Concurso de Projetos de Computação Avançada – 1ª edição

Relatório de execução

INT/2021/ AIA | CA

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INTRODUÇÃO

A consolidação e o reforço do Sistema Científico e Tecnológico Nacional (SCTN) constituem prioridades da política de ciência e tecnologia nacional. Estas prioridades visam aumentar a competitividade nacional e internacional da ciência e tecnologia, e o seu contributo para a inovação e transferência de conhecimento, assim como contribuir para a realização das aspirações globais definidas nos Objetivos para o Desenvolvimento Sustentável (ODS) das Nações Unidas. Neste contexto, assume particular relevância a promoção e o reforço de competências das instituições científicas e tecnológicas através da participação das suas equipas em projetos de computação avançada.

A execução computacional dos projetos de computação avançada efetua-se nos Centros Operacionais da RNCA. A RNCA é uma rede nacional colaborativa coordenada pela unidade FCCN da FCT, com um regulamento interno publicado em diário da república: Regulamento n.º 10/2022 e Regulamento n.º 470/2021. Mais informações na página WEB da RNCA em https://rnca.fccn.pt/

CONCURSO DE PROJETOS DE COMPUTAÇÃO AVANÇADA

PRINCIPAIS INDICADORES DA 1ª EDIÇÃO EM 2020

PRÉ-SUBMISSÃO

Submissões e Divulgação

- Plataforma de submissões: Formstack, com candidaturas redirecionadas para sistema de tickets OTRS via rnca@fccn.pt
- Página do concurso - https://www.fct.pt/apoios/Computacao/index.phtml.pt
- Divulgação junto dos canais FCT, FCCN, ANI, INCoDe.2030 via redes sociais, newsletters, sites

Modelos computacionais disponíveis

- High Performance computing (HPC)
- High Throughput computing (HTC)
- Cloud Computing

Tipologias de acesso disponíveis:

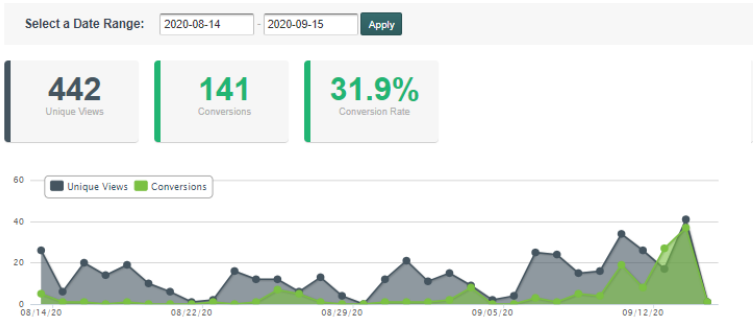
- **A1 (acesso preparatório)** - Este acesso está recomendado a todos os projetos científicos e de inovação sem experiência prévia em HPC ou HTC e/ou sem histórico de utilização nos recursos computacionais da RNCA. Destina-se primariamente à realização de testes de performance de software, testes de escalabilidade, benchmarking, re-factoring e projetos de curta dimensão que não ultrapassem o limite de tempo e recursos definidos no presente aviso. Limite de Recursos: 50 000 core.horas ou vCPU_core.horas. Limite de tempo máximo: 2 meses, prorrogáveis.
- **A2 (acesso projeto) -** Destina-se à utilização de recursos HPC, HTC ou Cloud Computing, para projetos com dimensão maior que 50.000 core.horas ou vCPU.horas até a um limite máximo de 3.000.000 core.horas ou vCPU.horas, com possibilidade de aprovação de pedidos de prorrogação. Limite de tempo máximo: 6 meses, prorrogáveis.

PÓS-SUBMISSÃO

Recursos a atribuir

CPU.Core horas disponibilizadas inicialmente= 27.300.000 CPU core.horas / vCPU.horas. Reforço durante a adequação técnica das plataformas MACC e INCD permitiu chegar a ~35.300.000 CPU core.horas / vCPU.horas.

Submissões e consultas do formulário

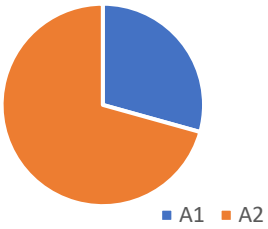


total de visualizações do formulário – 442

Candidaturas recebidas até 14/09 (12h) – 133

Candidaturas recebidas após 14/09, não consideradas para avaliação e ranking - 8

Candidaturas vs Tipologias de acesso:



A1	A2 e A1+A2	Total
39	94	133
29%	71%	100%

Plataformas

Candidaturas com 1ª Preferência nas plataformas

	Bob	Navigator	Oblivion	INCD
Preferência=1*	58	21	20	30

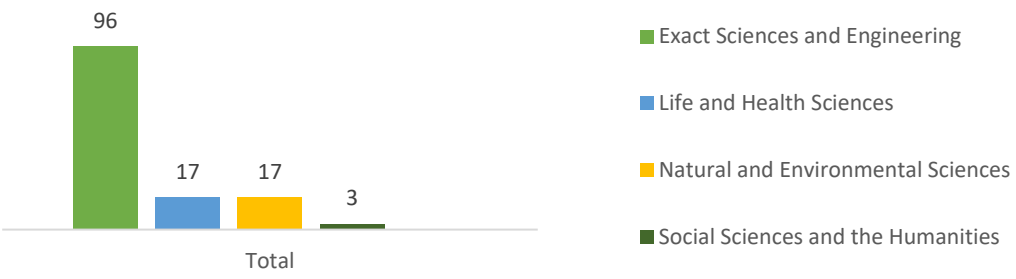
Avaliação

- Hierarquização do **A1 - Acesso Preparatório:**
  a) Ordem de submissão das candidaturas
- Hierarquização do **A2 - Acesso Projeto:**
  a) Exequibilidade do programa de trabalhos, nomeadamente a adequação técnica e razoabilidade dos recursos computacionais selecionados
  b) Existência de projeto científico ou tecnológico associado à candidatura do projeto de computação avançada, com avaliação prévia independente de mérito científico ou técnico, por entidade competente, nacional ou Europeia
  c) Ordem de submissão das candidaturas

- **Distribuição Avaliação técnica pelas equipas dos Centros Operacionais - A2 apenas:**

MACC	41
LCAUC	13
HPCUE	11
INCD	29

Domínios científicos

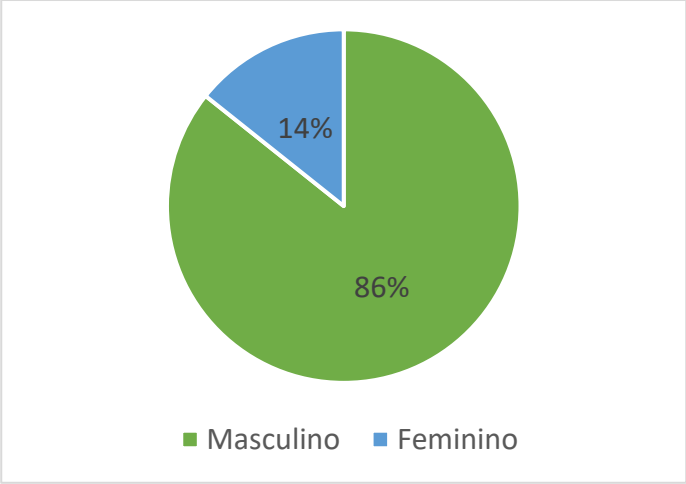


- Domínios científicos vs tipologias de acesso:

Domínio científico	Exact Sciences and Engineering	Life and Health Sciences	Natural and Environmental Sciences	Social Sciences and the Humanities	Total
A1	30	1	7	1	39
A1+A2 e A2	66	16	10	2	94
Total	96	17	17	3	133

Instituições: 31

Género: 19 candidaturas de mulheres

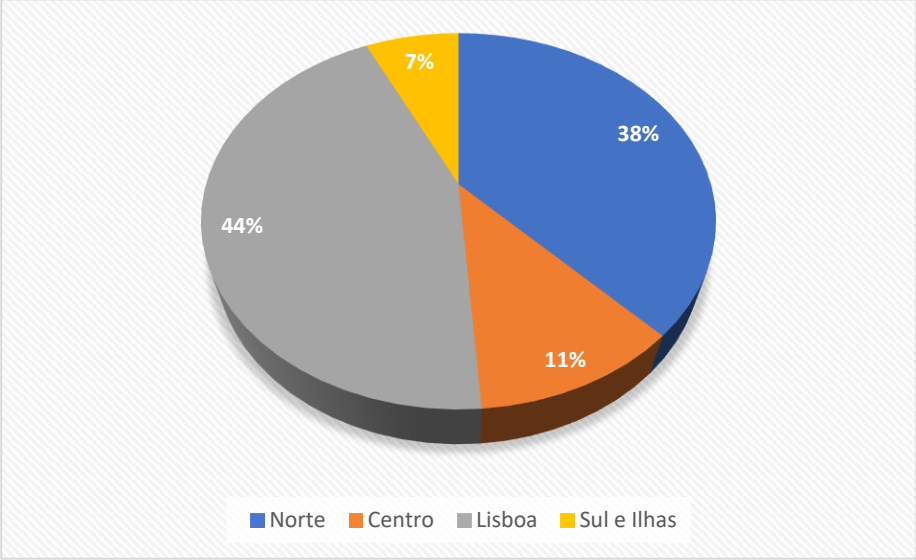


Sendo:

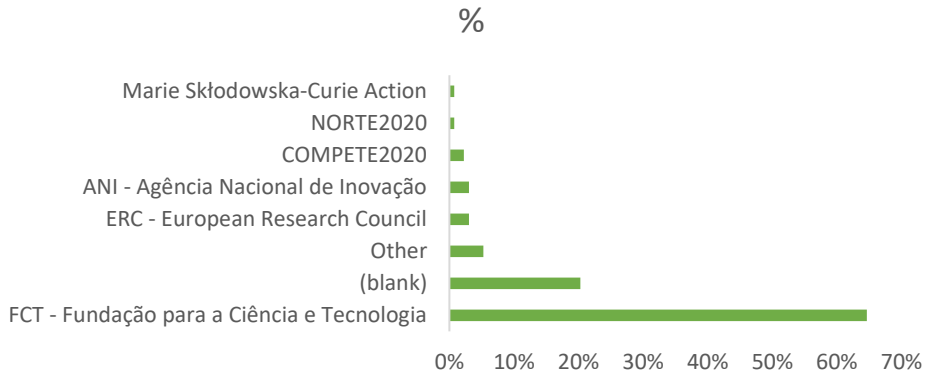
Nome da IR	Entidade	REGIÃO

Rafaela Nascimento Martins (n=2)	Universidade de Évora	ALENTEJO
Alexandra Teresa Pires Carvalho (n=2)	Universidade de Coimbra, CNC - Center for Neuroscience and Cell Biology, Institute for Interdisciplinary Research (IIIUC)	CENTRO
Rita Alexandra do Nascimento Cardoso Guedes	Universidade de Lisboa	AML
Sandra Cristina da Cruz Nunes	Universidade de Coimbra	CENTRO
Maria Leonor Nunes Ribeiro Cruzeiro	Centro de Ciências do Mar do Algarve	ALGARVE
Irina Sousa Moreira (n=2)	CNCB - Center for Neuroscience and Cell Biology	CENTRO
Anabela Pacheco de Oliveira	LNEC - Laboratório Nacional de Engenharia Civil	AML
Luísa Maria Sousa Mesquita Pereira	Instituto de Investigação e Inovação em Saúde	NORTE
Marija Vranic	Universidade de Lisboa, Instituto Superior Técnico	AML
Katharina Lorenz	Universidade de Lisboa, Instituto Superior Técnico	AML
Estelina Lora da Silva	Faculdade de Ciências da Universidade do Porto	NORTE
Mónica Sérvulo Correia Carneiro da Silva	Faculdade de Ciências da Universidade de Lisboa	AML
Diana Andreia Pereira Lousa	ITQB NOVA	AML
Tânia Firmino Guerra Guerreiro da Cova	Universidade de Coimbra	CENTRO
Sara Newbery Raposo de Magalhães	FCiências.ID - Associação para a Investigação e Desenvolvimento de Ciências	AML
Joana Gonçalves de Sá	Laboratório de Instrumentação e Física Experimental de Partículas e Departamento de Física, Instituto Superior Técnico, U. Lisboa	AML/NORTE

Distribuição geográfica:



Entidade financiadora do projeto associado ao projeto computacional:



PÓS-APROVAÇÃO

- # acessos A1 e A2 = 67
- # vouchers A0 e A00 = 62
- Total = 129 projetos apoiados
- Taxa de aprovação A1 e A2 = 50.4%
- Solicitado em candidaturas elegíveis = 80 M CPU core.horas
- Recursos computacionais atribuídos = 34,8 M CPU core.horas
- Valor económico estimado dos recursos atribuídos 428.087,77€
    - Sem contabilizar GPU.horas ou armazenamento em disco

Resumo dos resultados por Centro Operacional:

	BOB:MACC	NAVIGATOR:LCA-UC	OBLIVION:HPC-UÉ	CIRRUS-A:INCD	STRATUS:INCD	TOTAL
# CPU core.horas	**20 037 180**	**4 636 368**	**4 177 600**	**4 116 856**	**1 835 880**	**34 803 884**
# Projetos A1 e A2	**25**	**9**	**10**	**15**	**8**	**67**
# Vouchers A0/A00	30	8	7	14	3	62
TOTAL	55	17	17	29	11	129

PROJETOS DE COMPUTAÇÃO AVANÇADA

A2 - ACESSO PROJETO

A2- Destina-se à utilização de recursos HPC, HTC ou Cloud Computing, para projetos com dimensão maior que 50.000 core.horas ou vCPU.horas até a um limite máximo de 3.000.000 core.horas ou vCPU.horas, com possibilidade de aprovação de pedidos de prorrogação. Limite de tempo máximo: 6 meses, prorrogáveis.

> Projetos A2 encontram-se detalhados no Anexo I deste relatório.

