HR EXCELLENCE IN RESEARCH

UNIVERSIDADE DA CORUÑA

citic

3-i ICT – 3rd call

PhD projects

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1 About 3-i ICT PhD projects

All PhD projects will have a **supervision team** that will comprise:

- A main supervisor: a CITIC researchers qualified to guide a PhD thesis through to completion and provide the candidate with training and support of the highest standard.
- A secondary supervisor: an experienced researcher from other academic discipline, from any national or international academic institution, research organisation or private company.
- A non-academic supervisor to monitor intersectoral secondments and help prepare the candidate for life outside the academia.

Applicants can choose up to 4 PhD projects from the 8 offered in the 3rd call for candidates.

There are five thematic External Panels, each of them related to one of the five research areas of CITIC. Each PhD project is related to one of these five research areas:

- **Artificial intelligence** is mainly focused on designing and programming machines capable of performing tasks that require intelligence, with a wide range of crosswise applications in other fields.
- **Data science and engineering** are inherently multidisciplinary fields, with growing relevance in the big data era and interactions with several scientific disciplines.
- **High performance computing** is an essential tool for processing the large data sets needed to understand and meet social, scientific, and industrial challenges across a wide range of fields.
- **Intelligent Networks and Services** is a highly transferable, intersectoral area, especially in the field of Industry 4.0.
- **Cybersecurity** is a cross-disciplinary field that draws on and feeds into the other key areas of research at CITIC, including data processing and management, artificial intelligence systems, computation systems, and online services and communications.

CODE	Title	CITIC RESEARCH AREA	INTERDISICIPLINARY RESEARCH AREA
2024-C3-001	Addressing challenging optimization problems in cell signalling networks with High Performance Computing and Cloud-based approaches	High Performance Computing	Biochemistry and molecular biology
2024-C3-002	Supporting the European green transition by combining artificial intelligence methodology and psychological behaviour models	Artificial Intelligence	Social Psychology
2024-C3-003	Mathematical modelling and numerical simulation of adhesive joints for naval steel	Data Science and Engineering	Naval constructions
2024-C3-004	Augmentative and Alternative Educational Technology for Executive Functioning in Children with Autism	Smart services and networks	Computer Languages and Systems
2024-C3-005	Modelling complex biological phenomena via inverse optimal control and inverse reinforcement learning	Data Science and Engineering	Chemical engineering Biochemistry and Molecular Biology
2024-C3-006	Distributed and parallel algorithms for inference of cell lineage trees	High Performance Computing	Genetics
2024-C3-007	Software Engineering and Data Science Techniques for Urban Building Energy Modeling	Data Science and Engineering	Land Use and Urban Planning
2024-C3-008	Virtual Reality in Pediatric Surgical Care, Communication, and Education	High Performance Computing	Surgery; Pediatrics; Physiology; Pathology; Anatomy and Comparative Pathology; Radiology and Physical Medicine

2 PhD projects description

CODE	**2024-C3-001**
Title	Addressing challenging optimization problems in cell signalling networks with High Performance Computing and Cloud-based approaches
CITIC supervisor	Dra. Patricia González Gómez https://pdi.udc.es/en/File/Pdi/Z399E
Research lines	High Performance Computing / Biochemistry and Molecular Biology
Secondary supervisor	Dr. Julio Sáez Rodríguez Institute for Computational Biomedicine, Heidelberg University
Academic PhD programme	Information technology research https://estudos.udc.es/en/study/start/5023V01
Summary	Computational models have become very popular to analyze the functioning of complex biochemical networks such as those involved in cell signaling networks. Successful models build predictive logic models of signaling pathways by training a prior knowledge network to biochemical data obtained from perturbation experiments. This training shows up as an optimization problem that require efficient and robust solution methods. The use of High-Performance Computing (HPC) techniques may represent an effective strategy to speed up the time-to-solution. However, most of these methods, handled as algorithms, may have limited parallelism, while if they are tackled as problem solving methods, they offer other opportunities for large-scale parallel computing. In this project we will explore the use of HPC and Cloud-based techniques in the context of multimethod global optimization, in which multiple different search algorithms are performed concurrently and cooperate between them through information exchange. These algorithms will also be adapted to the specific problem structure of training models of signaling networks. To address this challenge, it is required to combine the complementary knowledge in the research areas of both supervisors of the Ph.D. project. This research will be addressed in a context of an already established international collaboration, having also in mind the potential technology transfer of the research results. More precisely, the methods developed here can be used in the pharmaceutical industry to construct signaling networks of diseases and use these models to find new targets for therapy as well as to better characterize the effect of existing drugs.
Foreseen secondments	Two research visits of at least three months each to the Institute for Computational Biomedicine. In addition, possible visits to IIM-CSIC (Marine Research Institute of the Spanish Council for Scientific Research), startups such as ProtAvio (https://www.multiplex-assays.com/) and Insilico Biotechnology (https://www.insilico-biotechnology.com/) could be carried out.

