

JANUARY 2025

# LNCC RESEARCH GROUPS PORTFOLIO

Laboratório  
Nacional de  
Computação  
Científica

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# NATIONAL LABORATORY FOR SCIENTIFIC COMPUTATION

LNCC researches, develops, and innovates in various areas of knowledge, using computational modeling for high-performance processing of studied phenomena.

Scientific computing is the optimization tool for research, as it reduces analysis time and increases result accuracy. It also reaches complex phenomena that could not be studied with the same speed and quality on conventional computers.

LNCC conducts research, trains Masters and PhDs, and offers high-performance computing platforms to the scientific community.

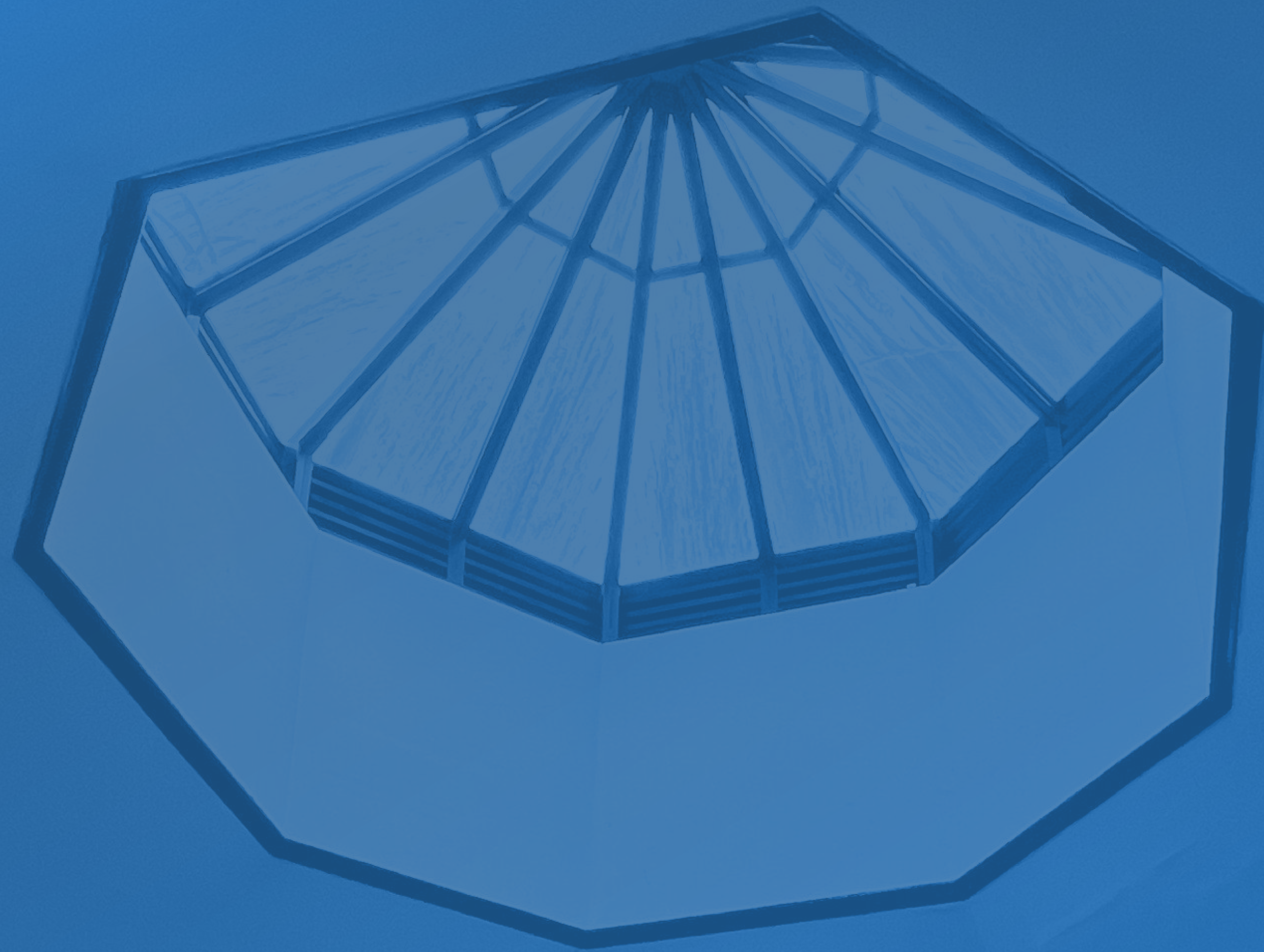
The high-performance processing platform, including the Santos Dumont Supercomputer, is open for use by the Brazilian scientific community, enabling them to simulate phenomena and advance research. Santos Dumont is the fastest academic supercomputer in Latin America, with a processing capacity of 5.1 quadrillion operations per second, equivalent to the capacity of thousands of home notebooks in theory. The 3rd expansion stage scheduled for 2024 will increase capacity by 17 Petaflops.



With the Computational Modeling Postgraduate Program, rated 7 by CAPES, training Masters and PhDs, coupled with courses, seminars, and events held regularly, LNCC promotes the diffusion of scientific computing in Brazil. Over 300 professionals trained in Computational Modeling at LNCC work in 14 Brazilian states, disseminating knowledge about scientific computing, to simulate phenomena, to analyze data and advance research. Its scientific output has received 17 honorable mentions since the start of the course in 2000.

