the HL-LHC, A. L. Moreira de Carvalho on behalf of the ATLAS Collaboration, PoS(LHCP2020)247
- Jet substructure modification probes the QGP resolution length, J. Casalderrey-Solana, G. Milhano, D. Pablos and K. Rajagopal, Nucl.Phys.A 1005 (2021) 121904, 10.1016/j.nuclphysa.2020.121904.
- Impact of LHC jet data on Parton Distribution Functions, João Pires, PoS LHCP2020 (2020) 145, 10.22323/1.382.0145.
- Gamma-ray Astrophysics in the MeV Range The ASTROGAM Concept and Beyond, A. De Angelis, V. Tatischeff, S. Brandt, A. Bulgarelli, R. Curado da Silva, I. Grenier, L. Hanlon, D. H. Hartmann, M. Hernanz, G. Kanbach, I. Kuvvetli, P. Laurent, M. Mariotti, M. N. Mazziotta, J. Mc Enery, A. Morselli, K. Nakazawa, M. Pearce, J. Rico, X. Wu, S. Zane, A. Zoglauer, Exp. Astron. 51 (2021) 1225-1254, 10.1007/s10686-021-09706-y.
- Deep Learning Versatility in New Physics Searches, Miguel Romão, PoS (ICHEP2020) 233, 10.22323/1.390.0233.

Conference posters produced with the support of INCD in 2021

- RODRIGO, A.P., GROSSO, A., MENDES, V.M., MANADAS, B., BATISTA, P.V., FERNANDES, A.R., COSTA, P.M. (2021). Unveiling venomous annelids by combining omics with ecological traits: The example of a phyllodocid. 12th European Conference on Marine Natural Products, Galway (Ireland), September 2021.
- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A study on whole-transcriptomes of two Polychaeta for discovering novel bioproducts with potential biotechnological applications. International Conference for YOUNG Marine Researchers. The Bremen Society for Natural Sciences, Berlin (Germany), September 2021.
- Integrated biochemical and computational approach reveals novel mechanisms underlying the antifungal activity of the milk-derived lactoferrin protein Cátia Santos-Pereira, María T. Andrés, Juliana F. Rocha, Henrique S. Fernandes, Susana R. Chaves, José F. Fierro, Hernâni Gerós, Stéphen Manon, Sérgio F. Sousa, Lígia R. Rodrigues, Manuela Côrte-Real XXI SPB National Congress of Biochemistry 14-16th Oct 2021, Évora, Portugal (online).
- Application of QM/MM methods for development of plastic degradation enzymes Jorge M. Cunha, Rita P. Magalhães, Henrique S. Fernandes, Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP) May 6th 2021, Porto, Portugal (online).
- Integrated in silico approach for the development of a new antipsychotic drug candidate to treat schizophrenia Rodrigo Andrade, Elina Marinho, Alba Iglesias, Jose Brea, Marián Castro, Filipe A. Almeida Paz, Filipe M. Areias, Maria I. Loza, Sérgio F. Sousa and M. Fernanda Proença Encontro de jovens investigadores da Universidade do Porto (IJUP) May 7th 2021, Porto, Portugal.