A1 – ACESSO PREPARATÓRIO

A1 – Este acesso está recomendado a todos os projetos científicos e de inovação sem experiência prévia em HPC ou HTC e/ou sem histórico de utilização nos recursos computacionais da RNCA. Destina-se primariamente à realização de testes de performance de software, testes de escalabilidade, benchmarking, re-factoring e projetos de curta dimensão que não ultrapassem o limite de tempo e recursos definidos no presente aviso. Limite de Recursos: 50 000 core.horas ou vCPU core.horas. Limite de tempo máximo: 2 meses, prorrogáveis.

VOUCHERS DE COMPUTAÇÃO AVANÇADA – A0 E A00

A0 - Voucher concedido aos projetos abaixo da linha de corte, após serem esgotados os recursos HPC/HTC, e que satisfaziam os critérios a) e b). Destinam-se ao incentivo da utilização de HPC, HTC ou Cloud Computing na RNCA. Recursos: ≤50.000 core.horas ou vCPU.horas. Duração máxima do projeto: 6 meses.

A00 - Voucher concedido aos projetos abaixo da linha de corte e que satisfaziam os critérios a) ou b) ou nenhum dos dois. Destina-se ao incentivo da utilização de HPC, HTC ou Cloud Computing na RNCA. Recursos ≤25.000 core.horas ou vCPU.horas. Duração máxima do projeto: 6 meses.

Bob

A2

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A2_2568_2020	Nuno Martins	Sim	Sim	Sim	Sim
CPCA_A2_2613_2020	Fernando Cruz	Sim	Sim	Sim[1]	Não
CPCA_A2_2640_2020	Pedro Ferreira	Sim	Não	Não	Não
CPCA_A2_3840_2020	Miguel Zilhão	Sim	Não	Sim[2]	Sim
CPCA_A2_4403_2020	Sergey Pyrlin	Sim	Sim	Sim[3]	Não
CPCA_A2_4513_2020	Luis Marques	Sim	Sim	Sim	Não
CPCA_A2_5804_2020	José Carlos Lopes	Sim	Não	Sim[4]	Sim
CPCA_A2_6052_2020	Célio Fernandes	Sim	Sim	Sim[5]	Não
CPCA_A2_6202_2020	João Miguel Nóbrega	Não			
CPCA_A2_6231_2020	João Miguel Nóbrega	Não			
CPCA_A2_6816_2020	Paulo Silva	Não			
CPCA_A2_7081_2020	Paulo Abreu	Sim	Sim	Sim	Não
CPCA_A2_7083_2020	Jorge Marques	Sim	Não	Sim	Não
CPCA_A2_7085_2020	Orlando Oliveira	Não			

[1] "Structure and Thermodynamics of Empty Clathrate Hydrates Below the Freezing Point of Water", Phys. Chem. Chem. Phys. [2021]

[2] Pedro Ildefonso, Carlos Herdeiro, Miguel Zilhao. "Evolutions of Dipolar Boson Stars ". To appear (2022).

[3] Pyrlin S.V. "Molecular dynamic model of bis-salphen chain deformation" (expected)

[4] Fernandes, I.S., M.S.C.A. Brito, Y.A. Manrique, M.M. Dias, J.C.B. Lopes, R.J. Santos, 2021. Computational Fluid Dynamics Model of Two-Phase Flow in NETmix Reactors. Chem. Eng. Technol. 44 (11), 2002-2010.
Matos, J., Dias, M.M., Santos, R.J., Lopes, J.C.B. 2021. Mixing in the NETmix Reactor. Frontiers in Chemical Engineering, 3, 771476.

[5] 1) C. Fernandes, S. A. Faroughi, R. Ribeiro, A. I. Roriz, and G. H. McKinley, Finite volume simulations of the inertia-less steady translation of random arrays of spheres in viscoelastic fluid flows: application to hydraulic fracture processes; 2) A.I. Roriz, S. A. Faroughi, G. H. McKinley, C. Fernandes, Digital-twin in Shear-thinning Viscoelastic Fluids: ML-based models to predict the drag coefficient of a sphere.

CPCA_A2_7087_2020	João Araújo	Sim	Sim	Sim	Sim
CPCA_A2_7181_2020	Luís Loura	Sim	Sim	Sim[6]	Sim
CPCA_A2_7269_2020	Cristóvão Dias	Sim	Não	Sim	Sim

A1

Ref. Projetos	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A1_4443_2020	Pedro Gardete	Sim	Não	Não	Não
CPCA_A1_6056_2020	Célio Fernandes	Sim	Sim	Sim	Sim
CPCA_A1_6058_2020	Célio Fernandes	Sim	Sim	Sim	Sim
CPCA_A1_6525_2020	Carlos Reis	Sim	Não	Não	Não
CPCA_A1_7015_2020	João Miguel Nóbrega	Sim	Sim	Sim	Sim
CPCA_A1_7017_2020	João Miguel Nóbrega	Sim	Sim	Sim	Sim
CPCA_A1_7070_2020	Ricardo Ribeiro	Sim	Sim	Não	Não

[6] 1 - Interaction of Rhodamines 123 and B with lipid bilayers (already submitted);2) Modelling of GdDOTA for molecular dynamics simulation (to be submitted before June 2022); 3) Interaction of GdDOTA with lipid bilayers (to be submitted during 2022); 4) Interaction of Hoechst 33342 with lipid bilayers (to be submitted during 2022); 5) - Interaction of Rifampicin with lipid bilayers (to be submitted during 2022).The following five communications have resulted from this project (others, concerning the rhodamine and Hoechst systems, are expected during 2022):
- Alexandre C. Oliveira, Hugo A. L. Filipe, Armindo Salvador, Carlos F. G. C. Geraldes, Maria João Moreno, Luís M. S. Loura. Modelling Gd-DOTA for molecular dynamics simulations in water and in presence of lipid bilayers. 7th International Iberian Biophysics Congress. 14-16th June 2021. Coimbra, Portugal. Oral communication.
- Rui M. S. Santos, Alexandre C. Oliveira, Hugo A. L. Filipe, Maria João Moreno, Luís M. S. Loura. Interaction of the antibiotic Rifampicin with lipid membranes: molecular dynamics simulations. 7th International Iberian Biophysics Congress. 14-16th June 2021. Coimbra, Portugal. Poster.
- Alexandre C. Oliveira, Hugo A. L. Filipe, Armindo Salvador, Rui Sun, Gregory A. Voth, Carlos F. G. C. Geraldes, Maria João Moreno, Luís M. S. Loura. Modelling Gd-DOTA for molecular dynamics simulations in water and in presence of lipid bilayers. Coimbra Chemistry Centre Day 2021. 15th December 2021. Coimbra, Portugal. Poster.
- Rui M. S. Santos, Alexandre C. Oliveira, Hugo A. L. Filipe, Maria João Moreno, Luís M. S. Loura. Interaction of Rifampicin with lipidic membranes - experimental characterization and Molecular Dynamics simulations. Coimbra Chemistry Centre Day 2021. 15th December 2021. Coimbra, Portugal. Poster.
- Alexandre C. Oliveira, Hugo A. L. Filipe, Armindo Salvador, Rui Sun, Gregory A. Voth, Carlos F. G. C. Geraldes, Maria João Moreno, Luís M. S. Loura. Modelling Gd-DOTA for molecular dynamics simulations in water and in presence of lipid bilayers. VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural). 20th December 2021. Coimbra, Portugal. Poster.

CPCA_A1_7240_2020	André Fortunato	Não			

A0 e A00

Ref. Projetos	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A0_7276_2020	Carlos Silva	Sim	Não	Não	Nâo
CPCA_A0_7287_2020	João Lopes	Sim	Sim	Sim	Sim
CPCA_A0_7290_2020	Guilherme Vaz	Não			
CPCA_A0_7291_2020	Gernot Eichmann	Sim	Não	Sim[7]	Sim
CPCA_A0_7299_2020	Vitor Duarte	Sim	Não	Não	Sim
CPCA_A0_7305_2020	Diana Lousa	Sim	Sim	Sim	Sim
CPCA_A0_7309_2020	Samuel Santos	Sim	Não	Sim	Não
CPCA_A0_7311_2020	Pedro Simões	Não			
CPCA_A0_7316_2020	Rui M. M. Brito	Sim	Sim	Sim[8]	Sim
CPCA_A0_7318_2020	José Carlos Monteiro	Sim	Sim	Sim[9]	Sim
CPCA_A0_7322_2020	Pedro Medeiros	Sim	Não	Sim	Sim
CPCA_A0_7324_2020	Ricardo Santos	Sim	Sim	Sim[10]	Sim
CPCA_A0_7329_2020	Manuel Simões de Melo	Sim	Sim	Sim	Sim
CPCA_A0_7348_2020	Nuno Silva	Sim	Sim	Não	Não
CPCA_A0_7356_2020	Pedro Castro	Sim	Não	Não	Não

[7] Gernot Eichmann, Jan M. Pawlowski, João M. Silva, "On mass generation in Landau-gauge Yang-Mills theory", e-Print: 2107.05352 [hep-ph]

[8] João P. Luís, Ana I. Mata, Carlos J. V. Simões, Rui M. M. Brito (2021), Analysis of the Conformational Dynamics of the Apo forms of Soluble and Membrane-Bound Interleukin-1 Receptor Type-1: insights into linker flexibility. (submitted for publication)

[9] "Optimization of Monte Carlo Methods for Matrix Functions Applied to Large Scale Problems", Gonçalo Santos, MSc thesis, IST, Sep 2021.

[10] Two papers on two-phase flow in NETmix. One is already under review: "Two-Phase Flow in NETmix Reactors", submitted to Chemical Engineering and Technology; The second paper will be a more thorough analysis of this flow and will be submitted to another Journal (ex: Chem. Eng. J.)

CPCA_A0_7361_2020	Rui Torres	Sim	Sim	Sim	Sim
CPCA_A0_7400_2020	Geoffrey Mitchell	Não			
CPCA_A0_7401_2020	Gonçalo Jesus	Não			
CPCA_A0_7402_2020	José Carlos Campos	Sim	Sim	Sim	Sim
CPCA_A0_7403_2020	Tânia Cova	Sim	Sim	Sim	Sim
CPCA_A0_7408_2020	José Carlos Campos	Sim	Sim	Sim	Sim
CPCA_A0_7420_2020	Tiago Oliveira	Sim	Sim	Sim[11]	

Ref. Projetos	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A00_6057_2020	Célio Fernandes	Sim	Sim	Sim[12]	Não
CPCA_A00_7094_2020	Sandra Nunes	Sim	Sim	Sim	Sim
CPCA_A00_7167_2020	António Costa	Sim	Sim	Sim	Não
CPCA_A00_7246_2020	Luísa Pereira	Sim	Sim	Sim	Não
CPCA_A00_6782_2020	Lucas Thomaz	Sim	Não	Sim[13]	Sim
CPCA_A00_7355_2020	André Silva	Não			
CPCA_A00_7358_2020	André Silva	Não			
CPCA_A00_7437_2020	Nuno Galamba	Sim	Sim	Sim	Sim

[11] Wind-wave characterization and modeling in the Azores Archipelago, Nuno Monteiro, Tiago Oliveira, Paulo Silva.
[12] Ahmad Fakhari, Željko Tukovic, Olga Sousa Carneiro, and Célio Fernandes. "A fast predictive moving mesh interface tracking method for simulating the extrudate swell phenomenon". Submitted to Polymers, 2021.
[13] J. M. Santos, L. A. Thomaz, L. S. Cruz, L. M. N. Tavora, P. A. A. Assuncao, S. M. M. Faria, "Hierarchical Lossless Coding of Light Fields with Improved Random Access". Signal Processing: Image Comumunication.

Navigator

A2

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A2_2524_2020	Manuel Mello-Franco	Sim	Não	Sim[14]	Não
CPCA_A2_6046_2020	José Laginha Palma	Sim	Sim	Sim[15]	Sim
CPCA_A2_6817_2020	José Gouveia	Sim	Sim	Sim[16]	Não
CPCA_A2_6972_2020	Rita Guedes	Sim	Sim	Sim	Sim
CPCA_A2_7219_2020	Irina Moreira	Sim	Sim	Sim[17]	Sim
CPCA_A2_7261_2020	Katharina Lorenz	Sim	Sim	Sim	Não

A1

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses

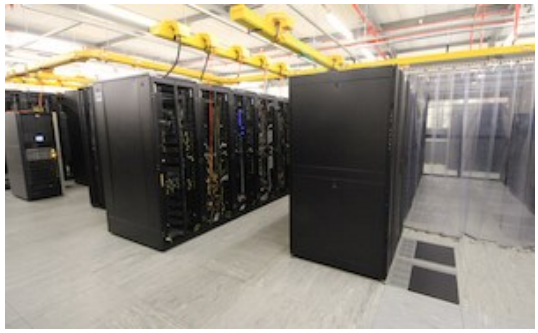
[14] . Zhan, G. et al., Observing Polymerization in Two-Dimensional Dynamic Covalent Polymers, Nature, accepted for publication (2022).
2.Dubey, R. K., Melle-Franco, M. & Mateo-Alonso, A. Inducing Single-Handed Helicity in a Twisted Molecular Nanoribbon. J. Am. Chem. Soc. (2022) doi:10.1021/jacs.1c12385.
3.Riaño, A. et al. An Expanded 2D Fused Aromatic Network with 90-Ring Hexagons. Angewandte Chemie International Edition 61, e202113657 (2022).
4.Dubey, R. K., Melle-Franco, M. & Mateo-Alonso, A. Twisted Molecular Nanoribbons with up to 53 Linearly-Fused Rings. J. Am. Chem. Soc. 143, 6593-6600 (2021).
[15] V.T.P. Batista and J.M.L.M. Palma. The three-dimensional flow over a double-ridge (to be submitted to Boundary-Layer Meteorology).
[16]José D. Gouveia, Ángel Morales-García, Francesc Viñes, José R. B. Gomes, Francesc Illas. "MXenes à la Carte: Tailoring the Epitaxial Growth Alternating Nitrogen and Transition Metal Layers". ACS Nano, 2021 (to be submitted)
[17] Beatriz Bueschbell, Pedro Magalhães, Carlos Barreto, Rita Melo, Anke C. Schiedel, Miguel Machuqueiro, Irina S. Moreira, DRD2 receptor homo-dimers - a world of possibilities - to be submitted.