The institution has been actively involved with society in solving national problems, such as genetic sequencing of viruses like SARS-CoV-2 (causing COVID-19) and Zika, Dengue, and Chikungunya agents - carried out by the LABINFO (Bioinformatics Laboratory) using state-of-the-art sequencers. Also in healthcare, LNCC collaborates on vaccine research in cooperation with Fiocruz; simulation of human cardiovascular systems to support medical assistance by the Hemodynamics Modeling Laboratory; DockThor portal, providing free access for protein coupling simulation for new drug projects, among other purposes; and computational models to simulate tumor growth in patients - projects that reinforce LNCC's national character.

Research, Development, and Innovation Projects developed at LNCC, such as computational models and programs developed for oil and gas reservoir simulation used by Petrobras in pre-salt exploration; applications of Big Data methods carried out by the DEXL Data Management laboratory; studies in cryptography and cyber security applied to sensor networks (with applications in IoT); research in Numerical Analysis, PDEs, stochastic systems and controls, digital signal processing methods, among others, complement this list of our assets. Its Incubator plays a unique role in integrating the local and regional entrepreneurial ecosystem and promoting technological innovation, serving as a link between the academic environment and the private sector, fostering interaction among researchers, entrepreneurs, investors, and government institutions. Among its actions are the search for local skills and strengthening of business partnerships. In its over 40 years of existence, LNCC and its body of researchers, technologists, analysts, professors, students, and collaborators have achieved recognition for their scientific, technological, and innovative activities, reaffirming their commitment to national science as a fundamental state policy for the country's strengthening.



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# MISSION

Considering its legal assignment and its capabilities, LNCC's mission is: i. To conduct research and development in scientific computing, particularly in the creation and application of mathematical and computational models and methods to solve scientific and technological problems; ii. To develop and manage high-performance computing environments that meet the country's needs; and iii. To train human resources, promoting technology transfer and innovation

# RESEARCH AREAS



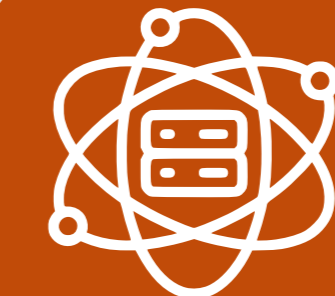
## BIOINFORMATICS AND COMPUTATIONAL BIOLOGY

- Molecular recognition modeling of receptor-ligand interactions;
- Protein structure prediction;
- Drug design;
- Biotechnological applications and genomic surveillance;
- Host-pathogen interaction study;
- Conceptual models of biological systems.



## HEALTH

- Tumor Growth Modeling;
- Medicine Assisted by Scientific Computing;
- Modeling in Hemodynamics;
- Human, Animal, and Plant Health.



## DATA SCIENCE

- Analysis and Management of Large Volumes of Data (Big Data);
- Artificial Intelligence (AI);
- Deep Neural Networks and Machine Learning;
- Metaheuristics in Engineering;
- Network Science;
- Reproducibility of Experiments;
- Management of Learning Models.



## HIGH-PERFORMANCE COMPUTING (HPC)

- Parallel and distributed computing methods;
- Collaborative and multimedia environments - virtual reality;
- Code and scientific workflow optimization;
- High-Performance Computing, Parallel Programming, and performance optimizations of scientific applications.



## ENERGY

- Computational Modeling of Reservoir Geological Fluid Extraction;
- Modeling of Geological Carbon Dioxide Storage;
- Subsurface Hydrogen Storage;
- Applications in Renewable Energy.



## MATHEMATICAL METHODS AND ALGORITHMS

- Mathematical modeling and computational simulation;
- Multiscale modeling;
- Topological optimization;
- Algorithms and numerical analysis;
- Epistemic uncertainty modeling.



## CRYPTOGRAPHY

- Post-quantum cryptographic algorithms;
- Computing in untrusted systems;
- Security and privacy;
- Artificial intelligence (AI);
- Quantum computing and quantum cryptography.



## SYSTEMS AND CONTROL

- Stabilization of dynamic systems;
- Stochastic control;
- Digital signal processing;
- Signal Processing Laboratory.

Supercomputador  
*Santos Dumont*

Research  
groups

**LNCC**

<https://www.lncc.br/grupodepesquisa>

## LABINFO

The LABINFO conducts research in Bioinformatics and Computational Biology and utilizes the processing infrastructure of LNCC, including the Santos Dumont supercomputer. It is associated with the Computational Genomics Unit "Darcy Fontoura de Almeida" (UGCDFA), a state-of-the-art sequencing facility. Due to the large amount of data generated by large-scale DNA sequencing, it employs High Performance Computing techniques and methodologies in the areas of Artificial Intelligence and Big Data, allowing for greater agility in processing and analyzing the generated data. With experience in Genomics, transcriptomics, metagenomics, exome, phylogenomics, and small RNAs, it conducts research in the areas of human, animal, and plant health, as well as in biotechnological applications. Since 2020, it has been involved in sequencing and genome analysis studies of the virus and samples from COVID-19 patients in collaboration with national institutions.

