Activities Report

2021

TABLE of CONTENTS

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 July 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 organized by FCT. Under this call and in the context of the National Advanced Computing Network (RNCA), INCD received an allocation of 40 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 harmonization 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 organization.

1. ACTIVITIES REPORT

The INCD is a digital infrastructure within the Portuguese roadmap of research infrastructures of strategic interest (RNIE). INCD aims at the establishment, continuous development and operation of a digital infrastructure, providing advanced computing and data-oriented services to the national scientific and academic community. The core infrastructure encompasses high performance computing (HPC), high throughput computing (HTC) and cloud computing complemented by block, object and file-system based data storage. The core infrastructure can be exploited directly by the end-users or indirectly through higher level services.

INCD supports research across all scientific and technological domains, enabling researchers to effectively participate in projects and related activities. INCD also supports researchers in the use of international resources by linking with international digital infrastructures and initiatives such as EGI, IBERGRID, WLCG and EOSC.

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 its operation and develop the activities summarized below.

The execution of the FCT research infrastructures contract (AAC 01/SAICT/2016 project nº 22153) continued along 2021. This project has been supporting most costs both in terms of human resources and equipment. In this context, INCD has improved and made available computing and data storage services to the scientific community, delivered through its operational centres in Minho and Lisbon. INCD supported its existing user base and further extended it namely through 40 new computational projects approved within the scope of the 1st call for advanced computing projects (CPCA) of 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. The infrastructure usage is further detailed in section 2.

In Lisbon, the phased migration of the high-performance and high-throughput computing services from the old SoGE batch scheduler to a newer Slurm batch scheduler, initiated in the summer of 2020, was completed. Similarly, the changes to the distributed computing middleware necessary for the federation of these services were also completed. These 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. The process of upgrading the Openstack and Ceph based cloud computing infrastructure was also started with a parallel test environment being deployed. The improvement of the internal virtualization platform based on KVM and internal monitoring systems continued. The implementation of a new Kubernetes cluster started to better support the internal services already relying on Linux containers.

In Minho, INCD continued to collaborate with FCT-FCCN and with the Minho Advanced Computer Center (MACC) in the management of the Bob supercomputer installed in Riba-de-Ave. INCD in partnership with LIP is supporting the management of the Lustre storage system and ensuring the management of part of the installed processing capacity. The availability of this resource was severely affected by power and cooling limitations in the commercial datacenter that houses the facility. Due to these limitations, the execution of several CPCA projects was extended until the end of 2021.

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 organization, among others.

Bridging with the IBERGRID and EGI activities, INCD also participated in the European Open Science Cloud (EOSC). Among others INCD is supporting 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 portfolio. Also in the EOSC scope, INCD continued its participation in the European project EOSC-Synergy, whose objective is the harmonization of policies, development of state-of-the-art tools to foster service integration through quality, and the integration of computing services, data repositories and thematic services in the context of EOSC. In the context of this project, INCD also 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. Additionally, 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. In C-Scale, the objective is the integration of earth observation services exploring data from the Copernicus system.

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 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/). Namely, INCD participated in the first CPCA as an operational centre supporting computational projects. INCD participated as well in the preparation of the second CPCA call and in

the technical evaluation of projects whose execution will take place in 2022. A formal protocol to join the RNCA was prepared and finally signed in January of 2022. Under this protocol INCD will continue 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 research data repository.

2. SERVICES

The main services delivered in 2021 can be summarized as follows.

High Performance Computing (HPC) Access to High Performance Computing clusters equipped with low latency interconnects. Delivered using conventional batch systems coupled with parallel file-systems and low latency networks. Available in Lisbon and Minho.
High Throughput Computing (HTC) Support for massive processing of independent tasks exploiting dedicated and opportunistic computing resources for massively computational and data intensive applications. Delivered using batch systems coupled with distributed filesystems.
Large Memory Computing Access to physical and virtual machines equipped with large RAM capacity tailored for computational tasks with large memory requirements. Delivered through the HPC, HTC or cloud services.
Accelerated Computing Scientific computing using specialized hardware e.g. GPUs, delivered using conventional batch systems and/or other solutions including cloud and containers orchestration systems. Suitable for machine learning and artificial intelligence applications.
Scientific Cloud Computing On-demand access to computing resources in cloud mode: Infrastructure-as-a-service, Platform-as-a-service, and Software-as-a-Service. Delivered using interoperable open source software solutions, coupled with block storage systems.
Federated Computing Access to the EGI, IBERGRID and WLCG distributed computing infrastructures, interconnecting computing clusters and data at international level. The INCD HTC and HPC computing services are federated in the EGI and IBERGRID computing services.
Federated Cloud Access to the EGI and IBERGRID federated cloud computing infrastructures, interconnecting cloud services and data at international level. The INCD cloud services are integrated in the EGI and IBERGRID federated cloud.
Containerised Computing Support for execution and orchestration of Linux containers for services and applications. Enabling portability, reproducibility and preservation of applications with their computing environments. Support for the delivery of complex containerised services and applications.

