National Laboratory for Scientific Computing











LNCC's Perspectives

on

Brazil-France Collaboration

after

HOSCAR







at a

GLANCE

Research and Development





LNCC

Focus on Computational Modeling in Sciences and Engineering and High-Performance Computing

Promote Excellence in R&D on Fundamental and Application Subjects

Offer an innovative Graduate Program in Computational Modeling

Provide Computing Facilities, Systems and Networking, to the National Academic and Research Community

History

LNCC was created in 1980 under the sponsorship of the Ministry of Science, Technology and Innovation (MCTI). Facilities are located in the city of Petrópolis, State of Rio de Janeiro since 1998

Upshot

LNCC is one of the 16 research units of the Ministry of Science, Technology and Innovation

LNCC is a reference in Scientific Computing in Brazil





Research and **Development**

Observation LNCC Physical Concepts Mathematical Model Mathematical Analysis Numerical Model Validation with Observation

Basics

Computational Modeling Fluid Dynamics and Porous Media Flow **Transport Phenomena** Geophysics

Numerical Methods **Finite Element Optimization and Inverse Algorithms**

System, Control and Signals **Control of Dynamic System Robust Signal Estimation**

Computation Bia Data **Complex Dynamics Network** HPC and Cloud Computing

Oil and Gas

Applications

Computational Biology

Medicine Assisted by **Scientific Computing**

Data Science





Oil and Gas

Multiscale Modeling of Porous Media Flow with Geomechanical



Goal

Development of new computational Models for solving multiscale flow in Oil and Gas reservoirs sensitive to stress changes in the rock matrix

Challenge

Improvement of the computational efficiency to describe fault activation in pre-salt and sandstone reservoirs

Partnership: PETROBRAS





Gas injection in heterogeneous media

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Tracer injection

Computational Biology

Bio-Informatics Molecular Modelling Neuroscience

Population Dynamics



Goals

Development and application of methods, algorithms and programs for

- Structure-Based Rational Drug Design
- Template-Free Protein Structure Prediction

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Challenge

Development of new algorithms and methods to free energy landscapes and extract information about ligandreceptor binding affinities and identify protein native structures.



Computational Biology

Bio-Informatics Molecular Modelling Neuroscience Population Dynamics

Goal

Innovative numerical methods of multiscale type ameliorates modeling heterogeneous dendrites







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Medicine Assisted by Scientific Computation

Imagery Reconstruction Scientific Visualization

Goal

Development of theoretical and computational predictive tools to quantify anatomic structure and physiologic response of the human vascular system

Visualização do interior da carótida - endoscopias virtuais-





Challenges

Diagnostics for the public heath system

Early warning systems for cardiovascular problems

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Planning of **chirurgical interventions**

Data Science

Goal

Exploring data management, representation and analysis techniques to support scientific applications

Challenges

Scientific Query Processing

Scientific Workflow Data Management

Semantic Data Modeling



LNCC's Perspective

for

2020

Major Challenges in Scientific Computing

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The Major Challenge in Scientific Computing

SOLVING

BIG

PROBLEMS (Strong Basics)



A shale gas problem: nano, meso, micro and macro scales presented

Growing size of scientific and technological problems

Modern computer technologies are based on **multi-processor machines**: massively parallel machines with combination of distributed memory, shared memory, vector processing, accelerators (like the GPU's)

Many problems are **not parallelized** or **scaling** to **large number of processes** as they are limited by memory transfer speed

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Major Challenge in Scientific Computing

Basics: To be continued, but...



A shale gas problem: nano, meso, micro and macro scales presented

Challenge

General View

To **adapt/develop** current applications to the new **massively parallel computer** architectures

The challenge will be even greater with the **exascale computers** (2020 ->) – Millions of simultaneous processes New ``**Divide and Conquer**'' **methodologies** are fundamental

Impact the design **of numerical methods and algorithms** to make full use of the new architectures

Integrated work between **computer** scientists and mathematicians/engineers





INRIA – LNCC Collaboration

at the

PRESENT

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Associate Team Projects

Long-Term Collaborations

HOMAR "High Performance Multi-Scale Algorithms for Wave Propagation Problems" (LNCC and NACHOS Project-Team)

Innovative high performance numerical methods particularly well suited to the simulation of multiscale wave propagation problems

MUSIC "MUltiSite Cloud data management" (LNCC and ZENITH Project-Team)

Develop a multisite cloud architecture for managing and analyzing scientific data, including support for heterogeneous data; distributed scientific workflows, and complex big data analysis

martin



Bio-Informatics

Dynamics Networks



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in the

HORIZON 2020





HPC4E Project

High Performance Computing for Energy

GOAL

Apply the new **exascale HPC** techniques to energy industry simulations and going **beyond the state-of-art** in the required HPC exascale simulations for different energy sources

APPLICATIONS

Oil and Gas

Wind

LNCC

Biomass

PARTNERS

BRAZIL: COPPE, LNCC, UFRGS, UFPE, ITA, PETROBRAS

EU: BSC, INRIA, LANCASTER UNIV., CIEMAT, REPSOL, IBERDROLA, TOTAL

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INRIA-BULL-LNCC partnerships

Identify common interests and propose **projects on demand**

- Big Data
- Massive Numerical Methods

Involve **interchange** of students and researchers

Establish partnerships with **Brazilian industry**

Petrobras, Embraer, Embrapa,...



1.1 Petaflop Computer Santos Dumont







Strengthening Cooperation

Promote novel Associate-Teams **Dynamics Network (Dante Team-Project) Oil and Gas Molecular Modeling** Cardio-Vascular System

Intensify interchange of researchers and students co-advising

Laboratório Nacional de Computação Científica



Modelagem Computacional Programa de Pós-Graduação do LNCC



Av. Getulio Vargas 333, Quitandinha . Petropolis, RJ . Tel.: 24 2233-6024

→) 10/08 a 23/10/2015 / 2016



Computação Científica Controle e Filtragem de Sistemas Dinâmicos Modelagem de Biossistemas e Bioinformática Modelagem de Circulação e Transporte Modelagem de Equilíbrio e Otimização

OFAPERJ

Master and Ph.d Program at LNCC



All Barland de

Gincia, Tecnologia e Brown, an

International Associate Laboratory





Inducing Multi-Lateral Collaborations

Building Bridges with Brazilian Labs

UNICAMP: Wave Propagation in Nano-Structures



Reinforcing Latin-American Cooperation (Stic- and Math-AMSUD)

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Chile Argentina Colombia





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Pedro Leite da Silva Dias

Director

diretoria@Incc.br

Frédéric Valentin

valentin@lncc.br

Head of the Dept. of Computational and Applied Mathematics

www.lncc.br



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