**Coordination: Ana Tereza Ribeiro de Vasconcelos**

<https://www.labinfo.lncc.br/#/>

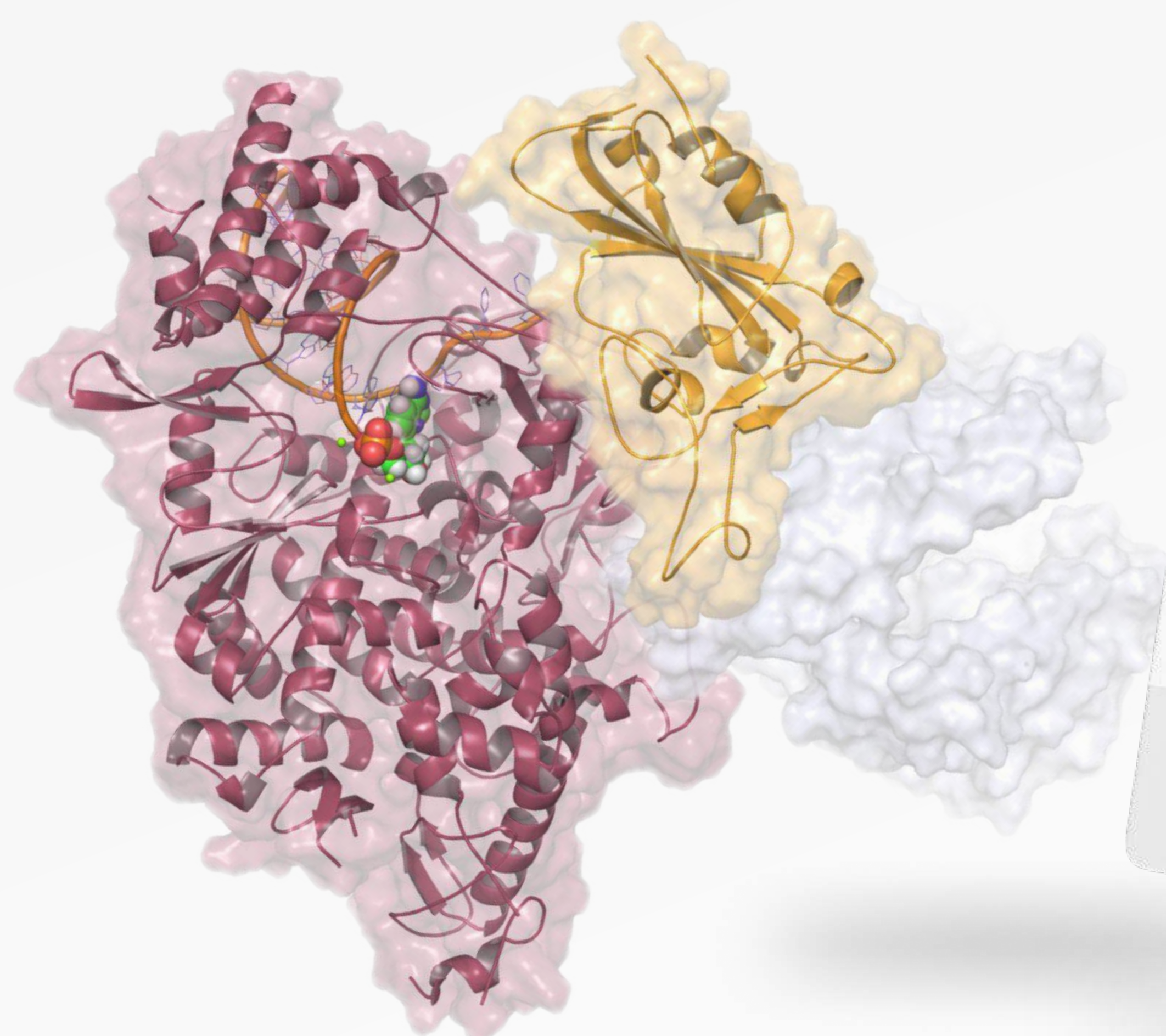


IMAGEM: LNCC E DOCKTHOR

## GMMSB

The GMMSB Group, part of the National Laboratory for Scientific Computing (LNCC) under the Ministry of Science, Technology, and Innovation (MCTI), is a dynamic, multidisciplinary research team based in the mountain city of Petrópolis, Rio de Janeiro. Established in 2002, the GMMSB brings together expertise in biology, physics, applied mathematics, artificial intelligence and high-performance computing. The primary focus lies in advancing computational methods for rational drug design, ab initio protein structure prediction, and quantum calculations of biological macromolecule electrostatic properties. We also play a pivotal role in LNCC's Computational Modelling post-graduate program, offering Master's and Ph.D. degrees to students from diverse scientific backgrounds, including biology, chemistry, physics, mathematics, computer science, and engineering.