Object Storage Access to cloud based object storage using interoperable cloud APIs for large scale highly reliable storage. Can be used as a standalone service or as a complement to the Scientific Cloud Computing and Federated Cloud services.
Distributed Read-only Filesystem Sharing of software environments and/or immutable files safely across the INCD sites and/or at other locations, via the INCD distributed wide-area read-only filesystem.
Data Repositories Provisioning of digital repositories for research data of general or community wide interest according to open science and FAIR data principles. Pilot service under development.
Data Protection Storage services suitable for data protection, long-term data storage, storage of critical data and disaster recovery. Delivered using tape and on-line data storage systems.
Scientific Portals and Gateways Access to scientific gateways and portals such as R-Studio, Jupyter notebooks, Galaxy and domain specific solutions for simulation and data analysis. Portals are community oriented services delivered on top of the INCD Scientific Cloud and/or in combination with other data or compute services.
High-Level Value-Added Services Provisioning of multiple services delivered through the INCD cloud (e.g. Sync&Share file services, databases, agenda meeting services, web servers, load balancers, proxies, container management frameworks, etc).
Integration of Services and Applications Support for the integration of generic or thematic software exploiting INCD capabilities. Higher scalability exploiting international partner infrastructures and initiatives at international level (EGI, IBERGRID and EOSC). Co-development and provisioning in partnership with the users.
Resource Management Management of virtual or physical resources integrated in the INCD platform, to benefit from the IT service management capabilities, experience and scalability of INCD.
Documentation, Support and consultancy Providing documentation about the services and their usage, Helpdesk service supporting the use of the INCD services and assisting users in exploiting the infrastructure and/or adapting their software. Generic and customized training oriented to the use of INCD services.

3. 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.

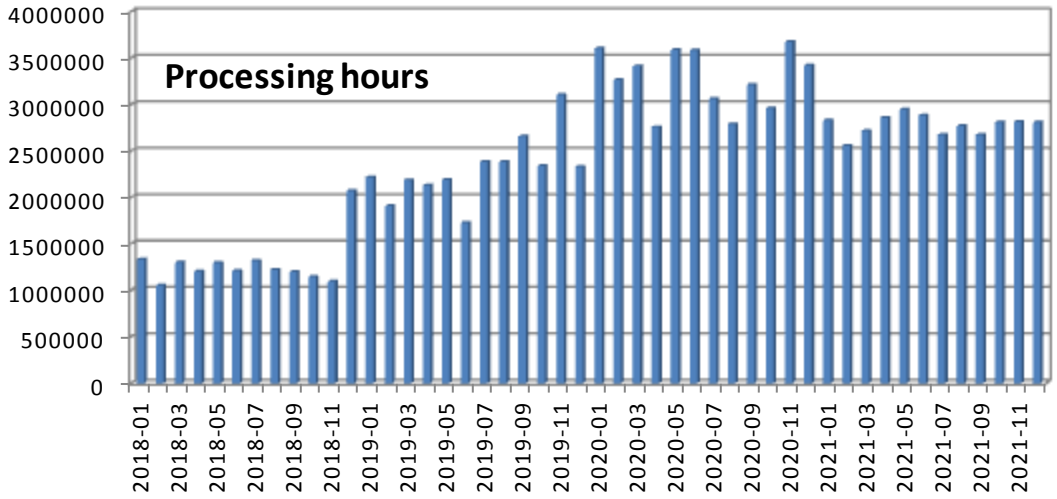

Figure 1: combined usage of all INCD services from January of 2018 to December of 2021.

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. Although the delivered capacity in Lisbon improved, issues in Minho resulted in a large reduction of the HPC capacity in 2021, particularly when compared with 2020.

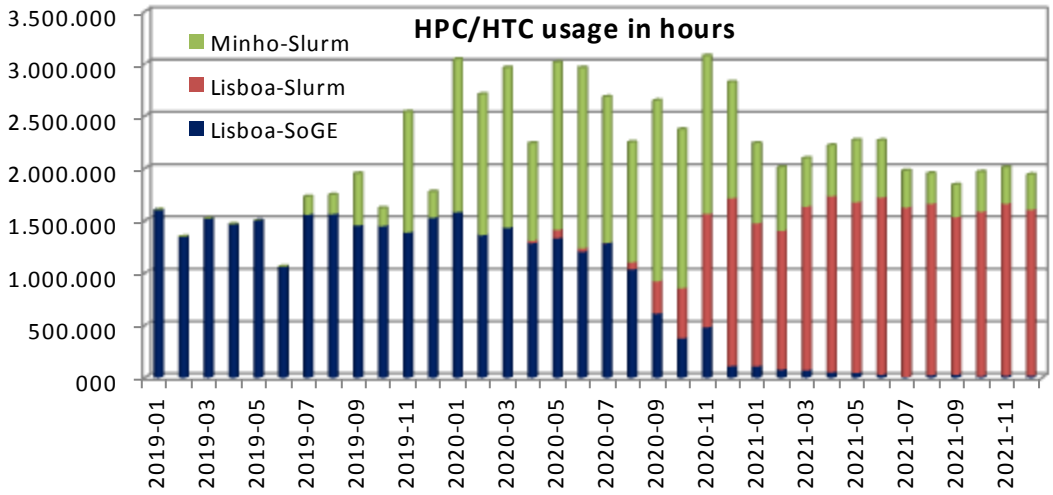

Figure 2: usage of both HPC and HTC batch services from January of 2019 to December of 2021.