CODE	**2024-C3-002**
Title	Supporting the European green transition by combining artificial intelligence methodology and psychological behaviour models
CITIC supervisor	Dra. Amparo Alonso Betanzos https://pdi.udc.es/en/File/Pdi/AF2AF
Research lines	Artificial Intelligence/Social Psychology
Secondary supervisor	Dr. Christian Klöckner Norges teknisk-naturvitenskapelige universitet (NTNU)
Academic PhD programme	Computational science. https://estudos.udc.es/en/study/detail/5009V01
Summary	Reducing energy consumption is the backbone of the European Green Transition and essential to combat climate change and ensure a sustainable future. Artificial Intelligence has the potential of being a powerful tool for achieving those goals by analysing traces of people's behaviour in big datasets and thereby identifying leverages for behaviour change. However, to assure that the insights produced by AI approaches are embedded in the state-of-the-art behaviour science, a multidisciplinary approach is mandatory to succeed. Machine Learning in particular can be used to identify patterns and trends in large databases of electricity consumption and segment the consumer base into different groups based on their usage patterns and demographics. After this initial step, the identified consumer groups will be analysed not only on the clustering basis, but also taking into account psycho-sociological theories, to identify opportunities for behaviour change, in other words, using a data-driven strategy to identify distinct segments of the population to then address these segments with interventions derived from behaviour science theory and practice. To simulate likely responses of the identified users, agent-based models will be used to model those clusters, and the interactions between the individuals that form part of them. Based on these simulations, personalized policy proposals will then be derived from general policies such as targeted education, incentive programs or time-of-use pricing based on empirically and theoretically based methodological tools from the social sciences.
Foreseen secondments	The student will be working at CITIC in Spain, in a technological centre with access to knowledge and tools in the field of Artificial Intelligence. However, the co-director is the head of a Psychology Department at NTNU, Norway, and thus the student will benefit from stays abroad, beside working closely to both co-supervisors in a regular basis, by videoconference. Also, both supervisors have connections with other research groups in UE, in which the student could make short stays, in the field of ABM for societal analysis. Some examples could be the James Hutton Institute, or the University of Groningen. At NTNU the student will have access to the members of NTNUs Energy Transition Initiative (NETI), which is an interdisciplinary collaboration of highly merited Norwegian and international energy scientists who are and have been involved in a substantial number of National and European research projects. The candidate will also be connected to the Norwegian Research Center for Environmentally Friendly Energy NTRANS.

CODE	**2024-C3-003**
Title	Mathematical modelling and numerical simulation of adhesive joints for naval steel
CITIC supervisor	Dra. María González Taboada https://pdi.udc.es/en/File/Pdi/LD49E
Research lines	Data Science and Engineering/ Naval constructions
Secondary supervisor	Dra. Ana Álvarez García Universidade da Coruña (UDC) https://pdi.udc.es/en/File/Pdi/9P98E
Academic PhD programme	Mathematical modelling and numerical simulation in engineering and applied science. https://estudos.udc.es/en/study/detail/5026V01
Summary	One of the main concerns of the Shipyard 4.0 is the weight of the ship. Lightening the weight of the ship would increase the efficiency and reduce greenhouse gas emissions, particularly CO2. In a ship, the weight of the weld represents at least between 5% and 7% of the total weight of the ship. The reduction of this weight can lead to huge savings in production costs every year. Moreover, it would help to improve the planet. This PhD project aims at studying from a mathematical perspective the use of adhesive joints in ships instead of welding. Specifically, the aim is to develop a mathematical model that enables to study an adhesive joint with naval steel in any position of the ship as well as to predict its behavior.
Foreseen secondments	The PhD student will be recommended to do research stays at prestigious research centers in the field, like the Jacques-Louis Lions Laboratory of the Sorbonne Université (France) -to improve the implementation of numerical methods-, and the Department of Mechanical Engineering at the University of Oporto (Portugal), to enhance the mathematical model.