**Coordination: Laurent Dardenne**

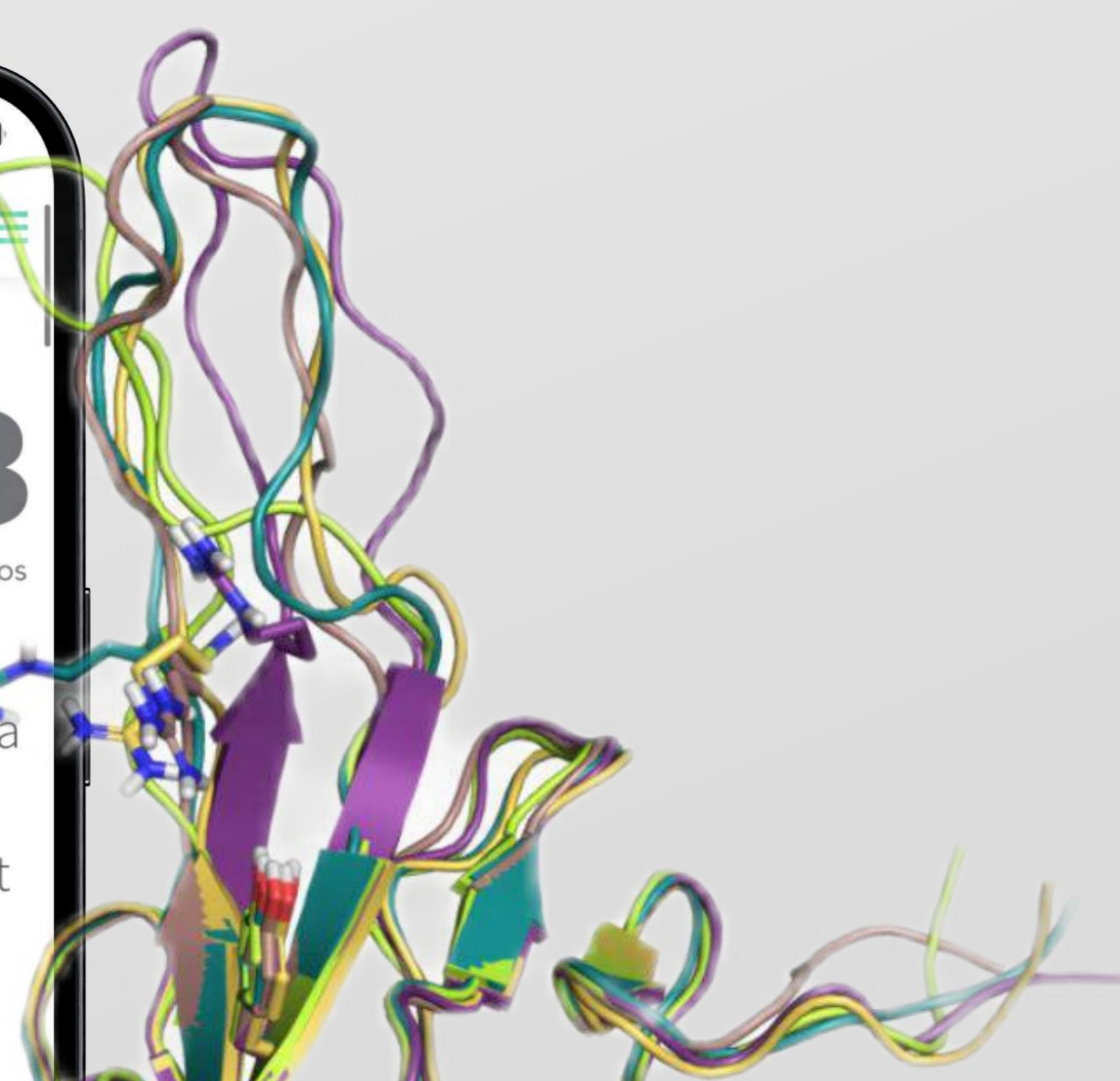
<https://www.gmmsb.lncc.br>

## DOCKTHOR-VS

The DockThor-VS web server is a platform developed for large-scale virtual screening of compounds to identify and design novel drug candidates. The DockThor-VS web server was developed by the Molecular Modeling of Biological Systems Group (GMMSB), which conducts interdisciplinary research spanning areas such as biology, physics, applied mathematics, artificial intelligence and high-performance computing. DockThor-VS is connected to the Brazilian supercomputer, Santos Dumont, providing a dedicated and freely accessible service to the scientific community.