CPCA_A1_4416_2020	Sergey Pyrlin	Sim	Não	Não	Não
CPCA_A1_6717_2020	Carlos Couto	Sim	Não	Sim[18]	Não
CPCA_A1_6759_2020	João Assis Dias	Não			

A0 e A00

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A0_7302_2020	Irina Sousa Moreira	Sim	Sim	Sim[19]	Sim
CPCA_A0_7326_2020	Carlos Silva	Sim	Não	Não	Não
CPCA_A0_7346_2020	Aurélio Araújo	Sim	Não	Não	Não
CPCA_A0_7347_2020	Aurélio Araújo	Sim	Não	Não	Não
CPCA_A0_7412_2020	Gerard Novell-Leruth	Não			
CPCA_A0_7429_2020	Henrique Cardoso	Sim	Não	Não	Não

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A00_7150_2020	Maria Leonor Cruzeiro	Sim	Sim	Sim[20]	Não
CPCA_A00_7317_2020	Sílvio Gama	Sim	Sim	Sim	Sim



Cirrus-A & Stratus

[18] 1) Couto C, Tong Q, Gernay T. "Predicting the capacity of thin-walled beams at elevated temperature with machine learning". Fire Safety Journal 2022 (submitted). 2) Couto C. "Neural network models for the critical bending moment of uniform and tapered beams". Structures 2022 (submitted). 3) Couto, C., Vila Real, P. (2021) - Modelos preditivos da resistência de vigas metálicas com base em inteligência artificial, atas do XIII Congresso de Construção Metálica e Mista, ISBN 978-989-99251-9-9, pp. 53-62, 25 a 26 de novembro de 2021.

[19] Beatriz Bueschbell, Pedro Magalhães, Carlos Barreto, Rita Melo, Anke C. Schiedel, Miguel Machuqueiro, Irina S. Moreira, DRD2 receptor homo-dimers - a world of possibilities - to be submitted.

[20] L. Cruzeiro, working title: "Effect of collision frequencies on the thermal stability of a small protein", to be prepared.

A2

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A2_4075_2020	Nuno Castro	Não			
CPCA_A2_4568_2020	Alexandra Carvalho	Não			
CPCA_A2_4595_2020	Alexandra Carvalho	Sim	Sim	Sim	Sim
CPCA_A2_5043_2020	Jaime Silva	Sim	Não	Sim	Não
CPCA_A2_6009_2020	Alcides Fonseca	Sim	Não	Não	Sim
CPCA_A2_6193_2020	Rui Caldeira	Sim	Sim	Sim[21]	Não
CPCA_A2_6986_2020	Lucas Thomaz	Sim	Não	Sim[22]	Sim
CPCA_A2_7192_2020	António Muralha	Sim	Sim	Sim	Não
CPCA_A2_7217_2020	Francisco Pina-Martins	Sim	Sim	Sim[23]	Não
CPCA_A2_7255_2020	José Lino Costa	Sim	Sim	Sim[24]	Sim
CPCA_A2_7257_2020	Marija Vranic	Não			
CPCA_A2_7407_2020	Pedro Medeiros	Sim	Não	Não	Não
CPCA_A2_7417_2020	Jorge Sinval	Sim	Sim	Sim[25]	Sim

[21] "Impact of Flash Flood Events on the Coastal Waters Around Madeira Island: The "Land Mass Effect"" with the doi: https://doi.org/10.3389/fmars.2021.749638

[22] J. O. Parracho, L. A. Thomaz, L. S. Cruz, L. M. N. Tavora, P. A. A. Assuncao, S. M. M. Faria, "Cross-modality Lossless Compression of PET-CT using Generative Auto-Encoders". International Conference on Image processing 2022.

[23] Francisco Pina Martins, Ana D. Caperta, Sofia I. R. Conceição, Vera Nunes, Isabel Marques, Octávio S. Paulo. "A first look at sea-lavenders genomics - can genome wide SNP information tip the scales of controversy in the Limonium species complex?". In Prep; 2) Pina-Martins F, Andaluz S, Janeiro M, Monteiro B, Paulo OS. "Natural selection detection revisited - challenges and insights from automating and massively scaling the process". In Prep

[24] Cereja, R., V. Brotas, J.P.C. Cruz, M. Rodrigues & A.C. Brito. 2021. Tidal and physicochemical effects on phytoplankton community variability at Tagus estuary (Portugal). Frontiers in Marine Science, 8: 675699. doi: 10.3389/fmars.2021.675699; 2) França, S., V.F. Fonseca, S.E. Tanner, R.P. Vasconcelos, P. Reis-Santos, A. Maia, M. Ruano, I. Cardoso, S. Henriques, M.P. Pais, P. Brandão, A.C. Brito, P. Castellanos, P. Chainho, B. Quintella, L. Costa, M.J. Costa, J.L. Costa & H.N. Cabral. 2021. Historical data in the CoastNet Geoportal: documenting fish assemblages in Portuguese estuaries. Frontiers in Marine Science, 8: 685294. doi: 10.3389/fmars.2021.685294

Castellanos, P., A.C. Brito, P. Chainho, B. Quintella, L. Costa, S. França, H.N. Cabral & J.L. Costa. In review. CoastNet dataset from Mondego, Tejo and Mira estuaries: multiparametric measurements during 2020. Frontiers in Marine Science.

[25] 1) Alves, S., Sinval, J., Neto, L., Marôco, J., Ferreira, A. G., & Oliveira, P. Burnout and dropout intention in medical students: The protective role of academic engagement. BMC Medical Education. (in press); 2) Sinval, J., Miller, V., & Marôco, J. Openness Toward Organizational Change Scale (OTOCS): Validity evidence from Brazil and Portugal. PLOS

CPCA_A2_7425_2020	Joana Gonçalves de Sá	Sim	Não	Não	Não

A1

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A1_2790_2020	César Capinha	Sim	Sim	Não	Não
CPCA_A1_3154_2020	Gareth Williams	Sim	Não	Sim	Não
CPCA_A1_5214_2020	Hugo Ferreira	Sim	Não	Não	Não
CPCA_A1_5613_2020	Alcides Fonseca	Sim	Sim	Sim	Sim
CPCA_A1_5903_2020	António Leitão	Sim	Sim	Sim	Sim
CPCA_A1_6717_2020	Carlos Couto	Sim	Não	Não	Não
CPCA_A1_7252_2020	João Amaral	Sim	Sim	Não	Não
CPCA_A1_7313_2020	Pedro Vieira	Sim	Sim	Sim	Sim
CPCA_A1_7350_2020	Tiago Paixão	Sim	Sim	Sim	Sim
CPCA_A1_7359_2020	Pedro Vieira	Sim	Sim	Sim[26]	Sim

A0 e A00

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A0_7288_2020	João Santos	Sim	Sim	Sim	Sim
CPCA_A0_7289_2020	João Lopes	Sim	Sim	Sim	Sim
CPCA_A0_7292_2020	João Santos	Sim	Sim	Sim	Sim

ONE, 2021, https://doi.org/10.1371/journal.pone.0249986; 3) Sinval, J., van Veldhoven, M., Oksanen, T., Azevedo, L. F., Atallah, Á. N., Melnik, T., & Marôco, J. Interventions for improving recovery from work. Cochrane Database of Systematic Reviews, 2021, https://doi.org/10.1002/14651858.CD014518; 4) Paolillo, A., Sinval, J., Silva, S. A., & Scuderi, V. E. The relationship between inclusion climate and voice behaviors beyond social exchange obligation: The role of psychological needs satisfaction. Sustainability, 2021, https://doi.org/10.3390/su13181025 5) Sinval, J., Aragão e Pina, J., Passos, A. M., & Marôco, J. Referee Self-Efficacy Scale (REFS): Validity evidence from Brazil, and Portugal. Measurement in Physical Education and Exercise Science, submitted; 6) Sinval, J., Vazquez, A. C. S., Hutz, C. S., Schaufeli, W. B., & Silva, S. Burnout Assessment Tool (BAT): Validity Evidence from Brazil, and Portugal. International Journal of Environmental Research and Public Health. submitted

[26] Marcos AL Teixeira, Pedro E Vieira, Joachim Langeneck, José C Hernandez, Bruno R Sampieri , Panagiotis Kasapidis, Torkild Bakken, Ascenção Ravara, Arne Nygren, Filipe O Costa. The small common European Platynereis worm is actually a large complex of at least 10 species.

CPCA_A0_7297_2020	Mónica Silva	Sim	Sim	Sim[27]	Sim
CPCA_A0_7303_2020	Vitor Conde e Sousa	Sim	Sim	Sim[28]	Sim
CPCA_A0_7304_2020	Daniel Santos	Não			
CPCA_A0_7323_2020	Mario Silva	Sim	Sim	Não	Sim
CPCA_A0_7363_2020	João Ferreira	Sim	Sim	Sim	Não
CPCA_A0_7416_2020	Sara Magalhães	Sim	Sim	Sim[29]	Sim
CPCA_A0_7429_2020	Henrique Cardoso	Sim	Não	Não	Não
CPCA_A0_7438_2020	Mario Ramirez	Não			

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A00_7188_2020	Lourenço Mendes				
CPCA_A00_7140_2020	Sergio Sousa	Sim	Sim	Sim[30]	Sim

[27] Afonso R, Pina-Martins F, Wang Z, Friesen VL, Campioni L, Madeiros J, Silva MC. in prep. Population genomics of the Cahow Pterodroma cahow. To be submitted to Conservation Genetics.

[28] 1) Paper (in preparation)describing the Approximate Bayesian Method (ABC - Task 2). Results from simulation study and application to simple empirical biological example. Target journals: Plos Genetics, Genetics; 2) Paper (in preparation) describing the implementation of the developed ABC method (Task 2) into an R package that will be freely available under GNU GPL3 license and deposited in VS's public repository ttps://github.com/vsousa/EG_cE3c). Target journals: Bioinformatics, Molecular Ecology Resources; 3) Paper (submitted) describing results from a theoretical study using simulations. Target journal: Molecular Ecology

[29] Fragata, I., Kozak, M., Ferreira, M., Sousa, V., Magalhães, S. "Analyses of genomic changes during cadmium adaptation in Tetranychus urticae and T. evansi." In preparation

[30] 1. 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; 2) 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, DOI: 10.3390/molecules26206162; 3) 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
4) 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; 5) 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; 6) 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; 7) 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; 8) Identification of new potential

CPCA_A00_7145_2020	Sergio Sousa	Sim	Sim	Sim[31]	Sim
CPCA_A00_7312_2020	Ricardo Ferreira	Não			
CPCA_A00_7319_2020	Daniel Santos	Sim	Sim	Sim[32]	Sim
CPCA_A00_7387_2020	Paolo Romano	Não			
CPCA_A00_7395_2020	Felipe Freitas	Sim	Sim	Sim[33]	Sim

inhibitors of quorum sensing through a specialized multi‐level computational approach Martins, F.G., Melo, A., Sousa, S.F. (2021) Molecules, 26 (9), art. no. 2600 DOI: 10.3390/molecules26092600

[31] 1) 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; 2) 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, DOI: 10.3390/molecules26206162; 3) 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; 4) 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; 5) 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; 6) 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; 7. 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; 8) Identification of new potential inhibitors of quorum sensing through a specialized multi‐level computational approach Martins, F.G., Melo, A., Sousa, S.F. (2021) Molecules, 26 (9), art. no. 2600 DOI: 10.3390/molecules26092600

[32] - L. Apolinário et al, "Deep Learning for the classification of quenched jets", JHEP 11 (2021) 219, https://doi.org/10.1007/JHEP11(2021)219; M.C. Romão et al, "Finding New Physics without learning about it: Anomaly Detection as a tool for Searches at Colliders", Eur.Phys.J.C 81 (2021) 1, 27, https://doi.org/10.1140/epjc/s10052-020-08807-w; N. Castro et al, novel signatures for monotop events at present and future colliders, in preparation.

[33] https://arxiv.org/pdf/2107.14165.pdf

Oblivion

A2

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A2_2500_2020	Rui Salgado	Não			
CPCA_A2_4377_2020	Rafaela Nascimento Martins	Sim	Sim	Sim[34]	Sim
CPCA_A2_4628_2020	Luis Marques	Sim	Sim	Sim	Sim
CPCA_A2_5649_2020	Veniero Lenzi	Sim	Sim	Sim[35]	Não
CPCA_A2_7242_2020	Anabela Oliveira	Sim	Sim	Sim	Não
CPCA_A2_7263_2020	Estelina Lora da Silva	Sim	Sim	Sim	Não

A1

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A1_2611_2020	Carlos Silva	Sim	Não	Não	Não
CPCA_A1_4630_2020	Carlos Silva	Sim	Não	Não	Sim
CPCA_A1_4781_2020	António Canto	Sim	Sim	Não	Não
CPCA_A1_7203_2020	Pedro Coelho	Não			

[34] Lucas G. Celia-Silva, Rafaela N. Martins, Alfredo J. Palace Carvalho, João P. Prates Ramalho, Pedro Morgado, Eduardo J. M. Filipe, Luís F. G. Martins. Influence of ionic liquids on the aggregation and pre-aggregation phenomena of asphaltenes in model solvent mixtures by molecular dynamics simulations and quantum mechanical calculations.
[35] 1) J. P. B. Silva, M. C. Istrate, M. Hellenbrand, M. T. Becker, A. Jan, J. Symonowicz, F. G. Figueiras, V. Lenzi, C. Ghica, K. N. Romanyuk, G. Di Martino, L. Marques, J. L. MacManus-Driscoll, Ferroelectric orthorhombic phase of pure ZrO2 thin films achieved through substrate orientation control. To be submitted.