CODE	**2024-C3-004**
Title	Augmentative and Alternative Educational Technology for Executive Functioning in Children with Autism
CITIC supervisor	Dra. Paula María Castro Castro https://pdi.udc.es/en/File/Pdi/WK6AF
Research lines	Smart services and networks/ Computer Languages and Systems
Secondary supervisor	Dra. María Luisa Gómez Taibo Universidade da Coruña (UDC) https://pdi.udc.es/en/File/Pdi/HX99E
Academic PhD programme	Information technology and mobile network communication. https://estudos.udc.es/en/study/detail/5029V01
Summary	This PhD project proposes the study of existing technologies and the state of the art in order to, on this basis, develop a free educational platform that integrates several applications for mobile devices aimed at the early years of children with some type of Autism Spectrum Disorder (ASD). Although this spectrum is very broad, the vast majority of children with ASD have communication problems with their environment (school, extracurricular activities, family, etc.), which affect both the performance of basic communicative functions (such as the expression of needs or desires or the development of language itself) and the organization of their daily life or variables involved in learning (memorization, concentration, acquisition of skills in certain specific areas, etc.). This project will aim to improve these aspects by means of a unique accessible environment that favors: 1) their integration both in the family and the educational environment through Augmentative and Alternative Communication (ACC) based on visual scenes embedded in videos, 2) the organization of activities through digital agendas and 3) the monitoring of their development with early warnings. Moreover, this project proposes the study of natural language processing methods, for lexical simplification or disambiguation of the meaning of words, and artificial intelligence techniques, for prediction of behavioral patterns, with integration of wearable devices, for communication and sensor purposes. This proposal is strongly interdisciplinary as it shares concepts, methods and technologies mainly from areas such as technology, engineering and AAC with many applications in sectors of health, education, ICT or smart environments.
Foreseen secondments	Throughout the completion of this thesis, contacts will be established with some of the American or European universities to carry out at least one stay and collaborate in the research work. In this sense, GTEC has a history of collaboration with European and American universities that could be taken advantage of: - Technical University of Munich - University of Maryland - Université Côte d'Azur

CODE	**2024-C3-005**
Title	Modelling complex biological phenomena via inverse optimal control and inverse reinforcement learning
CITIC supervisor	Dr. Carlos Vázquez Cendón https://pdi.udc.es/en/File/Pdi/DB58E
Research lines	Applied mathematics / Chemical engineering / Biochemistry and Molecular Biology
Secondary supervisor	Dr. Julio Rodríguez Banga Marine Research Institute – Spanish National Research Council (IIM-CSIC)
Academic PhD programme	Mathematical modelling and numerical simulation in engineering and applied sciences https://estudos.udc.es/en/study/start/5026V01
Summary	In recent years, the areas of molecular biology and biochemistry are witnessing a "data-deluge" due to major technological advances in genomics, proteomics and metabolomics. However, systematic analysis of these huge new experimental data sets from a mechanistic point of view remains an open question. In this thesis, we will develop novel methods to identify optimality principles from data in order to reverse engineer complex biological systems. In particular, these methods will be used to generate mechanistic understanding of the dynamics of biochemical pathways at the cellular level. The main idea is to bridge concepts and methods from numerical and mathematical optimization (inverse optimal control) and artificial intelligence (inverse reinforcement learning) to facilitate the dynamic modelling of these biological systems. These methods will be used to automatically infer the optimality principles that can explain the observed dynamic behaviour. The research will require tight interdisciplinary collaboration (involving the areas of applied mathematics, optimization, machine learning and cellular biology) to develop and apply novel methods and tools to fundamental problems in computational systems biology. These developments will be tested with case studies involving the metabolic response of microorganisms and human cells to environmental changes. As a result, a better mechanistic understanding of these bio-systems will be achieved. This new knowledge can have a major societal impact, improving intervention strategies in biomedicine (e.g. human metabolism and cancer) and industrial biotechnology (e.g. microbial fermentation bioprocesses).
Foreseen secondments	For this PhD project, the supervisors have carefully designed a list of high-quality international and intersectoral secondments tailored to complement different aspects of the research plan. In particular, research stays have been jointly agreed at the following research groups: - Mathematical Algorithmic Optimization group, leaded by Prof. Sebastian Sager (Otto-von-Guericke University Magdeburg, Germany), world-class researcher in optimal control theory and methods (more information at https://mathopt.de/). - Microcosme group at INRIA Grenoble (France), where Prof. Hidde de Jong is a leader in computational systems biology of microorganisms and its applications in industrial biotechnology (more information at https://team.inria.fr/microcosme/). - Systems and Data Analysis group at Fraunhofer-Chalmers Research Centre for Industrial Mathematics (Gothenburg, Sweden), leaded by Prof. Mats Jirstrand (Goteborg), a top-class group developing computational tools and techniques (including machine learning) for systems and data