**Coordination: Laurent Dardenne**

<https://dockthor.lncc.br/v2/>

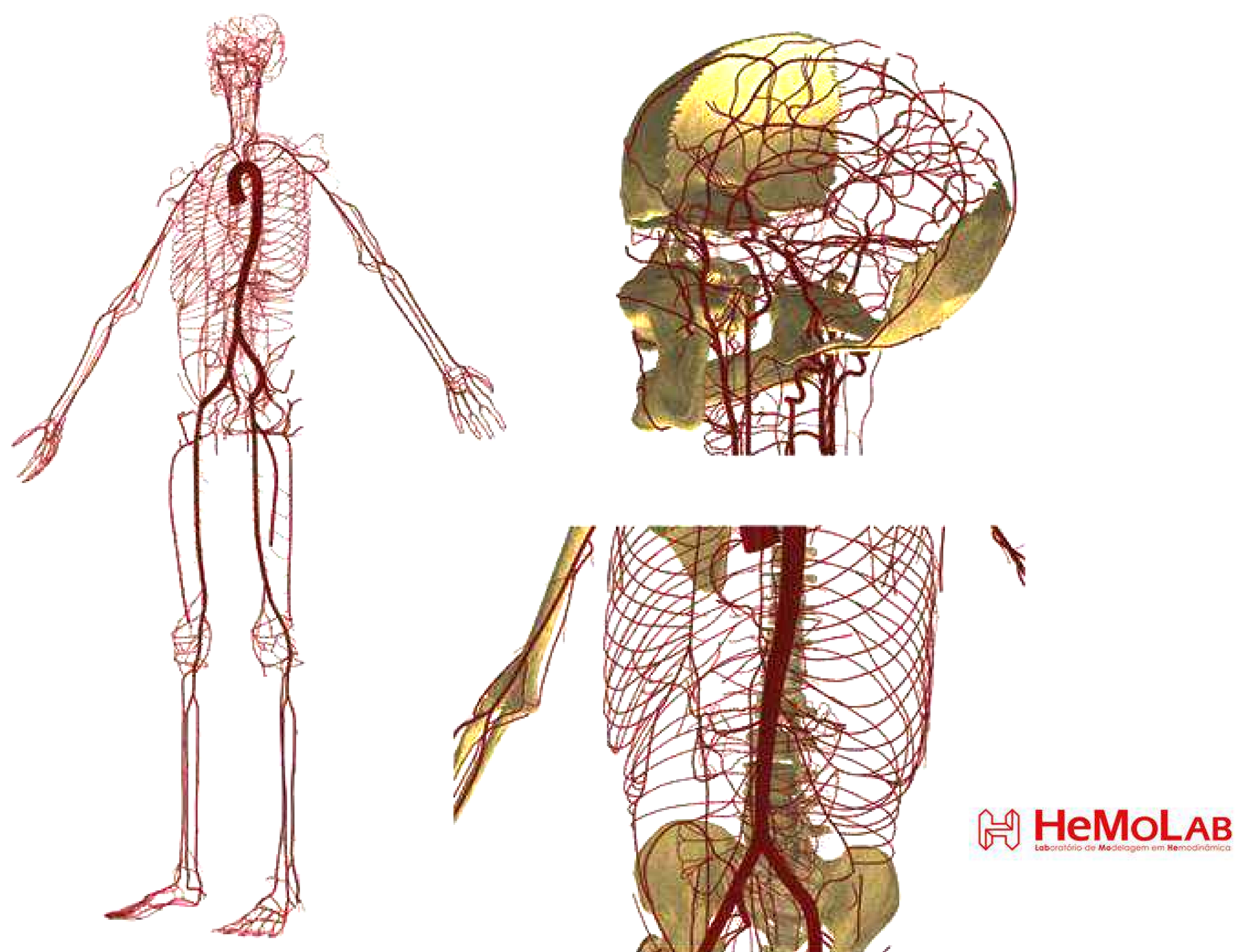




## BAMC

The aim of Research Group "Biology Applied to Mathematical and Computational Modelling" (BAMC) members is to create and develop mathematical and computational constructs, concepts, objects, and spaces that are better adapted to the description and study of life phenomena, indeed complex phenomena at large. To achieve this, we rely on knowledge gained from hands-on mathematical and/or computational modelling of biological and ecological phenomena, as well as of phenomena associated with diffusion of knowledge. If we consider phenomena as a set of interacting things that change due to interactions, there are at least two fundamental differences between physical or chemical phenomena and biological or complex ones. First, in physical and chemical phenomena, the possibilities of interaction between phenomenological components never vary with the unfolding of the phenomenon, whereas in biological and complex phenomena, the possibilities of interaction between elements in this set may vary widely at any instant. Second, biological phenomena are inherently multi-scale and occurrences at different scales cannot be studied separately as in most physical and chemical phenomena, given that phenomena at a given scale can be components of phenomena at another aggregation scale.

**Coordination: Maurício Vieira Kritz**



## HEMOLAB

The HeMoLab (Hemodynamics Modeling Laboratory) group is, since 2006, a R&D group within the National Laboratory for Scientific Computing (LNCC/MCTI). Background areas of HeMoLab team members and collaborators are Engineering, Computer Science, Mathematics, Physiology, Cardiology, Anatomy and Physics. Core activities are related to the modeling and numerical simulation of physiological systems, more specifically the cardiovascular system. Research efforts are concentrated towards developing coupled and multiscale physical models based on variational foundations, as well as to develop and implement numerical approximations based on the Finite Element Method, the Finite Volume Method and the Lattice-Boltzmann Method. Blood flow models, fluid structure interaction, wave propagation phenomena, medical image processing, constitutive multiscale modeling and parameter identification procedures are some of the activities of the group. Software development targeting distributed computing systems is a continuous concern with the aim of popularizing modeling and simulation tools and facilitate their use in real large scale problems