A0 e A00

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A0_7277_2020	José Coutinho	Sim	Não	Sim[36]	Sim
CPCA_A0_7296_2020	Roman Chertovskikh	Sim	Não	Sim	Sim
CPCA_A0_7308_2020	Bruno Amorim	Sim	Não	Não	Não

Ref. Projeto	Nome IR	Relatório	Dados	Publicações	Teses
CPCA_A00_4376_2020	Luís Filipe Martins	Sim	Sim	Sim	Não
CPCA_A00_7343_2020	Pedro Ribeiro	Sim	Sim	Sim	Não
CPCA_A00_7421_2020	Eduardo Castro	Sim	Sim	Sim	Sim
CPCA_A00_7439_2020	Alfredo Carvalho	Sim	Sim	Não	Não

TOTAL DE RECURSOS UTILIZADOS

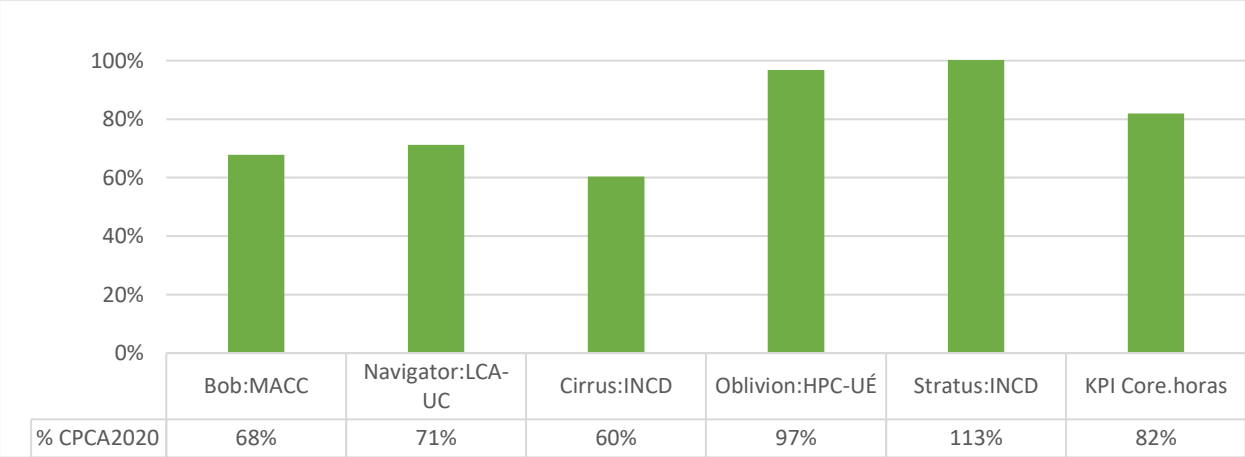


Gráfico: % de recursos utilizados por plataforma e a média geral de recursos utilizados em KPI Core.horas.

[36] 1) J. Coutinho et al., "The M-center in 4H-SiC is a carbon self-interstitial", about to be submitted (2021); 2) J. Coutinho et al., "Assignment of M-center to the carbon self-interstitial based on first-principles calculations and junction spectroscopy", to be presented at the International Conference on Defects in Semiconductors (Oslo, Norway, 2020); 3). J. Coutinho, "Performance of the Vienna Ab-initio Software Package (VASP) on the Oblivion Supercomputer", Public Report (2021).

Em números totais:

Bob:MACC	Cirrus B	Navigator:LCA-UC	Cirrus:INCD	Oblivion:HPC-UÉ	Stratus:INCD	Core.horas Totais
31 114 751	1 793 329	3 561 640	2 414 644	4 164 953	2 267 971	43 523 959

Tabela: Quantidade em Core.horas por plataforma para o CPCA 2020.

RELATÓRIOS FINAIS E OPINIÃO DOS UTILIZADORES

Relatórios finais preenchidos até 30 dias após término do projeto, no seguinte formulário simplificado: https://concursosfct.formstack.com/forms/cpca2020finalreport

Até **31/01/2022** foram entregues **114** relatórios finais, face a 129 projetos apoiados. Principais indicadores recolhidos:

Work plan and objectives (0-10) *	Platform performance (0-10) *	Operational center support (0-10) *	User satisfaction (0-10) *
7,4	7,8	9,0	8,0

*Média

Will DATA be publicly available and openly accessible?

Resposta	#	%
Yes	80	70%
No	34	30%

Did you prepare a Data Management Plan (DPM)

Resposta	#	%
Yes	18	16%
No	96	84%

Main DATA repositories: Github, Zenodo, others

Will the data produced with these resources be included in Journal ARTICLES, Reports or other Outputs?

Resposta	#	%
Yes	88	77%

No	26	23%

Do you plan to produce a Masters or PhD thesis linked with this project?

Resposta	#	%
Yes	64	56%
No	50	44%

Do you plan to apply for FUNDING with data generated under this project?

Resposta	#	%
Yes	45	39%
No	69	61%

Do you plan to register PATENTS associated with this project?

Resposta	#	%
Yes	3	3%
No	111	97%

Feedback on the Platform and Operational Center(s) (optional) - examples

- "The administrators at the INCD were very helpful and diligent in solving any issues with the calculations."
- "We would like to thank the support team, which was extremely helpful during the initial phase."(HPCUÉ)
- "Platform is super efficient; but too crowded for our needs."(MACC)
- "I am very satisfied with the Navigator Platform which has allowed me to run my simulations quickly and smoothly. I also appreciated the users workshop that was realized and which was very useful in instructing users about the the best practices on this platform. It has served me well in the past and I look forward to continuing to use it in the future."
- "The platform works fine, however the resources were limited during the time-frame of the project. For that reason we would like to use the core.hours we have requested, which were not yet spent completely, until the next couple of months. The operational center feedback is excellent."(MACC)
- "We were testing a large genetic dataset, and we realized that more resources would be necessary to obtain the final output files. However, this project was important to gain experience on the topic and test different solutions. The access to the platform was easy and fast. The support was good."(INCD)
- "Great Hardware and support." (HPC-UÉ)
- "The platform's configuration is intuitive and the available user wiki has been very helpful. Available resources allowed us to observe the performance of the code and resulted in high speed-ups compared to runs in our local system.The Operational Center's support was crucial for the setup and testing of the code.

Their feedback and insight have been much appreciated and contributed to more rigorous and complete work."(LCA-UC)

- "The platform worked well, but there were reductions to the available nodes/cores during the project."(INCD)

Feedback on the 1st Call on Advanced Computing Projects - CPCA (optional) - examples

- "This project was very beneficial to us. We learn a lot from it, and it will be a huge contribution to our research if we could keep using MACC, preferably with a large quota of CPU time."
- "Thanks for this initiative. It's a great support to fundamental science. Most of the fundamental science groups struggle with outdated equipment."
- "In the application form it was possible to chose the start date of the project. However, when the projects were aproved, this request start date was ignored and all projects had to start on the 1st of January."
- "We understand that the HPC resources are limited. Still, we were only granted 1/6 of the CPU time we applied for (50.000 CPU hours), which is very little and makes extensive production runs difficult to near impossible. It also does not justify very well the time"
- "The computer time granted was much less than needed to complete even a single task of the project. During the execution of the project several nodes of BOB were made unavailable, which impacted negatively the queueing time."
- "The resources made available from the CPCA project provided large speed-ups in the gathering and processing of results, which would not be possible under more localised systems."
- "The call was easy to understand and compile and I was fully satisfied with the management."
- "This first computational time call was very useful for the development of a substantial part of a project now funded by FCT. At a time when the acquisition of equipment is not easy to execute, having access to this type of infrastructure is paramount. The experience was so positive that I applied for the second call."
- "In general we believe it is essential to increase the HPC capacities in Portugal, in particular since the existing resources are in no relation to the high demand."

Would you apply again to a 2nd CPCA in 2021?

Resposta	#	%
Yes	101	**89%**
No	13	**11%**

PONTOS FORTES & PONTOS A MELHORAR DESTA 1ª EDIÇÃO

Aspetos positivos

- Suporte do Regulamento de projetos publicado em DR em setembro de 2020
- Procura superou oferta
- Baixo investimento com alto rendimento e muitos projetos
- Retorno resultados, dados, projetos, publicações em pouco tempo
- Disponibilidade *best-effort* das plataformas durante a avaliação técnica, início dos projetos e no seu decorrer
- Utilizadores relativamente satisfeitos com a capacidade já instalada e a possibilidade de acederem aos recursos em 4 plataformas e 3 modelos distintos
- 8-10 semanas desde fim da submissão até notificação dos candidatos
- Candidaturas decorreram sem sobressaltos
- Apenas 1 pedido AP, prontamente resolvido
- 31 instituições e 4 domínios científicos, revelando grande variedade
- Todos os 129 projetos assinaram TAs
- 95% beneficiários contataram COs nos primeiros 30 dias.
- Excelente suporte técnico por parte dos centros operacionais.
- Apesar de simples, as várias ferramentas de suporte foram suficientes (Formstack, Excel, Share, Email)

Aspetos a melhorar:

- Apenas 4 semanas com concurso aberto em agosto/setembro
- Divulgação podia ser melhorada
- Critérios demasiado simplificados e subjetivos, sem avaliação científica
- iniquidade de género – apenas 15% mulheres entre os candidatos
- Financiamento nem sempre garantido
- 6 meses revelaram-se curtos para projetos maiores; deveriam ter ciclos de 12 meses.
- Apesar do processo simplificado relativo a outros da FCT, ainda detêm alguma complexidade decorrente do cumprimento do CPA
- Alguns projetos A2 não justificaram o tempo computacional; e alguns sobre dimensionaram o seu pedido.
- Acessos A1 têm de ser simplificados, em regime contínuo de candidaturas
- Atrasos com limitações datacenter Bob e obras Navigator
- A melhorar formulário, integrando-o no myFCT

CONCLUSÕES FINAIS

A RNCA é uma rede colaborativa que se enquadra bem em iniciativas similares de outros estado-membros europeus, que tem reforçado e desenvolvido os seus centros e redes de computação avançada tais como, entre outros, a RES [37], em Espanha, a CINECA [38] na Itália, a GRNET [39] na Grécia, a CINES [40] em França ou a SLING [41] na Eslovénia. A listagem de membros do PRACE – *Partnership for Advanced Computing in Europe* [42] permite ter uma visão parcial do panorama europeu, mas que, ainda assim, identifica 26 participantes no PRACE, entre os quais Portugal, representado pela Universidade de Coimbra.

Considerando os custos elevados em disponibilizar recursos de computação avançada, bem como a complexidade inerente à sua utilização por parte dos utilizadores potenciais, como a comunidade de investigação, é essencial racionalizar a utilização dos recursos existentes. No caso português esse esforço consubstancia-se na RNCA que emergiu no setor da ciência e inovação. A RNCA é gerida e suportada pela FCT, sendo regulada pelos seguintes diplomas centrais:

- Regulamento n.º 1049/2020, Regulamento para a Rede Nacional de Computação Avançada e o Regulamento n.º 470/2021, requisitos mínimos para adesão à RNCA.
- Regulamento n.º 772-A/2020, Regulamento de Projetos de Computação Avançada.
- Despacho nº 4157/2019 que atualiza o Roteiro Nacional das Infraestruturas de Investigação de Interesse Estratégico (RNIE) com a RNCA.

Foram recebidas 133 candidaturas na 1ª edição do Concurso de Projetos de Computação Avançada que resultaram em 129 projetos de computação avançada, que correram numa das seguintes plataformas englobadas na RNCA – Rede Nacional de Computação avançada. Para as candidaturas recebidas, houve uma taxa de aprovação de 50,4% (n=67) para os projetos A1 e A2, valor que sobe para 97% (n=129) ao incluir os vouchers de experimentação atribuídos aos projetos abaixo da linha de corte (A0 e A00). As 4 propostas que não recebem qualquer apoio, não reúnem os requisitos mínimos para tal (preenchimento incompleto = 1; duplicação de formulário = 1; excede limite de candidaturas por PI ou co-PI = 2).

Sendo 05 plataformas distribuídas pelos 04 principais Centros Operacionais:

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37 https://www.res.es/en - Red Espanola de Supercomputacion
38 https://www.cineca.it/en
39 https://grnet.gr/en/services/computing-and-storage-services/hpc/
40 https://www.cines.fr/?lang=en
41 http://www.sling.si/sling/en/
42 https://prace-ri.eu/about/members/

Centro Operacional	Plataforma
Minho Advanced Computing Center	Bob
Laboratório de Computação Avançada da U. Coimbra	Navigator
High Performance Computing da U. Évora	Oblivion
INCD - Infraestrutura Nacional de Computação Distribuída	Cirrus-A
	Stratus

As candidaturas ao presente Concurso tiveram a seguinte distribuição por áreas científicas:

Domínio científico	Exact Sciences and Engineering	Life and Health Sciences	Natural and Environmental Sciences	Social Sciences and the Humanities	Total
A1	30	1	7	1	39
A1+A2 e A2	66	16	10	2	94
Total	96	17	17	3	133

(os acessos A1 e A2 são do tipo "Experimental", de menor dimensão computacional, ou "Projeto" com maior dimensão computacional)

Instituições distintas que se candidataram a recursos: 31

Género: 19 candidaturas de mulheres

A alocação de projetos computacionais por plataforma e centro operacional encontra-se resumida na tabela seguinte:

	BOB:MACC	NAVIGATOR:LCA-UC	OBLIVION:HPC-UE	CIRRUS-A:INCD	STRATUS:INCD	TOTAL
# CPU core.horas	20 037 180	4 636 368	4 177 600	4 116 856	1 835 880	34 803 884
# Projetos A1 e A2	25	9	10	15	8	67
# Vouchers A0/A00	30	8	7	14	3	62
TOTAL	55	17	17	29	11	129

Foram solicitados 2,3x mais recursos do que os disponíveis, ou seja, a procura foi superior à oferta. O valor estimado dos recursos atribuídos foi de 428.087,77€

A realização da 1ª edição de Concurso de Projetos de Computação Avançada registou uma procura muito elevada, que veio comprovar que a computação avançada é um instrumento muito relevante para as atividades científicas nacionais, pelo que a FCT abriu novo concurso a 19 de julho de 2021 que continua a decorrer. Em 2022 as

plataformas de computação avançada da RNCA terão um aumento de capacidade substancial com a instalação em Portugal do supercomputador Deucalion, que foi adquirido pelo organismo europeu EuroHPC JU, em resultado de um projeto conjunto entre Portugal e Espanha, em linha com a estratégia para a computação avançada disponível em https://www.incode2030.gov.pt/computacao-avancada

ANEXO I – DETALHE A2-ACESSO PROJETO

Bob

CPCA_A2_2568_2020

FLOW DYNAMICS IN STORAGE TANKS

Investigador Responsável: Nuno Miguel da Conceição Martins

Instituição: IST-UL

Recursos: 1 000 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Drinking water storage tanks are essential components of the network supply system, either to balance the pressure on the network or to guarantee emergency reserves in case of a fire. The storage tanks are operated to meet the daily demands of the distribution network. However, storage tanks are frequently pointed out as spots of quality degradation, mainly related to the design of the storage tanks that do not take into account the needed mixing and water renewal. The storage tanks design generates "dead zones", and these are responsible for the poor mixing and an extended Residence Time Distribution (RTD). An extended Residence Time Distribution combined with

differential temperatures between the incoming water (inflow) and the stored water result in thermal stratification, causing zonal of chlorine decay, biofilm development, sediment build-up. It exacerbated the formation of potentially carcinogenic toxic disinfection by-products, leading to an increase of consumption of chlorine. For these reasons, there is an urgent need to understand the hydrodynamics in tanks, regarding the design/geometry, configuration and operational conditions in order to improve mixing conditions.