CODE	**2024-C3-006**
Title	Distributed and parallel algorithms for inference of cell lineage trees
CITIC supervisor	Dr. Diego Darriba López https://pdi.udc.es/en/File/Pdi/4Y4NH
Research lines	High Performance Computing / Genetics
Secondary supervisor	Dr. David Posada González Universidade de Vigo
Academic PhD programme	Information technology research https://estudos.udc.es/en/study/start/5023V01
Summary	Recent advances in DNA/RNA sequencing technologies have allowed the generation of genomic data at single-cell resolution, promoting an unprecedented opportunity to better understand how somatic evolution works within our bodies and the evolutionary mechanisms behind diseases like cancer. Reconstructing cell lineage trees is essential to achieve this goal, but current algorithmic approaches have shortcomings: they cannot handle large data sets and/or they use simplistic models of somatic evolution. The aim of this project is to overcome the limitations of methods for inferring cell genealogies by developing new algorithms, tools and more biologically-realistic models. The massive amount of data currently generated thanks to Next-Generation Sequencing technologies brings up the importance of using High-Performance Computing techniques and environments. The results of this project will be publicly available as Open Access publications and Open Source software and will help researchers worldwide by increasing the power of hypothesis testing in the field of single-cell phylogenetics, thus increasing the knowledge about somatic evolution and its effects.
Foreseen secondments	**Torusware** is a technology company, spin-off of the Computer Architecture Group of the University of A Coruña, and it is specialized in Big Data and DevOps services. Collaborating with Torusware is interesting because of two aspects: on the one hand it may help provide additional parallel approaches, capable of handling larger data sets. On the other hand, their DevOps experience may help during the development and release of software to increase its scope (e.g., making it available to more platforms). The **Computational Molecular Evolution** (CME) research group belongs to the **Heidelberg Institute of Theoretical Studies** (H-ITS), a private, non-profit research institute in Germany. CME focuses on large-scale evolutionary biology data analysis and High-Performance Computing. Their experience in these fields can be extremely helpful for the development of this project.

