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Laboratório Nacional de Computação Científica
UNIDADE DE PESQUISA DO MCTI

Inria

Inria-LNCC-UDEC Workshop on Computational Fluids: Challenges and New Trends

March 14th, 2025

LNCC, Petrópolis

In the context of Inria's international initiatives in Chile (Inria Chile, the only Inria center abroad in Santiago since 2012, partner of many Chilean universities, including the Universidad de Concepción - UDEC) and in Brazil (Inria-Brazil program based on a partnership with LNCC, acting as a hub for the Brazilian research and innovation ecosystem), this Workshop aims to bring together research teams from Inria, LNCC and UDEC with expertise in computational simulation of realistic fluid flow problems with applications in areas such as energy, environment and medicine. The focus of this Workshop also includes the challenges and contributions of mathematical analysis, computational implementation on parallel machines and their interaction with machine learning techniques for the simulation of fluids.

Program

8:45-9:00 **Coffee**

9:00-9:15 **Welcome and introduction**

Fabio Borges de Oliveira (Director, LNCC), Patrick Valduriez (Director of Inria-Brasil, Inria) and Frédéric Valentin (Director of Inria-Brasil, LNCC)

9:15-10:45 **Session 1: Inria**

- Miguel Fernandez (Inria, France): *COMMEDIA: Computational Mathematics for Biomedical Applications*

- Géraldine Pichot (Inria, France): *SERENA: Simulation for the Environment: Reliable and Efficient Numerical Algorithms*

- Konstantin Brenner (Université Côte-d'Azur and Inria, France): *Preconditioned Newton's Method for Richards' Equation*

10:45-11:00 Coffee-Break

11:00-12:30 **Session 2: UDEC/UC and LNCC**

- Nicolas Barbafi (Universidad Católica, Chile): Fully Nonlinear Poroelastic Media: Approximation, Solution, and Applications

- Marcio Murad (LNCC, Brazil): *Computational Modeling of Porous Materials: 40 Years of the COMOPORE Team in Porous Media Science*

- Frédéric Valentin (LNCC, Brazil): *Computational Fluids in the Innovative Parallel numErical Solvers (IPES) Research Group*

12:30–14:30 Lunch

14:30-16:00 **Session 3: LNCC**

- Pablo Blanco (LNCC, Brazil): *Assessment of cerebral reperfusion during normothermic regional perfusion for organ transplant using a closed/loop anatomically detailed arterio-venous blood flow model*

- Antonio Tadeu Gomes (LNCC, Brazil): *On the Interplay of Scientific Machine Learning and Multiscale Numerical Methods: the Perspective of the IPES Research Group*

- Alexandre Madureira (LNCC, Brazil): *Spectral ACMS: A Robust Localized Approximated Component Mode Synthesis Method*

16:00-16:30 Coffee Break

16:30-17:30 Free Discussion on International Cooperation
Moderators: Miguel Fernandez, Rodolfo Araya and Frédéric Valentin

Scientific Committee

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COMMEDIA: Computational Mathematics for Biomedical Applications

Miguel Fernandez (Inria, France)

SERENA: Simulation for the Environment: Reliable and Efficient Numerical Algorithms

Géraldine Pichot (Inria, France)

I am part of the SERENA project team at Inria Paris, France. The SERENA project-team is concerned with numerical methods for environmental problems. The main topics are the conception and analysis of models based on partial differential equations, the study of their precise and efficient numerical approximation, and implementation issues with special concern for reliability and correctness of programs. We are in particular interested in guaranteeing the quality of the overall simulation process.
After an overview of the team, I will focus on simulating subsurface flow, particularly in fractured porous media. My main interest is in preserving the geometrical complexity of fracture networks when performing flow simulations. The discretization process leads to large-scale linear systems. I will present various methods we use to reduce computational costs, from efficient polytopal approaches such as Hybrid High-Order methods to robust domain decomposition preconditioners like HPDDM. Additionally, I will share some preliminary results that leverage a posteriori error estimates for adaptive mesh refinement and coarsening.

Preconditioned Newton's Method for Richards' Equation

Konstantin Brenner (Université Côte-d'Azur and Inria, France)

Richards' equation is essential in hydrogeological modeling. It serves as a generalization of the famous Darcy's law, allowing for the description of water movement in soils under both saturated and unsaturated conditions. However, despite its importance for practical applications, this equation has gained a poor reputation due to the difficulties encountered in its numerical resolution. In fact, solving the algebraic systems that arise from its discretization can become problematic due to the stiffness of the nonlinear closure laws. After a brief introduction to Richards' equation, from both hydrogeological and mathematical perspectives, I will present some nonlinear preconditioning methods aimed at improving the performance of the associated

Newton's method. Specifically, I will discuss traditional techniques based on the careful selection of primary variables, as well as more recent approaches involving domain decomposition methods. The latter are particularly interesting, both numerically and theoretically, as they allow for global convergence analysis.