CPCA_A2_2613_2020

CO_2 CAPTURE AND STORAGE USING NATURALLY OCCURRING H_2O ICES

Investigador Responsável: Fernando Jorge Araújo Lino da Cruz

Instituição: FCT-UNL

Recursos: 420 480 CPU core.hours

HPC V HTC x Cloud x GPU x

It is well known that CO2 concentration in the atmosphere has surged from 280 ppm (pre-industrial level) to 387 ppm today, raising major concerns regarding the corresponding greenhouse effect; such a climate crisis requires atmospheric carbon dioxide levels to be reduced. One idea currently under consideration to address this problem is the replacement of CH4 in natural clathrate hydrates (CHs, H2O ice polymorphs) with CO2, in order to simultaneously combine clean energy production with CO2 sequestration and storage. In order to access future industrial viability and ecological impact, the p and T equilibrium conditions of CH4/CO2/H2O mixtures (vapour, liquid, solid) need to be studied regarding the corresponding thermodynamical landscapes, at temperatures well bellow ice formation; experimental techniques are expensive and time consuming, owing to the cryogenic nature of CHs and slow kinetics of the sequestration/release mechanism (~2000 USD & 1 week/data point).

To address the aforementioned "big questions", we devise a molecular level and self-consistent methodology employing paralell computer calculations, spanning broad temperature and pressure ranges, T >100 K and p < 1000 bar. Samples of the 2 most common CHs polymorphs are employed, sI and sII, as well as several different guests with distinct sizes and chemical nature (CO2, CH4, C2H6, C2H4, electrolytes) to access the phase equilibria of naturally occurring and industrially relevant hydrates.

CPCA_A2_2640_2020

TRANSCRIPTOMICS-BASED PREDICTION OF HUMAN PHENOTYPES USING SCALABLE AND SECURE MACHINE LEARNING APPROACHES

Investigador Responsável: Pedro G Ferreira

Instituição: FCUP

Recursos: 48 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Unlike high-throughput genome sequencing, considered an invaluable tool for molecular characterization and clinical diagnosis, transcriptome sequencing remains largely unexplored as a clinical tool in spite of its potential. Therefore, we aim to develop predictive methods for medical, physiological, and other human phenotypes based on gene expression profiles. Machine learning methodologies will be applied to develop models based on the analysis of RNA-seq data obtained across dozens of tissues and organs, hundreds of individuals, and thousands of samples. The potential use of surrogate tissues for deducing information from less accessible tissues will be investigated. The use of complementary omics data, including DNA-seq and histopathological images, will be addressed, and results validated against external datasets. With this project, we aim to better understand the mechanisms behind phenotype prediction to develop individualized decision-making models. These models would complement those already in practice, resulting in less false positives and better health outcomes.

CPCA_A2_3840_2020

BLACK HOLES AND BOSONIC FIELDS

Investigador Responsável: Miguel Zilhão

Instituição: IST-UL

Recursos: 300 000 CPU core.hours

HPC V HTC x Cloud x GPU x

This project takes place in the context of the long-term research that our team has been developing concerning studying the dynamics and interaction between bosonic fields and black hole binaries. Driven by the direct gravitational wave detections of LIGO and Virgo, the next decade will see an unprecedented exploration of the strong-field regime of general relativity, both with electromagnetic telescopes such as Event Horizon and with advanced gravitational wave detectors such as LISA. Such studies have applications even beyond astrophysics. For instance, a very elegant connection with particle physics comes about through fundamental fields--essential for

cosmological models used to model dark matter--which can form mini-halos around supermassive black holes.An open question is how such fields will behave in the vicinity of black hole binaries. The long-term development of massive fields in these geometries is unknown, with potential very interesting effects in particular when the mass of the field resonates with the angular velocity of the binary. This is something we now have the tools to explore, and will use the provided computational time to perform extensive explorations of these systems.

CPCA_A2_4403_2020

SATRAP: Rational design of Self-Assembling networks for TRansparent electrode Applications

Investigador Responsável: Sergey Pyrlin

Instituição: UM

Recursos: 332 800 CPU core.hours

HPC V HTC x Cloud x GPU x

Quest for better transparent electrode materials for flexible opto-electronic (OE) devices is one of the most pursued goals in materials science. In this project, we propose to avoid the high costs of conventional fabrication by exploiting the phenomenon of self-assembly of neuron-like molecular networks to align very small amounts of carbon nanotubes into highly transparent conductive films. This will enable cost-effective, printable solar or OLED panels, which can be mass-produced on "roll-to-roll" basis. To achieve this we will investigate the effect of chemical structure of self-assembling molecules on the morphology of the self-assembled network. This will allow us to optimize transparency and conductivity of deposited films as well as their performance as electrodes of an OE device by modifying the self-assembling block molecular structure. The in silico part of this project implies using a combination of molecular dynamics and Monte Calro simulations to study the relations between molecular structure, dynamics of self-assembled fibers and sparsity and connectedness of the deposited network. Simulations will be verified by experimental fabrication and characterization of self-assembled films. On a later stage these data will be used for machine learning the relation between structure graph of already known molecules and the parameters of the self-assembled networks, enabling solutiom of inverse problem: tailoring molecular structure for optimal electrode morphology.

CPCA_A2_4513_2020

NANOSCALE MATERIAL DESIGN FOR ADVANCED CUTTING TOOLS

Investigador Responsável: Luis Silvino Alves Marques

Instituição: UM

Recursos: 1 000 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Increasing requirements on high speed and dry cutting applications open up new demands on the quality of cutting tool materials. This is particularly important in the aerospace and automotive industries where easy and premature degradation of the cutting tools is observed during the machining of hard-to-difficult materials. Workpiece materials and coating materials for machining tools often show complex structures and chemical compositions, exhibiting many different diffusion and deformation mechanisms, requiring extensive Finite element (FEM) simulation studies. The fundamental material parameters for these simulations are embedded in constitutive models, which can be obtained either experimentally or using molecular dynamics (MD) /density functional theory(DFT) calculations.The modelling component of the proposed project will serve three major purposes:

-The evaluation of the diffusion and deformation mechanism(s) in self-lubricating coatings (TiSiN:Ag) using MD simulations.

- Development of macroscopic material constitutive models to be used in finite element simulation of cutting process.

- FEM simulations to optimize the size, geometry as well as to predict the right machining parameters to improve the performance of the cutting tools for hard-to-machine materials.

This project results from a collaboration between university of Texas - Austin and Minho and Coimbra Universities.

CPCA_A2_5804_2020

3D SIMULATIONS OF NETMIX FOR CARBON CAPTURE, CHEMICAL REACTION, AND COMBUSTION

Investigador Responsável: José Carlos Lopes

Instituição: coLAB Net4CO2

Recursos: 1 024 000 CPU core.hours

HPC V HTC x Cloud x GPU x

The objective of this 36-month project is to perform 3D structural and fluid dynamics simulations for the research and design of chemical reactors, based on the NETmix technology, for the carbon dioxide capture and re-use in a

carbon dioxide circular economy. The project is divided in 3 work packages and this is the first time RNCA Resources are being requested. WP1 is focused on the 3D dimensionalization of current planar reactors for carbon dioxide capture via hydrate formation. Carbon re-utilization processes involve the catalytic reaction steps and thus, WP2 consists in the modelling of the hydrodynamics of NETmix reactor with a catalytic chemical reaction, where either the catalyst is present on the solid surface of reactor walls or it is transported with a fluid carrier within the reactor. In WP3 the occurrence of combustion and reforming reactions in parallel NETmix reactor plates will be considered, with the goal of improving the energy efficiency of the reforming steps. The work requires 3D computational fluid dynamics simulations (CFD), with chemical reaction and multiple phase flows, which require a strong computational power. The work will be presented at national and international conferences and scientific publications are also expected, according to the CoLAB NET4CO2 dissemination plan.

CPCA_A2_6052_2020

DEEP LEARNING FOR PARTICLE-LADEN VISCOELASTIC FLOW MODELLING

Investigador Responsável: Célio Bruno Pinto Fernandes

Instituição: UM

Recursos: 1 638 120 CPU core.hours

HPC V HTC x Cloud x GPU x

Many industrial operations involve the processing of particle-laden viscoelastic fluids (PLVF), in which the continuous or matrix phase possesses a viscoelastic character. Simulating the dynamical response of these systems is a current challenge of computational rheology (CR).This project aims at exploring the possibility of using Deep Learning (DL) techniques to disentangle the complex non-linear interactions, and develop expressions to evaluate the drag coefficient of particles translating in non-linear viscoelastic fluids. At the first step, the results obtained from DNS for different values of parameters are collected. This step is computationally expensive and should be done using high-performance computing (HPC) facilities. For that purpose, the access level proposed for the work is the A2-Project Access. Then, these results will be used to train a deep neural network to classify the calculated sequence data. Finally, the results obtained will be incorporated in a 3D Eulerian-Lagrangian viscoelastic code. This project is directly connected to a main FCT project (MIT-EXPL/TDI/0038/2019), under which the envisaged tools should be employed to support the HPC activities. Concluding, this project presents a key step towards modeling the flow of PLVF, and due to the open nature of the tools to be employed will surely contribute to a more complete

understanding of many advanced manufacturing and industrial operations, and their general dissemination and exploitation.

CPCA_A2_6202_2020

EXPLOITATION OF OPEN-SOURCE COMPUTATIONAL FLUID DYNAMICS IN HPC SYSTEMS

Investigador Responsável: João Miguel de Amorim Novais da Costa Nóbrega

Instituição: UM

Recursos: 1 095 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Computational Fluid Dynamics maturely used in engineering design and analysis across several industry sectors is ubiquitous. The algorithmic technology-base is known, well established and universally applied. Continued widespread exploitations, in the next decade and beyond, are hampered by performance scaling bottlenecks on massively parallel HPC systems, rendering this technology as not fully fit to take best advantage of recent major developments. The computational library OpenFOAM is one of the most successful open-source projects in the area of computational modelling, and has a large user base across most areas of engineering and science, from both commercial and academic organizations. As a technology, OpenFOAM provides an extensive range of features to solve anything from complex fluid flows to solid dynamics, among several others. Additionally, the OpenFOAM technology offers complete freedom to customize and extend its functionalities. This project, which is integrated in the European Project exaFOAM (H2020-JTI-EuroHPC-2019-1/956416), main aim is to contribute to enable the OpenFOAM Community to exploit efficiently and fully the current and evolving HPC systems.The University of Minho (UMinho) contributions in exaFOAM, are related to development and improvement of algorithms for rheologically complex fluids. UMinho is also the leader of the Work Package (WP) "Dissemination, Impact and Exploitation".

CPCA_A2_6231_2020

GREENSHOES - VIRTUAL PROTOTYPING, ARTIFICIAL INTELLIGENCE AND ADDITIVE MANUFACTURING IN THE FOOTWEAR INDUSTRY

Investigador Responsável: João Miguel de Amorim Novais da Costa Nóbrega

Instituição: UM

Recursos: 372 300 CPU core.hours

HPC V HTC x Cloud x GPU x

The industrial footwear sector in Portugal has managed to remain in a prominent position in the international markets, essentially due to the knowledge acquired over the many years of experience and a substantial creativity. However, the worldwide competitiveness of the sector has been increasing significantly. In fact, the increasingly demands of a market regarding individualized products, have promoted the incorporation of innovative manufacturing techniques, as is the case of additive methods. As happens in several fields the possibility of resorting to appropriate computational modelling tools, may help to optimize production processes and products and the introduction of new processes. This project is related to the mobilizer project GreenShoes 4.0- "Footwear, leather goods and Advanced Materials, Equipment and Software Technologies". The Greenshoes 4.0 project joins 23 entities, including 15 companies from the Portuguese Footwear industry and aims at contributing to their digital transformation. The work to be done comprises the application of previously developed codes to support the design of current manufacturing processes and products, and the implementation, verification and test of new codes to model novel manufacturing processes. In some of the cases under study the simulation codes will be coupled with Artificial Intelligence (AI) algorithms to implement automatic optimization procedures of both process and products.

CPCA_A2_6816_2020

MULTI-GLUON VERTICES IN LATTICE QCD

Investigador Responsável: Paulo de Jesus Henriques da Silva

Instituição: UC

Recursos: 2 978 400 CPU core.hours

HPC V HTC x Cloud x GPU x

Lattice QCD is one of the most successful approaches to understand QCD, the theory of quarks and gluons. The study of the low energy regime of this quantum field theory requires non-perturbative methods, like the formulation of QCD in a space-time lattice. Indeed, a space-time lattice provides a natural regulator of the theory. Together with the imaginary time formalism, it allows for a first principles numerical simulation of QCD. Lattice QCD research requires the use of HPC resources. This Advanced Computing Project aims to improve our previous study of the three-gluon vertex and perform a first lattice study of the four-gluon vertex in Landau gauge. These correlation functions can improve our description of the forces in multiple particle states (e.g. glueballs, tetraquarks). Furthermore, from these vertices one can compute the running coupling constant. The investigation of higher order

correlation functions in lattice QCD, due to the large fluctuations, demands ensembles with a very large number of gauge configurations and the development of methods that improve the signal to noise ratio for the vertices.