The reduction of HTC/HPC capacity was caused by power and cooling limitations imposed at the Minho Riba-de-Ave commercial datacenter 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 considerably the INCD users 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 since mid 2020. In December 2021 there were 60 projects registered in the Openstack cloud service.

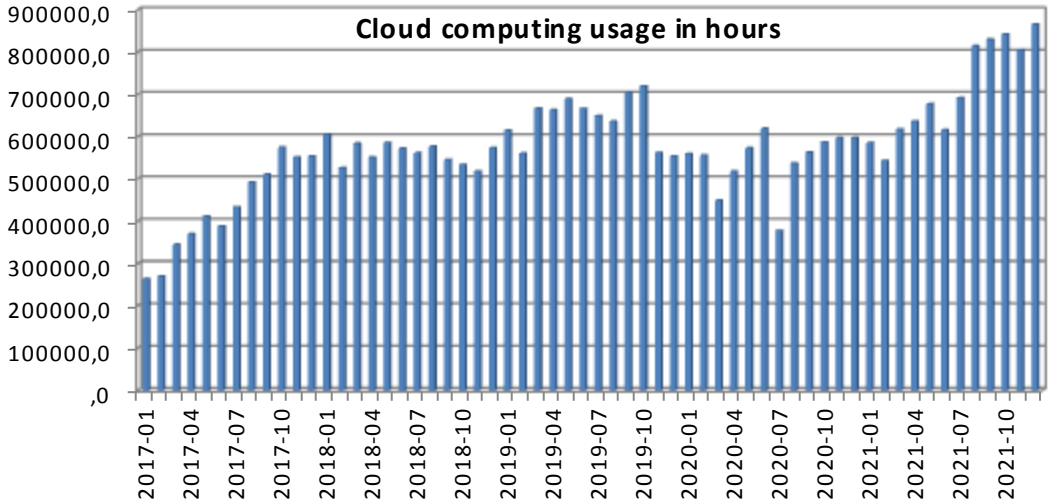

Figure 3: usage of the INCD cloud computing service from January 2017 to December of 2021.

Table 1 provides a list of 62 organizations, 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)
Centro de Ciências do Mar e do Ambiente (MARE)
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: organizations, infrastructures and research units that used INCD provided services in 2021.

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.

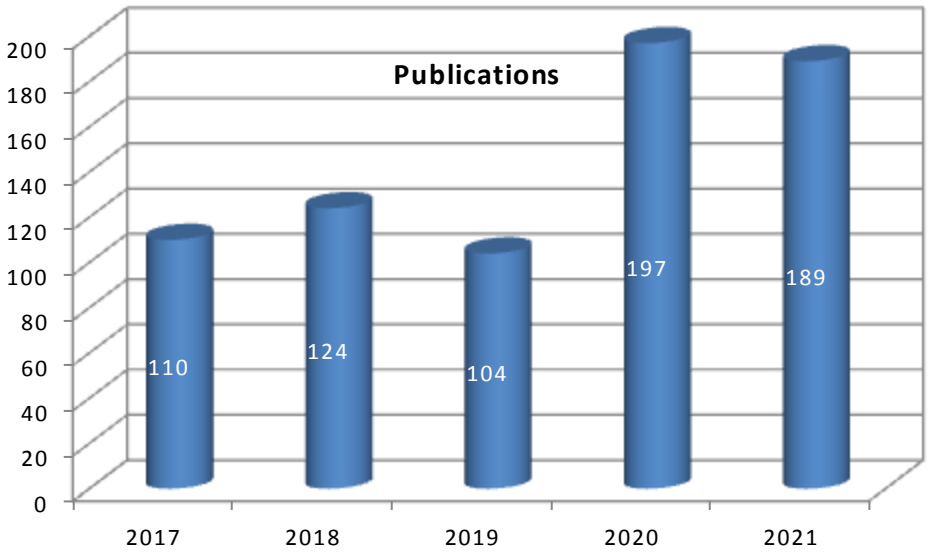

Figure 4: publications that benefited from INCD from 2017 to 2021.

4. 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 $B0 \rightarrow K*0\mu+\mu-$, 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.

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- 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.
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- 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.
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- 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).
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- 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).
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- 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).
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- 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.
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