CODE	**2024-C3-007**
Title	Software Engineering and Data Science Techniques for Urban Building Energy Modeling
CITIC supervisor	Dr. Miguel Ángel Rodríguez Luaces https://pdi.udc.es/en/File/Pdi/6U69E
Research lines	Data Science and Engineering/ Land Use and Urban Planning
Secondary supervisor	Dr. Jorge Rodríguez Álvarez University of A Coruña (UDC) https://pdi.udc.es/en/File/Pdi/5R5LF
Academic PhD programme	Computational science https://estudos.udc.es/en/study/start/5009V01
Summary	This doctoral research proposal aims to develop a novel methodology to model urban building energy flows based on urban morphology, construction specifications and user behavior thus enabling meaningful analysis of the likely impacts of energy plans and policies at building, city, and regional scale. The project will apply variability management techniques and data science methods to define a sound, flexible and scalable energy model framework that can be easily deployed on different cities and for multiple intended uses. Despite the growing interest in urban energy performance in the last decade, few Urban Buildings Energy Models (UBEMs) are available to evaluate the energy implications of plans and policies. Most of the existing models have one or more of the following limitations: (a) they require time-consuming geometric modeling, (b) they are based on building-scale thermodynamic models and are therefore limited to a few blocks, (c) they are based only on statistical correlations and do not take into account the specific characteristics of buildings and the urban fabric, and (d) they have been designed ad hoc for specific cities and are not generalizable. The research will systematize the process of adapting and combining thermodynamic and daylighting models with original morphological analysis algorithms, thus creating the core structure for mapping energy demand patterns in large urban areas. In addition, software engineering techniques will be applied to create a framework that can be deployed in cities with varying requirements and characteristics. The research results will greatly facilitate the modeling process, thus expanding the scope for innovative planning support systems (PSS). Applications range from energy mapping to interactive analysis of alternative scenarios.
Foreseen secondments	It is expected that the potential PhD candidate will complete a research stay in some of the most important academic institutions in the field such as: - The Bartlett Centre for Advanced Spatial Analysis (CASA) – University College London, London, UK. - The Building 2050 Innovation Research and Integration Support Group- École Polytechnique Fédérale de Lausanne (EPFL, Switzerland). - Sustainable Environmental Design Programme (SED)– Architectural Association School of Architecture. London, UK. - Data and Web Science Lab at Aristotle University of Thessaloniki. - Fraunhofer Institute for Experimental Software Engineering

CODE	**2024-C3-008**
Title	Virtual Reality in Pediatric Surgical Care, Communication, and Education
CITIC supervisor	Dr. José A. Iglesias-Guitián https://pdi.udc.es/en/File/Pdi/FG72G
Research lines	High performance computing/ Surgery/ Pediatrics/ Physiology/ Pathology/ Anatomy and Comparative Pathology/ Radiology and Physical Medicine
Secondary supervisor	Dr. Manuel Gómez-Tellado SERGAS (Galician health service)
Academic PhD programme	Information and communications technology https://estudos.udc.es/en/study/detail/5032V01
Summary	Augmented and virtual reality (AR/VR) technologies can be used in pediatric healthcare to create simulations of complex surgeries, improve patient communication, or even be used as a therapeutic tool helping to alleviate anxiety and pain in children facing medical procedures. This proposal aims to explore further this trend by exploring the potential benefits that advanced scientific visualization and AR/VR technologies can bring together in pediatric healthcare. This project will research novel automated transfer functions (TFs) to provide novel interactive tools that can perform advanced volume rendering visualizations without requiring prior volume segmentation. Having fast interactive TFs for volume exploration can be critical when analyzing medical images just before an urgent pediatric surgery. Complementary, this project will explore natural interfaces leveraging AR/VR technologies for analyzing complex pediatric medical data streams, e.g. in pediatric surgical planning or augmented implant surgery. This project will explore further applications of AR/VR technology in pediatric surgery, facing three main challenges: i) improving understanding and planning in pediatric surgery procedures through advanced volume rendering techniques, e.g. integrating cinematic rendering in AR/VR; ii) developing novel approaches for advanced scientific visualization in education and developing narrative storytelling approaches for communicating healthcare data with patients; iii) exploring applications of VR in preoperative and post-operative phases, for example tailoring audiovisual content for children in AR/VR to create immersive experiences aimed to reduce and alleviate preoperative anxiety and stress.
Foreseen secondments	For this PhD project, supervisors would like to propose a list of potential secondments aimed to complement different aspects of this research project. In particular, the following research stays have been jointly agreed: - University Hospital of A Coruña (CHUAC). The Ph.D: candidate will work closely with healthcare professionals at CHUAC in order to perform any experiment involving real pediatric patients. - University of Bergen, Norway. Either with Prof. Stefan Bruckner, a well-known expert (11 Best Paper Awards) in illustrative volume rendering and scientific visualization and/or Prof. Noeska Smit, a radiologist with experience in scientific visualization research and narrative healthcare storytelling. - Geneva School of Health Sciences, Switzerland. Since he is an expert in medical imaging and regularly trains radiologist in the use of medical visualization software. ARSoft, a Spanish company aimed to deploy AR/VR technology across industries, including healthcare.