- Development of a Structural Database of Insecticide Targets Maria F. Araújo, Tatiana F. Vieira, Elisabete M.S. Castanheira Coutinho and Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP), May 7th 2021, Porto, Portugal.
- Molecular Docking, Molecular Dynamics, and Free Energy Calculations for Identification of New Drugs Against Biofilm Formation in P.aeruginosa Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa Hünfeld 2021: Workshop on Computer Simulation and Theory of Macromolecules April 23-24 2021 (online).
- Identification of Biofilm Formation Inhibitors in Pseudomonas aeruginosa through Virtual Screening, Molecular Dynamics, and Free Energy Calculations Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online) Best Poster Communication.
- Bioinformatic applications for the development of plastic degradation enzymes using QM/MM Jorge M. Cunha, Rita P. Magalhães, Henrique S. Fernandes, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online).
- Development of a Structural Database of Insecticide Targets Maria F. Araújo, Tatiana F. Vieira, Elisabete M.S. Castanheira Coutinho, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online).
- 3D Prediction of Non-B DNA Conformations Associated with MtDNA Genomic Instability André F. Pina, Sérgio F. Sousa, João Carneiro X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online).
- In silico methodology for the identification of new drugs against biofilm formation in P. aeruginosa Tatiana F. Vieira, Rita P. Magalhães, Sérgio F. Sousa Affinity 2021: The 24th meeting of the International Society for Molecular Recognition 22-24 June 2021 (online).
- Discovery of New Drugs Against Biofilm Formation in P.aeruginosa through Molecular Docking, Virtual Screening, Molecular Dynamics and MM/GBSA calculations Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa Affinity 2021: The 24th meeting of the International Society for Molecular Recognition 22-24 June 2021 (online).
- Elucidating the interaction of lactoferrin with V-ATPase towards understanding its mechanisms of action Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes, Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa. The 24th meeting of the International Society for Molecular Recognition, Affinity 2021, 22-24 June 2021 Note: Young investigator award.
- A Multi-Level Computational Approach in the Discovery of New Quorum Sensing Inhibitors for P. aeruginosa Tatiana F. Vieira , Cristina Sousa, Sérgio F. Sousa Paul Ehrlich (PE) Euro-PhD Network virtual meeting, MedChem2021 26-28 July 2021 (online).
- Development of a Classification Model for the Identification of Targets to Known P.aeruginosa Biofilm Formation Inhibitors Rita P. Magalhães, Victor de la Oliva, João Carneiro, Sérgio F. Sousa Machine Learning in Quantum Physics and Chemistry Summer School 24 August to 3 September 2021, Warsaw, Poland Note: Award for 3rd Best Poster.
- Specialized Multi-Level Computational Approach For The Identification of Novel Quorum Sensing Inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexcel (online).
- Optimization of a Drug Discovery Computer Aided Workflow for Identification of P.aeruginosa Quorum-Sensing Inhibitors Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexcel (online).
- The catalytic mechanism of Nitrilase 2: the role of the Cys-Glu-Lys catalytic triad Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa 18th European Symposium on Organic Reactivity (ESOR2021) 21-23 September 2021, Vrije Universiteit Amsterdam, The Netherlands (online).

- The Cys-Glu-Lys catalytic triad from the nitrilase superfamily: a QM/MM study on Nitrilase 2 Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexel (virtual).
- Unveiling the catalytic mechanism of the Cys-Glu-Lys catalytic triads using the Nitrilase 2 as a case study Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) 7December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Unraveling the Catalytic Mechanism of Threonine Aldolase, a potential biocatalyst for industrial application Juliana F. Rocha, Sérgio F. Sousa, Nuno M. F. S. A. Cerqueira FEBS 2021 Advanced Course - Computational Approaches to Understanding and Engineering Enzyme Catalysis October 19-22st 2021, Oulu, Finland (online) - Flash Talk.
- The Catalytic Mechanism of the SARS-Cov-2 Main Protease Henrique S. Fernandes, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Optimization of Classification Models for Identification of Ligand-Target Inhibition Pairs in Biofilm Formation in P.aeruginosa Rita P. Magalhães, Victor de la Oliva, João Carneiro, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- A computational study on the catalytic mechanism of Pdx2: a glutaminase containing the Cys-His-Glu triad André F. Pina, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Specialized Multi-Level Computational Protocol for the Identification of Potential New Drugs Fábio G. Martins, Tatiana F. Vieira, Joel P. Moreira, Tiago Barbosa, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Unraveling the catalytic mechanism of Threonine aldolase - a critical enzyme in the pharmaceutical industry Juliana F. Rocha, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Bridging the gap between lactoferrin and V-ATPase through a multi-stage computational approach Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes, Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal.
- Molecular detection of species from the Boraginaceae family to safeguard food and feed safety, integrity, authenticity, and quality Inês Carvalho Leonardo, Jorge Capelo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021.
- The complete genome sequence of Alicyclobacillus acidoterrestris DSM 3922T, a food spoiler taint producing strain Inês Carvalho Leonardo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021.
- Adaptation of SPARK to atmospheric-pressure micro-plasma jet flow conditions Duarte Gonçalves, João Santos Sousa, Stéphane Pasquiers, Mário Lino da Silva, Luís Lemos Alves PLATHINIUM 2021.