CPCA_A2_7081_2020

MOLECULAR DYNAMICS OF CRYSTALLIZATION OF HONEY-LIKE SYSTEMS

Investigador Responsável: Paulo E. Abreu

Instituição: UC

Recursos: 96 000 CPU core.hours

HPC V HTC x Cloud x GPU x

The first part of this task will be focused on defining models than can describe honey crystallization by MD simulation. Several models containing varying proportions of water and sugars present in honey (glucose, fructose and sucrose are the sugars in largest quantity and will be the focus of this project) will be prepared and the topology generated for use with the GROMACS program. Classic MD trajectories will be used to verify if the system crystallizes under several temperatures by running long simulations (more than 500 ns).

CPCA_A2_7083_2020

MICROSOLVATION OF IONS IN ATOMIC AND MOLECULAR SOLVENTS

Investigador Responsável: Jorge Manuel Campos Marques

Instituição: UC

Recursos: 192 000 CPU core.hours

HPC V HTC x Cloud x GPU x

In this computing project, we are using the microsolvation approach to study the solvation phenomena at the molecular level. Such approach consists on the stepwise addition of solvent species to the ion. The clusters so formed are then studied by computational means according to the following steps: (i) modeling the interaction potential of the cluster by fitting a set of ab initio energies to an empirical function; (ii) application of global optimization algorithms to obtain low-energy structures of the clusters; (iii) re-optimization of the low-energy structures at a high level of theory to get more reliable insights about the energy landscapes of the clusters; (iv) calculation of thermodynamic properties of phase transitions of the clusters by applying Monte Carlo techniques; (v) study

transitions among the most relevant low-energy structures by employing molecular dynamics simulations. The methodology will be used to study the microsolvation of alkali-metal ions with different solvents. First studies will use atomic solvents such as rare-gases, while small solvent molecules (e.g., O2, N2 or CO2) will be employed in a second stage.

CPCA_A2_7085_2020

DYNAMICAL LATTICE QCD SIMULATIONS AT FINITE TEMPERATURE

Investigador Responsável: Orlando Olavo Aragão Aleixo e Neves de Oliveira

Instituição: UC

Recursos: 2 995 200 CPU core.hours

HPC V HTC x Cloud x GPU x

Lattice QCD is one of the most successful approaches to understand QCD, the theory of quarks and gluons. The study of the low energy regime of this quantum field theory requires non-perturbative methods, like the formulation of QCD in a space-time lattice. Indeed, a space-time lattice provides a natural regulator of the theory. Together with the imaginary time formalism, it allows for a first principles numerical simulation of QCD. Lattice QCD research requires the use of HPC resources. This Advanced Computing Project focus on the computation of the gluon, the ghost and the quark propagators in the Landau gauge and at finite temperature, including the effect of dynamical fermions via the use of Clover fermions. The first step towards this goal is to generate several dynamical configuration ensembles, at different temperatures below and above the deconfinement transition, using the Hybrid Monte Carlo method.

CPCA_A2_7087_2020

NATURAL LAYERED PEROVSKITE OXIDE ENGINEERING FOR GREEN TECHNOLOGIES

Investigador Responsável: João Pedro Esteves de Araújo

Instituição: UP

Recursos: 2 064 000 CPU core.hours

HPC V HTC x Cloud x GPU x

An important challenge of this century, within the goals of the 2030 Agenda for Sustainable Development, is to search for new materials allowing the development of novel sources for sustainable energy harvesting. In fact, lead-free photovoltaics (PV) and photoelectrochemical (PEC) cells, applied for water splitting and Hydrogen production, comply with these aforementioned challenges. Perovskite oxides (PVO), such as those with ABO3 stoichiometry (A=alkaline or rare-earth metals; B=transition metals) are an important class of functional materials, due to their structural and compositional flexibility, providing a direct impact to the proposed technologies. However, to enhance the capabilities of such systems it is necessary to guide and tune the design for achieving maximum efficiencies. For example, through substitutional doping with cations that present different oxidation states and differ in ionic radii, lattice distortions may occur enabling structural phase transitions. These variations cause a direct impact to the crystal-field splitting of the PVO, thus altering the opto-electronic properties of the system. Band gap engineering in PVO systems may allow for the tuning of the photogenerated charge carriers through variation of the absorption coefficients and electron-hole diffusion lengths. This project aims the search for promising perovskite systems, which evidence efficient optical and electronic properties for applications to environment-friendly PEC and PV devices.

CPCA_A2_7181_2020

IN SILICO OPTIMIZATION OF BRAIN IMAGING PROBES WITH ENHANCED PERMEATION

Investigador Responsável: Luís Miguel Santos Loura

Instituição: UC

Recursos: 2 943 360 CPU core.hours

HPC V HTC x Cloud x GPU x

Technological advances in imaging have led to tremendous progress in medical sciences in the last few decades. Among these techniques, Magnetic Resonance Imaging (MRI) stands out as a versatile technique with outstanding spatial resolution and that does not involve the use of X-rays or ionizing radiation. However, clinical utilization of MRI often requires the use of contrast agents. Among these, paramagnetic gadolinium(III) chelates such as gadoteric acid (GdDOTA, Dotarem) are widely used. Because of their hydrophilicity, these complexes do not cross the blood-brain barrier, unless the latter is compromised. They are therefore useful in the detection of brain tumors, but cannot be used in diagnosis of neurodegenerative diseases such as Alzheimer's and Parkinson's. We believe that one of the main reasons for this failure is that intermediate evaluations in model studies, which would allow a more quantitative characterization - e.g., in terms of energy barriers or permeation rates - have not been carried out. Our

project will solve this problem by starting at the most fundamental level: molecular simulation at the atomic or quasi-atomic scales. In silico methodologies based on molecular dynamics simulations will be carried out to calculate permeability coefficients, which will allow a first rank of possible GdL candidates (L denotes a DOTA-based ligand, with structural modifications aiming at enhancing membrane permeation), for subsequent synthesis and experimental testing.

CPCA_A2_7269_2020

HIGH-PERFORMANCE COMPUTATIONAL DESIGN OF BIOCOMPATIBLE CELL SCAFFOLDS FOR TISSUE ENGINEERING

Investigador Responsável: Cristóvão de Sousa Dias

Instituição: FCUL

Recursos: 256 000 CPU core.hours

HPC V HTC x Cloud x GPU x

The ultimate goal of tissue engineering is to grow human tissues in a controlled manner. A critical step is to produce 3D matrices (scaffolds) that support and guide the growth of the tissue. From 3D printing to fiber bonding, impressive techniques have been developed to assemble the scaffolds. However, all require implanting the final scaffold in vivo, through surgery, which may lead to several complications. Alternatively, a group performing experiments at University of Aveiro devised a protocol to obtain the scaffolds directly in vivo from the self-organization of colloidal particles. The scaffolds should be mechanically stable, low-density structures to yield a large surface/volume ratio for the tissue growth, with the porosity required to deliver nutrients to the bulk. This is in principle possible to design with the optimal combination of experimental conditions (e.g. surface chemistry of the colloidal particles, concentration, selectivity). However, exploring the parameter space experimentally is time consuming and inefficient. To tackle this challenge, we have been collaborating with the experimental group to develop a numerical model. The model has been successfully parameterized and validated using our in-house computer cluster. But, to access the relevant time and length scales, we need larger and longer simulations, which are not accessible with our cluster. This project aims at accessing these resources.

Navigator

CPCA_A2_2524_2020

NEW GRAPHENE MATERIALS FOR ELECTRONICS

Investigador Responsável: Manuel Mello-Franco

Instituição: UA

Recursos: 400 000 CPU core.hours

HPC V HTC x Cloud x GPU x

The discovery of graphene has opened up new exciting possibilities for the so-called 2D materials. Remarkably, graphene displays a high electron and hole mobility at room temperature due to its extended conjugation, with reported values in excess of 15,000 cm^2/V/s on SiO2. Additionally, it possesses a unique set of properties, such as transparency, lightweight and flexibility. However, graphene is a zero-gap semiconductor, which constitutes a hurdle in its implementation into electronic devices. This project aims to computationally study and design bottom-up graphene-based materials with suitable properties for new electronics devices. We will explore different novel and prospective graphene materials and molecules reachable by organic chemistry, namely graphene nanoribbons, flakes and related molecules as well as Covalent Organic Frameworks (COFs). The innovative part of this project lies in the combination of solid-state physics, computational chemistry and high-performance computing to compute, with high accuracy and thus predictively, the structure and electronic properties of several carbon-based molecular materials. For this, we will follow an ad-hoc multiscale approach based on a battery of technologies ranging from molecular mechanics and dynamics models to tight-binding, density functional theory and multideterminant ab-initio calculations.

CPCA_A2_6046_2020

HIGH PERFORMANCE COMPUTING OF WIND FLOWS OVER FORESTED MOUNTAINS

Investigador Responsável: José Manuel Laginha Mestre da Palma

Instituição: FEUP

Recursos: 200 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Wind flow in the Perdigão region is characterised by a strong daily cycle, and highly unsteady complex interaction of flow separation, forest canopy drag and thermal stratification [1]. Our objective is to model this flow during 24h starting at 18h of the 14th of May 2017.The software employed for the purpose is VENTOS/M [2,3], an atmospheric flow simulation code featuring the appropriate physics modelling capabilities, but that requires considerable computational resources and input data to reproduce flow behaviour adequately. Comparatively to existing model results [4], increased temporal and spatial resolution and the addition of surface cover will reveal more intricate flow phenomena near the ground. The simulation results should provide insights into multiple areas of interest associated with projects LIKE and WindscannerPT, such as wind energy, micro-meteorology, mountain flows and forest fires. Access to larger HPC cluster should also provide the chance to test the software's performance with larger thread count and various node/core configurations.The higher targeted simulation complexity will lead to additional demand in computational resources. After optimizing configurations for speed or efficiency, a more powerful system (compared to UPORTO's) will allow both to reduce the turnaround time and release our resources for less demanding tasks.

CPCA_A2_6817_2020

EPITAXIAL GROWTH OF MULTIMETALLIC MXENES VIA NITROGEN DISSOCIATION

Investigador Responsável: José Daniel Lago da Silva Neves Gouveia

Instituição: UA

Recursos: 420 480 CPU core.hours

HPC V HTC x Cloud x GPU x

The discovery of two-dimensional transition metal carbide and nitride surfaces (MXenes) has generated great interest due to their promising applications in catalysis, including electrocatalysis, photocatalysis, and heterogeneous catalysis. MXenes are composed of alternating layers of M and X elements, where M is a transition metal element, and X can be carbon, nitrogen, or both. The number of atomic layers is usually 3, 5 or 7, the thinnest

ones having the general formula M2X. MXenes can be bimetallic, i.e., comprise two distinct metallic elements: one occupying the two outer M layers and the other one occupying the remaining M layers. Our recent computational studies have shown that bare M2X (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W) surfaces strongly activate N2, some reducing its dissociation energy barrier by over 90%, a remarkable feature among catalysts of this reaction. This suggests that, in a nitrogen-rich atmosphere, one may be able to completely cover an MXene surface by a layer of nitrogen, resulting in an M2XN2 material. In turn, a layer of metallic atoms, of either the same M element or a different M' one, could be deposited on top of the outer nitrogen layer, finally yielding a surface with formula M'2M2XN2, a bimetallic MXene, via epitaxial growth. In this project, we aim employ computational methods based on density-functional theory to predict the thermodynamic and kinetic feasibility of this process.

CPCA_A2_6972_2020

EXPANDING THE DRUGGABLE TARGET SPACE

Investigador Responsável: Rita Alexandra do Nascimento Cardoso Guedes

Instituição: UL

Recursos: 4320 CPU core.horas + 4620 GPU horas

HPC V HTC x Cloud x GPU V

Despite the large chemical space enumerated to date, there are no known modulators for half of the human proteome associated with diseases. This project envisions the exploration of currently neglected protein targets of the human proteome. Using bioinformatics, cheminformatics, and computational chemistry (Molecular Docking and Molecular Dynamics simulations) we will focus our analysis on targets for which there are no tested (reported) compounds. This will address the large portion of the human proteome which is potentially druggable but currently neglected. We will carry out a series of feasibility filters to select a new target among the understudied targets and then submit it to different computational studies to establish its ability to interact with a diverse set of compounds. Among these studies, molecular dynamics produces highly informative data at the expense of also high computational cost. As a result we would greatly benefit from additional GPU+CPU computation time to ensure that the selected protein target is tested against a sufficiently large compound set, and therefore yield meaningful results. The outcome of this project will be an essential starting point for the follow-up experimental testing of this target with a select set of compounds. In addition, we believe this project will serve as a proof of concept for a methodology to explore new targets, which can be adopted by the community mitigate the large number of neglected proteins targets.

CPCA_A2_7219_2020

DISSECTING DOPAMINE RECEPTOR 2 FUNCTIONAL MECHANISM

Investigador Responsável: Irina Sousa Moreira

Instituição: CNC-UC

Recursos: 2 999 808 CPU core.hours

HPC V HTC x Cloud x GPU x

G protein-coupled receptors (GPCRs) are a superfamily of membrane proteins that have key roles in the transduction of extracellular signals as sensory stimuli, hormones, neurotransmitters or paracrine factors into the intracellular environment through the activation of one or more heterotrimeric guanine nucleotide binding proteins (G-proteins) or Arrestins (Arr-s). In particular, our project aims to understand a specific GPCR, the dopamine receptor 2, as the wide spectrum of three-dimensional oligomers and signalling pathways available for this receptor provide many possibilities for selectivity of the functional response. To address how GPCR signalling is modulated by "functional selectivity", we first need to pinpoint and explore at the atomic-level how D2R interacts with its two signalling partners: G-proteins and Arr-s, by exploring the dynamic properties of the complex systems in their natural environment. The members of the team have worked on GPCRs, dimers, and G-protein interactions on large computing clusters, and are eager and well prepared to continue the work on such a captivating biological question in a HPC setting.