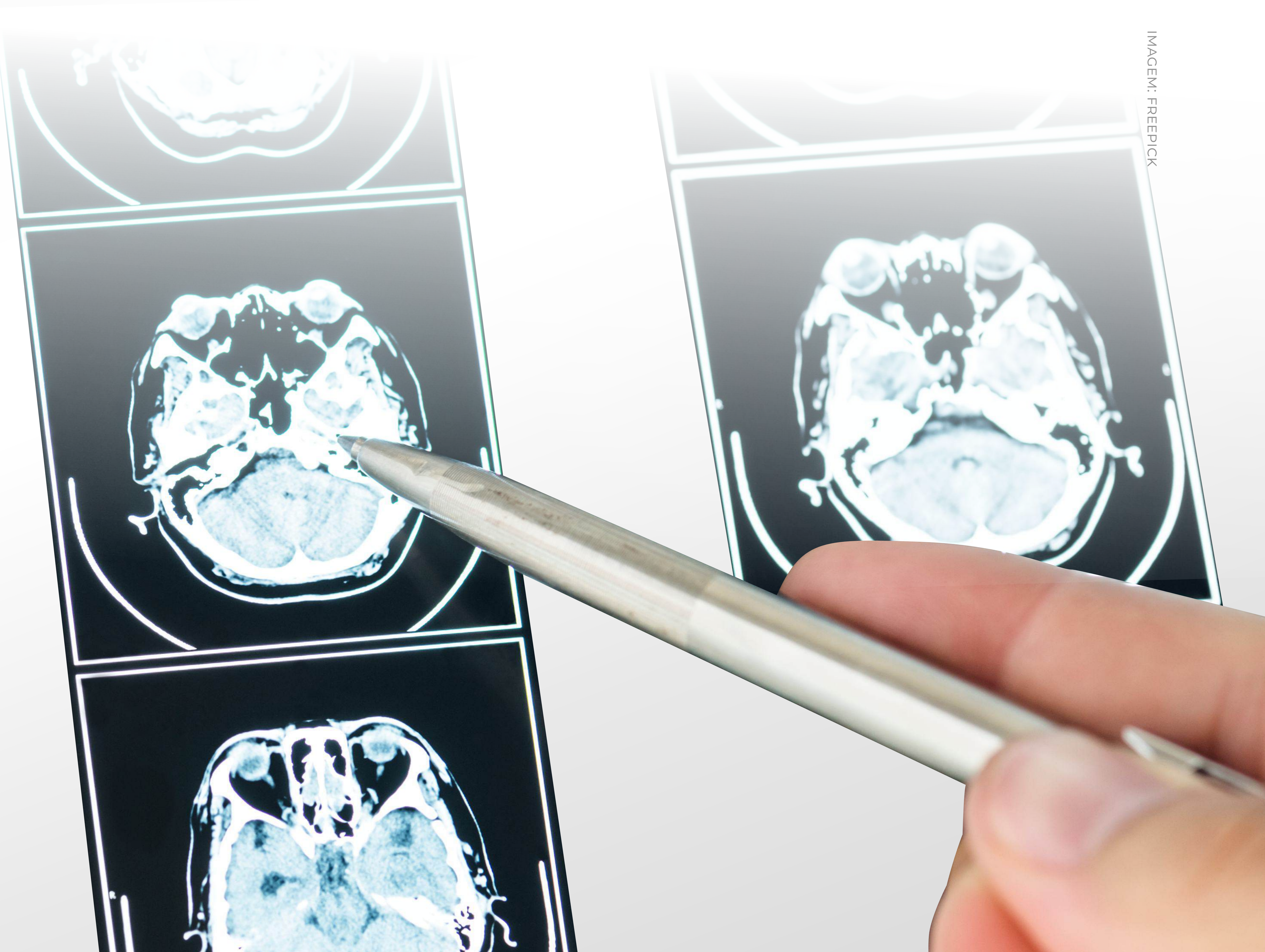
**Coordination: Pablo Javier Blanco**

<http://hemolab.lncc.br/>

## TMG

The main goal of the Tumor Modeling Research Group is to develop predictive mathematical and computational models for the initiation, growth, and decline of tumors in response to various treatment modalities. Using a theoretical framework based on biological and physical principles, the cancer hallmarks, and empirical data, we integrate a variety of components of predictive science that enable dealing with the selection, calibration, and validation of models in the presence of uncertainties. We develop classes of hybrid models and numerical methods that are employed to represent events at the molecular, cellular, and tissue levels. Our central hypothesis is that the new methodologies developed by the team can provide a valuable approach to cancer therapies, contributing significantly to reducing deaths. The research results from interdisciplinary efforts in different areas, including essential knowledge of applied mathematics, numerical and computational methods, and theoretical cancer biology.

***Coordination: Regina C. Almeida***



## DEXL

The Data Extreme Lab is a research group of the National Laboratory of Scientific Computing (LNCC) involved in research, development and graduate studies in Data Science, Artificial Intelligence and Big Data. Our work is founded in Computer Science principles, techniques and methods to be applied to problems raised in different disciplines, such as: Astronomy, Biodiversity, Oil and Gas, Sport Science, Smart Cities etc. The DEXL group was granted the coordination of the National Institute of Science and Technology (INCT) in Data Science, a national initiative to orchestrate the development of Data Science in Brazil involving Universities and Research Institutes. In 2018, the DEXL Lab organized the 34th International Conference in Very Large Data Bases, held in Rio de Janeiro, and attracting more than 800 top researchers from all around the world.

**Coordination: Fábio Porto**

<https://dexl.lncc.br/>

**DEXL**  
DATA EXTREME LAB

## IIA-LNCC

The advancements in artificial intelligence have broad implications across various spheres such as economy, society, education, and the environment. Therefore, it is crucial for the Brazilian scientific community to be aligned with innovations worldwide and be able to attract and retain talent both in institutions and in higher education universities.

In this context, the creation of the Artificial Intelligence Institute at LNCC (IIA-LNCC) emerges as an initiative aligned with the goal of boosting research and technological development in the country, especially through support for initiatives led by the Ministry of Science, Technology, and Innovations (MCTI). This aims to establish an effective channel of communication with the national and international community in the field, representing an initial milestone in this journey.

**Coordination: Fábio Porto**

<https://instituto.ia.lncc.br/pt>



Instituto de  
Inteligência Artificial



## COMCIDIS

The ComCiDis group has been working since 2002 on the topic of Distributed Scientific Computing and Applications, focusing on the development of the computational environment, interfaces, and applications, with the aim of facilitating execution within the deployed environment. The group's mission is the development and study of distributed scientific computing environments at the national level, integrated through a scalable computational infrastructure of clouds, grids, and geographically distributed clusters in different centers of the country, capable of providing reliable, consistent, and cost-effective access to computational resources (equipment, applications, and services).