- Sinval, J.; Vazquez, A.C.S.; Hutz, C.S.; Schaufeli, W.B.; Silva, S. Burnout Assessment Tool (BAT): Validity Evidence from Brazil and Portugal. Int. J. Environ. Res. Public Health 2022, 19, 1344. https://doi.org/10.3390/ijerph19031344.
- Collective dynamics of heavy ion collisions in ATLAS, Helena Santos, on behalf of the ATLAS Collaborations, ISMD2021 - International symposium on multiparticle dynamics.
- Collective dynamics of heavy ion collisions in ATLAS, Helena Santos, on behalf of the ATLAS Collaboration, 50th International Symposium on Multiparticle Dynamics.
- Evidence for local acceleration of heavy >10 MeV/n oxygen and sulphur in Jupiter's innermost radiation belts, Elias Roussos, Christina Cohen, Peter Kollmann, Marco Pinto, Patricia Gonçalves, Norbert Krupp, and Konstantinos Dialynas, Europlanet Science Congress 2021, https://doi.org/10.5194/epsc2021-603.
- Gamma/hadron discrimination using a small-WCD with four PMTs, R. Conceição et al., for the SWGO collaboration, 37th International Cosmic Ray Conference (Berlin).
- Modeling the radiobiological effects of gold nanoparticles in proton therapy of glioblastomas, J. Antunes, F. Mendes, A. Paulo and J. M. Sampaio, PANIC 2021, Particles and Nuclei International Conference.
- Monitoring Gamma-Ray Burst VHE emission with the Southern Wide-field-of-view Gamma-ray Observatory, G. La Mura, U. Barres de Almeida, A. De Angelis, R. Conceição, F. Longo, M. Pimenta, E. Prandini, E. Ruiz-Velasco, B. Tomé on behalf of the SWGO Collaboration, 37th International Cosmic Ray Conference (Berlin).
- The BepiColombo Radiation Monitor, Pinto, M., Gonçalves, P., Cardoso, C., Sanchez-Cano, B., Moissl, R., Vainio, R., Oleynik, P., Huovelin, J., Korpela, S., Lehtolainen, A., Grande, M., and Marques, A., Europlanet Science Congress 2021, https://doi.org/10.5194/epsc2021-20.

Datasets produced with the support of INCD in 2021

- MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Comparative transcriptomics between two potential toxin-secreting marine annelids: Glycera alba and Hediste diversicolor. GenBank OL606744-OL606747 (embargo pending).
- Crispim Romao, Miguel; Castro, Nuno F.; Pedro, Rute; Simulated pp collisions at 13 TeV with 2 leptons + 1 b jet final state and selected benchmark Beyond the Standard Model signals. DOI: 10.5281/zenodo.5126747.

Patents produced with the support of INCD in 2021

- EP21306547 / BNT231376EP00 - Vincent Parissi, Sérgio F. Sousa, D. Lapaillere, O. Delelis, L. Meertens, S. Gallois-Montbrun, S. Routier - Pharmaceutical composition, its use as a drug and new compounds, especially for treating SARS-CoV-2 infection (Indole derivaties), 04 November 2021
- EP21306521 / BNT231394EP00 - Vincent Parissi, Sérgio F. Sousa, D. Lapaillere, O. Delelis, L. Meertens, S. Gallois-Montbrun, M. Teulade-Fichou, R. Lartia, G. Bordeau - Pharmaceutical composition, its use as a drug and new compounds, especially for treating SARS-CoV-2 infection (triphenylamine derivatives), 29 October 2021