CPCA_A2_7261_2020

TWO-TEMPERATURE MODEL - MOLECULAR DYNAMCIS SIMULATIONS OF QUANTUM WELLS UNDER STRONGLY IONISING IRRADIATION

Investigador Responsável: Katharina Lorenz

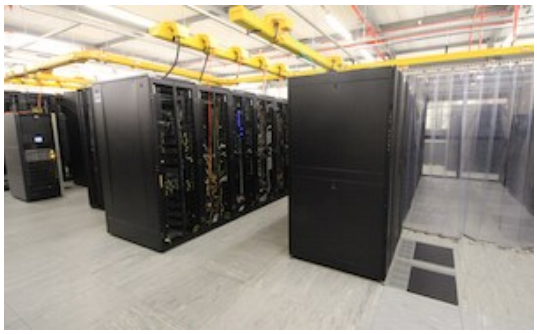
Instituição: IST-UL

Recursos: 140 400 CPU core.hours

HPC V HTC x Cloud x GPU x

The necessity of robust electronics working in extreme environments is driving the research on alternatives to the ubiquitous silicon-based devices. Group-III-nitride wide bandgap semiconductors are considered for the next generation of space electronics due to their remarkable thermal and chemical stability as well as radiation

resistance. However, their response to strongly ionising radiation such as highly energetic heavy ions (in the following called swift heavy ions - SHI) is still poorly understood. These SHI make part of the intense radiation field in space and can cause considerable damage to electronic devices due to their high ionisation power and long-range. In a running project, NASIB, we are investigating the effect of SHI on III-nitride semiconductors combining experimental and computational techniques. In particular, a simulation scheme combining the thermodynamic Two-Temperature-Model with Molecular Dynamics simulations (TTM-MD) was shown to successfully predict radiation damage in GaN. In order to run MD cells of actual device structures and using more realistic cell sizes, more computation power is needed. Therefore, in this project, we propose to apply the developed modelling scheme to typical heterostructures used in III-N light-emitting diodes (LED) and lasers containing several InGaN quantum wells. The effects of SHI irradiation on the InGaN/GaN crystal and interfaces will be studied in detail and MD simulations will be compared to ongoing experiment.



Cirrus-A & Stratus

CPCA_A2_4075_2020

GETTING READY FOR THE UNEXPECTED: SEARCHING FOR NEW PHYSICS PHENOMENA AT THE CERN LARGE HADRON COLLIDER

Investigador Responsável: Nuno Filipe da Silva Fernandes de Castro

Instituição: UM

Recursos: 150 000 CPU core.horas + 4380 GPU horas

HPC V HTC x Cloud x GPU V

High Energy Physics generates extraordinary amounts of complex data and its full exploitation requires equally complex analysis techniques. The goal of the current proposal is the development of advanced techniques in machine learning to be used to analyse the data collected by the experiments of the Large Hadron Collider (LHC) and by detectors searching for dark matter interactions. For this purpose, extensive simulated samples, describing both the already known Standard Model processes, as well as new physics processes, will have to be generated and simulated using Monte Carlo methods. Given the high luminosity expected at the next phase of the LHC, hundred of millions of collision events will have to be simulated in order to have a representative sample of the data to be collected. Such simulations, which require significant CPU time (of the order of hundred thousand hours) and disk space (or the order of 10 Tb) to be obtained, will be used to train supervised and semi-supervised machine learning methods. These methods, relying on complex deep neural networks, will contribute to advance of the exploration of the LHC data, where Portugal has a strong presence. In particular, this will contribute to improve the generality of the searches for new phenomena, ensuring that an eventual discovery is not missed simply because the details of searches processes are not known.

CPCA_A2_4568_2020

ENZYMATIC SYNTHESIS OF BIOPOLYMERIC CONJUGATES FOR ADVANCED AND TARGETED THERAPIES

Investigador Responsável: Alexandra Teresa Pires Carvalho

Instituição: UC

Recursos: 47 616 CPU core.hours

HPC V HTC V Cloud x GPU x

The extension of life expectancy is increasing the need for new treatments. Despite intensive efforts, the number of effective treatments is still low. However, directed therapeutics may prove to be a potential tool to overcome the drawbacks of current strategies. We aim at developing delivery systems of biodegradable amphiphilic polymer-drugs (PDC) and RNA-peptide conjugates as potential therapeutics for cancer and COVID-19. We will test the enzymatic esterification of anticancer drugs with amphiphilic polyesters using their hydroxyl and carboxylic acid groups, expanding the scope of bioresorbable PDCs for selective and controlled delivery systems. We also aim at designing bioconjugates that interact with nucleic acids, acting as delivery and therapeutic agents, binding more effectively to their targets. The enzymatic synthesis will be assessed by testing lipase CalB, as well as other hydrolases and transpeptidases, such as SortA. Compared with conventional chemical routes, enzymatic catalysis represent a greener approach as they act at mild temperatures and conditions, do not require the use of toxic reagents and give

a more precise construction of well-defined structures. We will perform QM/MM MD simulations to access the reaction free energy barriers, enabling us to subject the studied enzymes to rational design for properties enhancement. The increase of complexity of the Quantum Mechanical models will increase the computing power required to achieve our aims.

CPCA_A2_4595_2020

ROLE OF METAL IONS IN DNA RECOGNITION BY PROTEINS

Investigador Responsável: Alexandra Teresa Pires Carvalho

Instituição: UC

Recursos: 64000 CPU core.horas + 4000 GPU horas

HPC V HTC V Cloud x GPU V

In this project, which is a follow-up of past and ongoing projects within our work group, we will study bacterial Transcription Factors (TFs) belonging to the GntR superfamily and develop new programmable TFs. Understanding the allosteric mechanism of TFs is essential for several medical and biochemical applications, given the importance of TFs in the regulation of the natural cell circuits and for the development of new ones. We will use computational chemistry as our main tool. To clarify: the role of Zn2+ ion binding to the effector domain, the mechanism of allosteric regulation in GntR repressors and activators that employ Zn2+ ion, and the conformational changes that affect DNA binding. After a detailed study of these specific TFs, it will be possible to characterize more accurately the metal-binding subfamily of GntR TFs and understand how the substrate specificity can be changed to design new synthetic programmable TFs through computational and experimental methods. Another important aspect that will be studied is the role of metal ions in the conformational changes that allow the DNA cleavage by different endonucleases. Our computational approaches include ion motif parameterization, Molecular Dynamic and Quantum Mechanic/Molecular Mechanic simulations. To complete our project, it is necessary to use a range of highly complex computational approaches with different needs. The software performance used is highly dependent on a constant high computational power.

CPCA_A2_5043_2020

AB INITIO COMPUTATIONAL DESIGN OF A PLASMONIC SPINTRONIC MATERIAL

Investigador Responsável: Jaime Pedro Oliveira da Silva

Instituição: UC

Recursos: 46 080 CPU core.hours

HPC V HTC x Cloud x GPU x

The field of spintronics is one of the most promising subfields of condensed matter physics for the development of the next generation of electronic devices. In fact, the onset of spintronics started with the observation of the giant magnetoresistive effect (GME) in the 80's. In the GME the resistance of the material, alternate ferromagnetic and nonmagnetic layers, is lowest when the magnetic moments are aligned and highest when they are anti-aligned. The main advantage of spintronics devices is their reduced power consumption and their operational frequency, which should be higher than that of conventional devices due to the fact that they are not limited by the velocity of the electric charge . Even if this would not apply, as there are two spin currents as found in the pioneering work of Mott, spintronics would allow more information to be transmitted in the same time interval.Plasmonic spintronics is a promising and emerging field that integrates plasmons into spintronics. Plasmonic spintronic devices have applications as solar cells, sensors, and as a new class of electronics where the current can be directly controlled by light. The aim of this project is to study the feasibility of a carbon nanotube based plasmonic spintronics device. This device will rely on the results of a previous work where it is shown that a surface plasmon with optical frequency can be excited in a carbon nanotube (CNT) using light.

CPCA_A2_6009_2020

CAMELOT – Cloud

Investigador Responsável: Alcides Miguel Cachulo Aguiar Fonseca

Instituição: FCUL

Recursos: 140 160 vCPUcore.horas

HPC x HTC x Cloud V GPU x

The CAMELOT (autonomiC plAtform for MachinE Learning using anOnymized daTa) project aims at developing an innovative machine learning platform, which will tackle three key issues that hinder the efficiency and accuracy of modern AI applications:

- Ensuring real-time constraints during both the training and inference phases of machine learning models, while minimizing operational costs deriving from the use of cloud resources.

- Enabling learning over anonymized data, thus circumventing the privacy issues that currently prevent the reuse of information across models trained on datasets belonging to different entities (e.g., different financial institutions).
- Integrating information from different, independent and heterogenous data plataforms (e.g., key-value stores, relational and graph databases) in an automatic approach that maximizes the performance of machine learning applications.

CPCA_A2_6193_2020

OCEAN-ATMOSPHERE DYNAMICS OF ISLAND WAKES

Investigador Responsável: Rui Miguel Andrade Caldeira

Instituição: ARDITI - Madeira

Recursos: 207 360 CPU core.hours

HPC V HTC x Cloud x GPU x

The Oceanic Observatory of Madeira (OOM) uses a numerical modeling framework to study the interaction between the atmosphere and the ocean. Previous studies indicate that the uncoupled models are insufficient to reproduce the regional phenomena in mountainous archipelagos such as Madeira. The main objective of this project is to use Coupled-Ocean-Atmosphere-Wave-Sediment Transport (COAWST) Modeling System to study: (i) the wind effects (wakes; jets) generated by the island as well as the ocean response; (ii) the impact of climate change on wind-jets generation; (iii) deep-sea ocean circulation; (iv) improve the forecasting of the coastal ocean circulation system. COAWST numerical framework has three main models: the Weather Research and Forecasting (WRF), for atmosphere; the Regional Ocean Modeling System (ROMS), for ocean circulation; and the Simulating Waves Nearshore (SWAN), for waves. All of these three numerical components are computationally expensive thus require sufficient HPC resources (including MPI capabilities). Our plan is to use/analyse the simulation results to write at least one scientific article in the next 6 to 12 months and also to make forecasts available to the general community. Our meteo-oceanographic forecasts are currently being processed on our webpage (https://oom.arditi.pt/forecasts). An automated validation system compares model results with observations every 15 days and reports are publicly available https://oom.arditi.pt/modelvalidation.php

CPCA_A2_6986_2020

CIBME - COMPRESSÃO DE IMAGENS BIOMÉDICAS DE MODALIDADES EMERGENTES (COMPRESSION OF IMAGES FROM EMERGENT BIOMEDICAL MODALITIES)

Investigador Responsável: Lucas Arrabal Thomaz

Instituição: IT

Recursos: 175200 CPU core.horas + 2190 GPU horas

HPC V HTC V Cloud x GPU V

Motivated by recent technological developments in bioimaging systems, this project aims to alleviate technical requirements for bioimage archiving and transmission, which are emerging as operational bottlenecks in imaging facilities due to growing adoption of advanced optical and electronic imaging systems. One possible solution to maximize storage capacity and enable efficient transmission of dense image data relies on image compression. Hence, the main goal of this project is the development of robust coding approaches to compete with general-purpose image/video compression standards, which are still not able to optimally exploit the properties of volumetric image data. In fact, the versatility offered by the current data compression algorithms motivates the central idea of this project which involves the development of a set of standard-compatible modules (optimal color transformations, semantic segmentation, and content-adaptive and saliency-oriented image partitioning) aimed to provide better contexts and thus, optimal operation. A different research line will be also exploited in order to promote data-driven approaches for bioimage compression. To this, deep learning (DL) based methods will be investigated to i) define alternative image representations more suitable for compression and transmission purposes ii) pave the way to lossy image compression optimized to preserve the performance of common bioimage analysis tasks.

CPCA_A2_7192_2020

HIGH VELOCITY WATER JETS: COMBINED COMPUTATIONAL FLUID DYNAMICS (CFD) AND EXPERIMENTAL APPROACHES TO CHARACTERIZE THE SCOURING PROCESS

Investigador Responsável: António Maria de Afonseca Portela Roseira Muralha

Instituição: LNEC

Recursos: 1 120 000 CPU core.hours

HPC V HTC x Cloud x GPU x

This project is part of an ongoing PhD thesis of the research fellow António Muralha, supervised by Prof. Helena Ramos from IST and Dr. José Melo from LNEC. Dams over the world involve very specific features, namely in what concerns the hydraulic safety appurtenances such as the spillways. Spillways generate high velocity water flows, a particular case being water free jets strongly impacting rocky river beds downstream. The flow conditions, velocity and pressure, at the jet impact zone may lead to scour of the river bed. The present research focuses on scour due to high velocity jet actions based on suitable CFD simulations calibrated and validated by means of experimental simulations. A new methodology to characterize the scouring process will be implemented in the CFD simulations using OpenFOAM. The main goals of the numerical CFD simulations are: simulate flow conditions of the existing experimental facility at LNEC; compare the experimental results with the ones obtained numerically, validate the CFD parameters; implement a technique that allows a simulation of the rock scouring process; finally, validation of the developed methodology for scouring analysis considering field data from real an existing dam with jet spillway produced scouring. As a major expected result one can expect the definition of procedure to assess the scouring process, applicable either in the project of new dams, as well as in the assessment of spillway operation safety of existing dams.

CPCA_A2_7217_2020

PATHOGENOMICS OF COFFEE LEAF RUST TO PROBE VIRULENCE MECHANISMS AND DIAGNOSTIC MARKERS

Investigador Responsável: Francisco Pina-Martins

Instituição: FCUL

Recursos: 320 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Coffee agroecosystems have been under siege with the repeated resurgence of fungal epidemics during the last decade. Focusing on the devastating fungal pathogen Hemileia vastatrix, the main threat to Arabica coffee production worldwide, this project intends to apply an integrative pathogenomics approach to dissect the molecular mechanisms underlying virulence divergence and evolution of pathotypes, and to develop molecular markers for high-throughput discrimination of races. To achieve this goal, a high-quality reference genome will be assembled and annotated and then used in combination with comparative genomics, genome-wide association and transcriptomic analyses to identify SNPs, genomic changes and candidate effector genes, that can be linked to rust virulence profiles. Based on generated markers, diagnostic tools and a web platform will be developed serving as a

basis for the much needed design of sustainable disease control practices and establishment of worldwide disease surveys.