**Coordination: Bruno Schulze**

<http://comcidis.lncc.br/>



## PIVC

In the Image Processing and Scientific Visualization group, research is conducted in the area of image processing and analysis, focusing on segmentation, restoration, classification, synthesis, and feature extraction. For these tasks, both traditional techniques and machine learning methods are applied. Additionally, we also work with computer graphics techniques and modeling for scientific visualization and computational animation.

**Coordination: Gilson Antonio Giraldi**

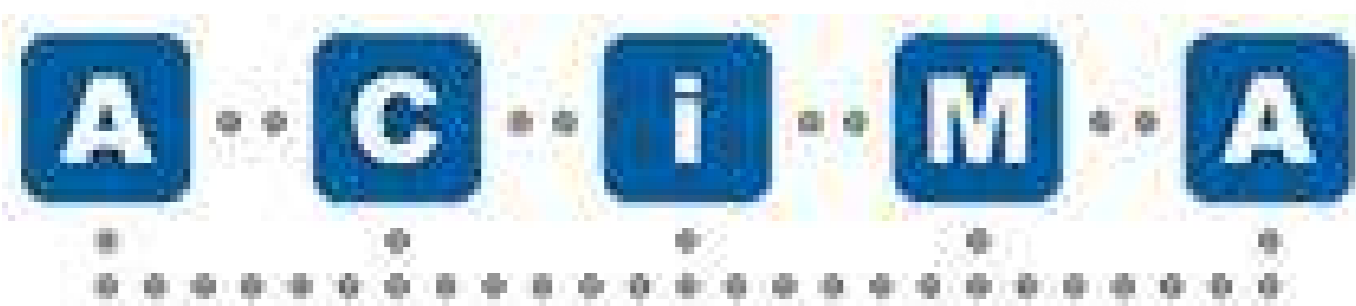


## ACIMA

Virtual environments are implementations of Virtual Reality systems, where a user is immersed in a synthetic world controlled by computers. In such synthetic world, the user can have experiences of interest. Training and motor rehabilitation have been areas of exploration for such environments, which can also be collaborative, when a group of users interact with one another through the system. Another type of system that can also be explored in such context is one that uses augmented reality, where instead of the user being immersed in a completely synthetic world, virtual content of interest is simply added to the real world.

**Coordination: Jauvane Oliveira**

<http://acima.lncc.br/>



## CAD

The development of software enabling efficient utilization of computational resources from SDumont and High-Performance Computing (HPC) machines, in general, is a complex task requiring highly specialized human resources. The CENAPAD/LNCC research group aims to assist in the development of efficient and scalable applications on HPC machines in collaboration with scientific computing research groups and to offer human resource training courses in the field of HPC. The group conducts research in parallel programming, distributed programming, parallel data I/O, scientific workflows, and Artificial Intelligence applied to HPC. Finally, the HPC group also conducts research to enable efficient utilization of computational resources offered by the web portal for users lacking expertise in parallel programming.