Fully Nonlinear Poroelastic Media: Approximation, Solution, and Applications

Nicolás Barnafi (UC, Chile)

Fully nonlinear poroelastic equations provide a daunting task for scientific computing, as they are the coupling of two difficult problems: nonlinear elasticity and generalized porous media equations. In this talk I will give an overview of the model, and show some difficulties that are intrinsic to the nonlinear structure of the problem. After this, we will see how these equations can be robustly discretized and solved with Krylov subspace methods in an HPC framework through block partitioned strategies relying on a spectrally equivalent approximation of the Schur complement. The talk will close with some on-going research on thermo poroelastic media and applications in biomedicine.

Computational Modeling of Porous Materials: 40 Years of the COMOPORE Team in Porous Media Science

Marcio Murad (LNCC, Brazil)

We present the fundamental principles underlying the research conducted by our group, which has been at the forefront of Computational Modeling of geobodies with particular emphasis on coupled processes. Our work has focused on understanding and describing the behavior of rocks in the context of energy extraction and CO_2 sequestration in subsurface environments. We explore several key areas of this research, including the coupling of multiphase flow in deformable porous media, with an emphasis on the complexities and challenges associated with modeling carbonate rocks, which are critical in various energy-related applications. Additionally, we highlight our ongoing efforts in the development of Mixed-Dimensional flow models, particularly as they apply to fractures within subsurface formations. These models incorporate both fluid dynamics and geomechanical effects, enabling a more comprehensive understanding of fracture behavior and its impact on energy extraction and CO_2 storage. The integration of these diverse modeling approaches is crucial for advancing our ability to predict and optimize subsurface processes, with significant implications for sustainable energy practices and environmental management.

Computational Fluids in the IPES (Innovative Parallel numErical Solvers) Research Group
Frédéric Valentin (LNCC, Brazil)

The IPES Research Group at LNCC aims to develop, analyze and validate new numerical methods for solving differential equation models using modern mathematical and computational approaches for use in massively parallel architectures combined with artificial intelligence techniques. In this talk, we present the IPES Research Group and the group's latest advances in computational fluid simulation with particular emphasis on multiscale finite element methods applied to the Darcy and (Navier-)Stokes equations.

Assessment of Cerebral Reperfusion during Normothermic Regional Perfusion for Organ Transplant Using a Closed/Loop Anatomically Detailed Arterio-Venous Blood Flow Model

Pablo Blanco (LNCC, Brazil)

In this presentation, we will apply an anatomically detailed closed-loop model of the cardiovascular system to assess potential brain reperfusion during normothermic regional perfusion (NRP). Normothermic Regional Perfusion (NRP) is a rapidly growing organ recovery technique. However, there remain concerns that NRP could result in meaningful cerebral perfusion. We compare different scenarios: 1) Reference model (living); 2) NRP (distal aortic and caval cannulation, thoracic clamp and distal ligation of cava and aorta); 3) NRP with aortic arch drainage to reservoir (0mmHg). Results will be discussed in detail, providing insight into best NRP practices for brain reperfusion risk minimization.

On the Interplay of Scientific Machine Learning and Multiscale Numerical Methods: the perspective of the IPES research group

Antonio Tadeu Gomes (LNCC.Brazil)

In this talk, we discuss some of the initiatives of our IPES research group in integrating scientific machine learning techniques with domain decomposition strategies typically employed in multiscale finite element methods. We argue that such integration benefits both areas by making learning more scalable and at the same time leading to less computationally expensive numerical simulations. We are particularly interested in such integration involving neural network-based machine learning (e.g. physics-informed neural networks, deep operator networks) and the family of hybrid-mixed multiscale methods (MHM, for short).

Spectral ACMS: A robust Localized Approximated Component Mode Synthesis Method

Alexandre L. Madureira (LNCC, Brazil)

We consider two methods based on the Approximated Component Mode Synthesis approach to compute numerical solutions for two-dimensional symmetric elliptic partial differential equations with heterogeneous rough coefficients. The methods are based on submeshes, and we decompose the finite element spaces into bubble and harmonic components, which are orthogonal with respect to the bilinear form inner product. The bubble problems are local, and here we focus on how to efficiently solve the remaining global problem.

Our first method works for the low-contrast situation, and is based on LOD (Local Orthogonal Decomposition) ideas. The second method works for the high contrast case as well, and is constructed by adding to the multiscale space edge modes corresponding to carefully developed generalized eigenvalue problems.