CPCA_A2_7255_2020

CoastNet RESEARCH INFRAESTRUTURE

Investigador Responsável: José Lino Vieira de Oliveira Costa

Instituição: FCUL

Recursos: 420 480 vCPU core.horas+ 4380 GPU horas

HPC x HTC x Cloud V GPU V

The Portuguese Coastal Monitoring Network - CoastNet (https://coastnet.pt/) is an RI focused on monitoring coastal ecosystems through relevant chemical, physical and biological parameters, which are available in the infrastructure's geoportal (http://geoportal.coastnet.pt). This information allows a better understanding of their functioning through the assessment of long-term trends and spatial-temporal variability. It includes four main lines of action: (i) a Coastal Remote Sensing System, providing a range of Earth Observation innovative products for the Portuguese coast; (ii) an Environmental and Biological Monitoring System, providing autonomous and continuous measurements of environmental and biological variables; (iii) the Portuguese Tracking Network, collecting data on animal movements through arrays of biotelemetry acoustic receivers; and (iv) a geoportal which integrates and processes real time and historical data, and provides them in open access. CoastNet offers access to a wide variety of services related to coastal monitoring, including research and innovation, advanced training, consultancy, laboratory support and databases and biological collections. The innovative nature of this infrastructure relies on the capacity to monitor environmental and biological components of coastal aquatic systems autonomously, displaying and providing the whole dataset in near real time, and also allowing the integration of different types of information.

CPCA_A2_7257_2020

NOVEL RADIATION SOURCES FROM LASER-PLASMA INTERACTIONS

Investigador Responsável: Marija Vranic

Instituição: IST-UL

Recursos: 1 152 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Intense lasers excite ultra-relativistic plasma waves that can accelerate electrons and positrons to very high energies in cm-scale plasmas. These electrons can emit high-brilliance photon beams through betatron radiation or via Compton scattering. Adjusting the energy of the relativistic particles (emitters) allows varying the critical frequencies of the broadband output radiation from X-ray to Gamma-ray spectrum. This technology offers an outstanding opportunity to construct affordable, table-top radiation sources that could be widely available, at a fraction of the size and the cost of the conventional synchrotrons. The aim of this project is to explore several configurations relying on the interaction of ultra-intense lasers with matter, focusing on the radiation output. We aim to evaluate brilliance and luminosity of the potential sources, as well as establish reliable scaling laws to ensure tunability. To that end, we will perform massively parallel particle-in-cell modeling, which allows taking into account the finite-size effects, collective dynamics etc., thus providing a roadmap for the development of novel sources for industrial and medical imaging applications. This project was granted by FCT in the Individual call for junior researchers (Dec. 2018). It was ranked first in physics in Portugal.

CPCA_A2_7407_2020

PERFORMANCE EVALUATION OF PARALLELIZATION STRATEGIES IN DERIVATIVE-FREE OPTIMIZATION ALGORITHMS

Investigador Responsável: Pedro Abílio Duarte de Medeiros

Instituição: FCT-UNL

Recursos: 280 320 vcpu core.horas

HPC x HTC x Cloud V GPU x

This proposal is framed on a ongoing research project whose main is to develop efficient and robust algorithms for Global and/or Multi-objective Derivative-free Optimization. This type of optimization is typically required in complex scientific/industrial applications, where the function evaluation is time-consuming and derivatives are not available for use, neither can be numerically approximated. We intend to address the inherent problem of the huge execution times by resorting to parallel/cloud computing and carrying a detailed performance analysis. As a result of the parallelization efforts harder Derivative-free Optimization problems, with more variables for example, could be tackled. A goal of the project is the availability of integrated toolbox for solving single/multi objective, local/global Derivative-free Optimization problems. The main goal of the toolbox is to ease the use of the optimization algorithms by problem specialists that are not experts in high performance computing. An aspect of the toolbox is the issue of

recommendations for taking advantage of parallelization and cloud computing, providing easy access to the optimization algorithms. The type of recommendations issued are related with the number of CPUs to be used in a given problem. To these recommendations, a detailed performance and scalability analysis is mandatory and this will be possible through the use of these advanced computing facilities.

CPCA_A2_7417_2020

MEASURING AND ADAPTING TEAM-LEVEL CONSTRUCTS: CHALLENGES AND OPPORTUNITIES

Investigador Responsável: Jorge Fernando Pereira Sinval

Instituição: ISCTE-IUL

Recursos: 560 640 vcpu core.horas

HPC x HTC x Cloud V GPU x

Validity assessment of team-level instruments is mostly performed using procedures designed for individual-level measures. However, the study of team-level instruments should include the possible inequality in the within- and between-level structure and should also consider information about scale item's ability to differentiate groups (Bliese et al., 2019). We based our application in the most recent proposals related to multilevel theory, measurement, and validation. The first goal is to validate multilevel constructs, i.e., constructs that emerge from the interactions between individuals but that exist at both levels. The second goal concerns the assessment and validation of emergent team constructs, which can be different in their nature (Mathieu & Luciano, 2019) and also in their measurement (Jebb et al., 2019). The last goal is to evaluate the longitudinal validity of dynamic team constructs (Luciano et al., 2018). This proposal clear contributes to advance team-level construct validation by integrating different approaches, implemented with top international collaboration and using advanced statistical methods.

CPCA_A2_7425_2020

FAKE NEWS AND REAL PEOPLE - USING BIG DATA TO UNDERSTAND HUMAN BEHAVIOUR (FARE)

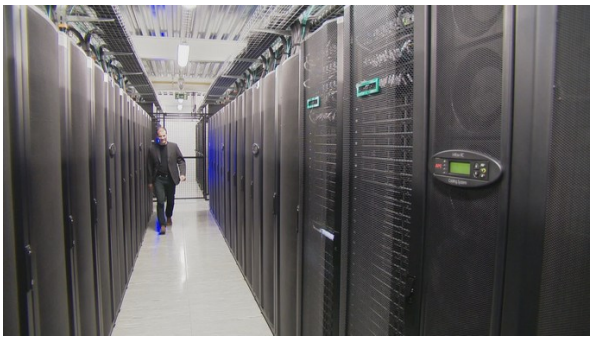
Investigador Responsável: Joana Gonçalves de Sá

Instituição: IST-UL

Recursos: 4000 CPU core.horas + 35 040 vcpu core.horas

HPC V HTC x Cloud V GPU x

The FARE project aims to quantitatively study human behavior by leveraging the large scale data generated daily in online activities. It will use fake news as a model to probe the spread of information through social networks. The group also focuses on the ethics of research involving humans, including privacy-preserving machine learning, which requires computationally expensive encryption. We will need computing power to analyze large scale social media data - text and metadata - using standard NLP techniques: descriptive statistics, TF-IDF, topic extraction and sentiment analysis, among others. Statistical and machine learning methods will be used to classify social media content and characterize populations.



Oblivion

CPCA_A2_2500_2020

PYROCONVECTION

Investigador Responsável: Rui Paulo Vasco Salgado

Instituição: Universidade de Évora

Recursos: 50 000 CPU core.hours

HPC V HTC x Cloud x GPU x

The objective of the present project is to use HPC to perform simulations of wildfires events with atmospheric-fire coupled models in order to study and model a fire induced atmospheric phenomenon still poorly known: the pyroconvection, which in turn change the spread of the fires. So, the main objective of the simulations is about how to obtain a better representation of pyroconvection in numerical weather modelling. This will be of great importance to improve the understanding of pyroconvection, as well as its impact in the atmospheric dynamics (i.e., troposphere-stratosphere transport of particulate matter), as well as cloud microphysics and atmospheric chemistry.

CPCA_A2_4377_2020

DISPERSION OF ASPHALTENES IN MODEL MIXTURES BY IONIC LIQUIDS - A THEORETICAL APPROACH

Investigador Responsável: Rafaela Nascimento Martins

Instituição: Universidade de Évora

Recursos: 1 200 000 CPU core.horas

HPC V HTC x Cloud x GPU x

In this project, the ability of selected ionic liquids to be used as additives in order to alter aggregation properties of asphaltenes (particularly dispersing them) in model mixtures resembling oil will be tested using molecular dynamics simulations and quantum mechanical calculations. The additives used will be alkyl methyl imidazolium, alkyl pyridinium and alkyl isoquinolinium based ionic liquids along with anions such as chloride, bromide and acetate. The "oil" environment will be obtained using mixtures containing toluene and n-heptane in different proportions. This proposal will investigate the aggregation phenomenon of asphaltenes in solution with different concentrations of additives (ionic liquids) but also the direct interactions between asphaltenes and ionic liquids. The former will be studied by molecular dynamics simulations, following the asphaltene aggregation over time. The latter will be investigated by calculating the energetics of binary interaction asphaltene/ionic liquid using quantum mechanical calculations (DFT method). Both the study of the aggregation dynamics of asphaltenes in model mixtures and the calculation of the interaction energetics asphaltenes and ionic liquids are important data to contribute to the screening procedure needed to choose the best additive to disperse asphaltene in oil and that the main objective of the project. The results obtained will be object of scientific publications in international journals with peer-reviewing.

CPCA_A2_4628_2020

OPTIMAL SURFACE TEXTURING PATTERNS FOR GREENER AND MORE ENERGY EFFICIENT SLIDING CONTACTS

Investigador Responsável: Luis Silvino Alves Marques

Instituição: UM

Recursos: 50 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Nowadays, the reduction of friction in combustion engines has been almost exclusively achieved with the use of lubricant and additives, however EU regulations require the elimination of P and Zn containing additives in automotive industry. The main objective of the project is the reduction of the friction in lubricated mechanical contacts through the synergy between adaptive self-lubricant coatings, based on transition metal dichalcogenides (TMD), deposited onto textured surfaces. The experimental approach needs to be supported and complemented with theoretical studies based on Finite Element simulations and or ab-initio DFT calculations to design the optimal nanostructured surfaces. The modelling component of the proposed project will serve two major purposes:

- Understanding of the contact conditions in lubricated conditions and discrimination of the contribution of each of the following part on the overall tribological performance: the texturing and the low friction coating;

- Optimize the surface texturing pattern in terms of distribution and dimensions of topographic features.

This projects results from the collaboration of theoretical and experimental research groups from the Universities of Coimbra and Minho, which joined an institute of interface with Industry (IPN), and a manufacturing company of parts for combustion engines (Mahle), for accomplishing this important goal for the society.

CPCA_A2_5649_2020

TiSiNAg-o-Learn

Investigador Responsável: Veniero Lenzi

Instituição: UM

Recursos: 410 000 CPU core.hours

HPC V HTC x Cloud x GPU x

Self-lubricating coatings have enormous potential to protect working part in extreme temperature and pressure conditions. In particular, nanocomposite TiSiN/Ag systems, in which silver is the lubricating agent, were shown to have very promising performance. However, the behaviour of such coating is greatly influenced by their nanostructure and composition. In order to optimize the coating's performance, a complete understanding of how silver is diffusing within the TiSiN matrix is fundamental. To study the Ag behaviour under realistic conditions, a classical Molecular Dynamics force field is required, but whereas parametrizations exists for some of the element pairs, e.g. TiN and TiAg, none is currently available for TiN/Ag and TiSiN/Ag nanocomposites. The ultimate goal of this project is to develop and test a classical force field for TiSiN/Ag coatings, employing fast On-the-fly Machine Learning techniques which rely on ab-initio calculations to train the force field. Firstly, the method will be tested with TiN, for which many experimental and computational works already exists, thus making it simple to check its

accuracy. TiN/Ag systems will be addressed after the method is verified, and TiSiN/Ag nanocomposites will be treated as the last part. The accuracy of the developed force-field will be tested by comparison with full ab-initio molecular dynamics simulations of the studied systems.

CPCA_A2_7242_2020

SINERGEA@RNCA - scenarios database for decision support of the integrated and optimized management of energy, bathing water quality and inundation in coastal cities

Investigador Responsável: Anabela Pacheco de Oliveira

Instituição: LNEC

Recursos: 347 200 CPU core.hours

HPC V HTC x Cloud x GPU x

The ANI-funded SINERGEA project targets an intelligent platform for decision-support of the integrated and optimized management of energy, bathing water quality and inundation in coastal cities. Framed in a smart city view, this work will: 1) minimize drainage infrastructures' energy consumption; 2) protect urban beaches by minimizing bathing waters' contamination by urban discharges; 3) contribute to urban flood events risk management. Based on innovative ICT methods, the system will provide the real-time optimization of infrastructure operation, merging a database of pre-defined environmental scenarios and operational alternatives, and the real-time water forecast of the catchment, urban and coastal areas and of energy. The city of Albufeira and its coast will be the demo site. SINERGEA@RNCA targets the development of the pre-defined scenarios for the demo site, using the computational model SCHISM in the RNCA infrastructure. The scenarios database accounts for several parameters that control the hydrodynamics and water quality of the Albufeira area, namely: tidal amplitude, wind magnitude and direction, short wave magnitude and direction, discharge patterns and their lag relative to tides, precipitation, and seasonal variation of air temperature and solar radiation. The proposed work will be included in SINERGEA's dissemination plan, namely through the open-access publication of a journal paper on the scenarios database and its presentation at a major coastal conference.

CPCA_A2_7263_2020

LATTICE THERMAL CONDUCTIVITY OF BIASED BILAYER GRAPHENE SYSTEMS

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Recursos: 1 670 400 CPU core.hours

HPC V HTC x Cloud x GPU x

Between several derivatives of the monolayer graphene system, special interest is given to its bilayer alloptrope. Two known modifications of bilayer graphene (BLG) can coexist with different stacking environments: the AB structure (Bernal) and its alternative, the AA structure. The interest in BLG is mainly due to the possibility of inducing a semiconductor with a tunable band gap, for which the most reliable structure for external tuning has been observed for the AB system[1,2]. The tuning of the gap occurs through the application of an electric field normal to the layers[1,2]. When an external field is applied to the AB system, breaking of the continuous symmetry to a triangular lattice is observed[2]. Therefore variations of the electronic properties occur for this configuration. For the unbiased system the electronic band-structure presents a parabolic dispersion at the Fermi energy. A tunable band-gap is evidenced with applied electric field and, for increasing amplitudes of the bias, different scaling behavior as a function of momentum is observed[2]. The present proposal will consider calculations of the lattice thermal conductivity (κ) for the AB-BLG with different amplitudes of applied bias, for which variations of κ is expected since disorder is introduced to the systems.