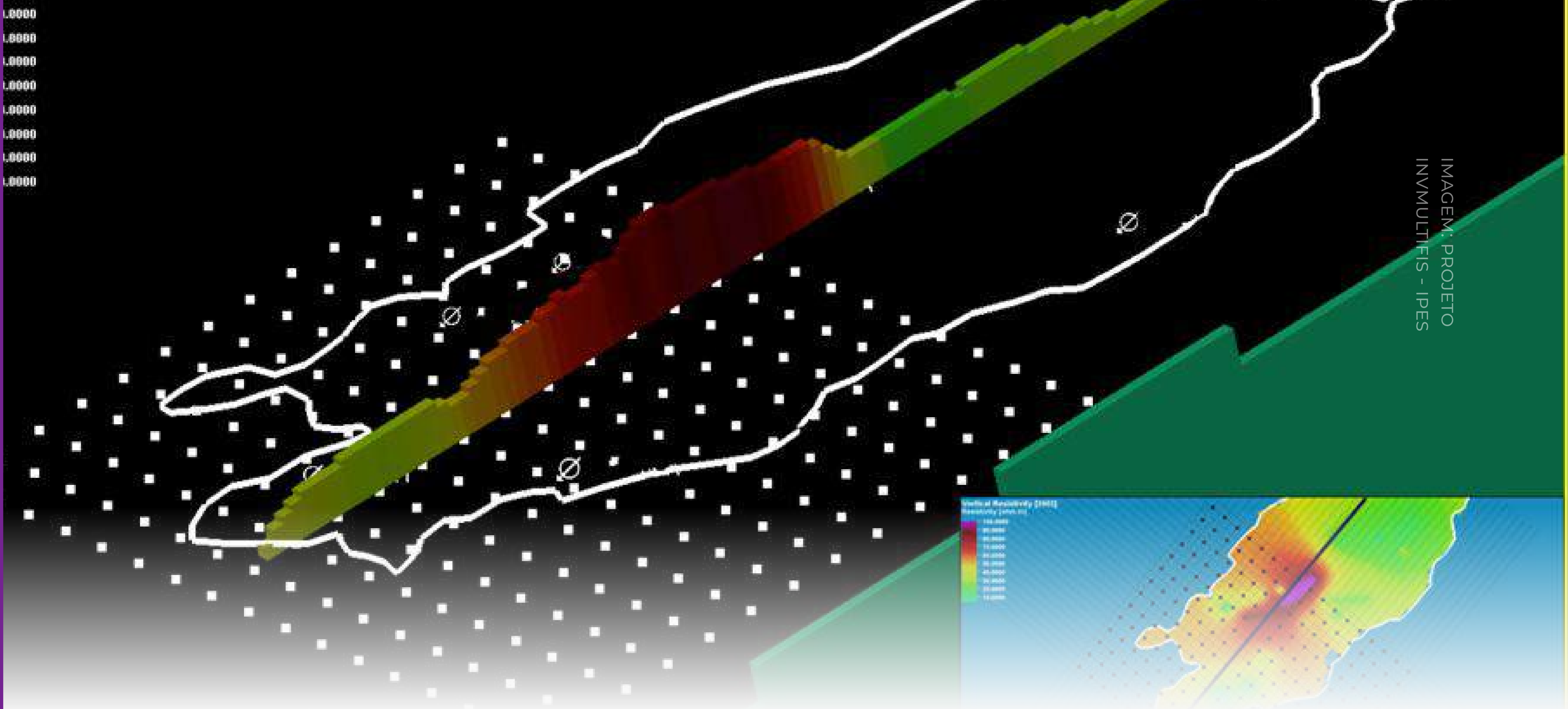
**Coordination: Carla Osthoff**

## COMOPORE

The mission of the COMOPORE group (Computational Modelling of Porous Materials) is the development and implementation of new multi-scale computational models to describe the hydro-mechanical coupling in processes related to hydrocarbon prospecting in petroleum reservoirs, as well as the construction of computational tools to integrate fine scale information in commercial simulators used by industry.

**Coordination: Márcio Murad**

<https://comopore.lncc.br/>



## ESDA

The research group on Dynamic Systems Stabilization and Applications (ESDA) aims to study vibration problems by investigating the physical modeling of oscillation issues and their stabilization, with applications to engineering. Our primary focus is on the Optimal Design problem. This problem involves determining the location where a dissipative mechanism should be applied so that, at that position, the mechanism stabilizes oscillations in the shortest time possible. This problem is extensively studied by engineers in the construction of bridges or long structures where oscillations are amplified and can grow uncontrollably, thereby compromising the structure. From a mathematical perspective, this problem is still not highly developed. Engineers solve these problems through high-precision models where stabilization tests are conducted. Therefore, both the mathematical problem and computational modeling are currently under active development, giving a high degree of relevance to the problem we are addressing.

**Coordination: Jaime Rivera**

## IPES

The Innovative Parallel numerical Solvers (IPES) Research Group aims to develop, analyze, and validate new multiscale numerical models and methods through modern mathematical and computational techniques and strategies for use in massively parallel architectures, contributing to the development of state-of-the-art scientific research and training of human resources with a strong multidisciplinary character.

**Coordenação: Antônio Tadeu A. Gomes**

<http://ipes.lncc.br/>

## MIE

In the Uncertainty Modeling Research Group (MIE), the aim of this project is to study how these uncertainties can be determined and how to incorporate the knowledge of these factors into simulations to obtain reliable solutions, including considering uncertainties in the choice of physical/mathematical model.

**Coordination: Renato Simões Silva**



IMAGEM: PROJETO MULTIFIS - IPES

IMAGEM: FREEPICK

## MACS2E

The objectives of this group are mathematical and numerical modeling, mathematical and numerical analyses, and computational simulation to solve problems in sciences and engineering. The activities of this group are part of the Brazil-China Cooperation in Scientific Computing and the China-Brazil Center for Scientific Computing (CBCSC).

**Coordination: Jiang Zhu**

## GCQC

The mission of LNCC's Quantum Computing group is to conduct original research in the areas of quantum computing and quantum information, supervise master's and doctoral students, seek national and international collaborations to enhance the quality of the group's research, propose new techniques, and, if possible, participate in the development of quantum hardware. To achieve this mission, the quantum computing group develops and implements quantum algorithms based on quantum walks on IBM quantum computers and conducts computational simulations of quantum systems and quantum computing using high-performance computing (HPC) employing the following languages: Python, C, OpenCL, CUDA, and Nebula. The group also develops simulators for HPC platforms aimed at researchers working in both quantum computing and quantum mechanics. Group members also use algebraic computing languages, with advanced knowledge in languages such as Mathematica and Maple.

***Coordination: Renato Portugal***



## GCON

Signals and Systems (or Systems and Control) research encompasses, fundamentally, mathematical-computational problems involving differential and difference equations, often arising from the mathematical representation of analysis and decision problems in engineering and economics. Some emblematic problems in this area are those of analyzing the stability and performance of systems and synthesizing controllers, estimators, and filters for signal processing, as well as financial modeling. These problems can be investigated using various mathematical models for systems, which can be deterministic or stochastic, in continuous time or discrete time, linear or nonlinear, with constant or time-varying coefficients, finite or infinite dimension, and involving different types of uncertainty ("set-theoretic" or probabilistic, parametric or non-parametric). At LNCC, this research area has been active since the early 1980s, focusing today on the general themes of system stability, stochastic control and applications, control and filtering in the presence of modeling uncertainties, acoustic and electrical signal processing, and stochastic methods in finance.

***Coordination: Marcos Todorov***



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