New Challenges in the Numerical Simulation of Partial Differential Equations - V

Minisimposium at CNMAC 2024, September 16-20 - Porto de Galinas, PE https://www.cnmac.org.br/novo/

1 Introduction

As computational capacity continues to advance, the application of numerical formulations (e.g. using finite elements) emerges as a viable and attractive approach for obtaining reliable approximations of multiple quantities related to various physical phenomena in Science and Engineering. This progress opens the door for the application of innovative formulations, combined with advanced computational resolution techniques, to enhance the precision of studying complex problems involving singularities, coupled phenomena at various scales, etc.

Building upon the successes of previous events at CNMAC in 2010, 2016, and 2018, as well as at a workshop at UNICAMP in January 2020, this minisymposium aims to convene Brazilian researchers and esteemed foreign guests specialized in this field. The current fifth version will occur withing the activities of CNMAC 2024.

CNMAC (National Conference in Applied Mathematics) is a congress organized every year, since 1979, by the The Brazilian Society for Applied Mathematics (SBMAC). The scope is quite general and there are activities for a wide range of participants, from undergraduate and graduate students to young and more experienced researchers, including plenary guest talks, short courses, mini-symposia, contributed talks, and posters. CNMAC 2024 will happen in September 16-20 at Porto de Galinhas, a very nice beach in Pernambuco, in the northeast of Brazil (https://en.wikipedia.org/wiki/Porto de Galinhas).

1.1 Objectives

The primary objective of the mini-symposium is to facilitate a comprehensive discussion on participants' recent endeavors, ongoing projects, encountered challenges, and potential avenues for new collaborations. Furthermore, it is expected to spark interest among young researchers, comprising the majority of CNMAC participants, by providing a platform for insightful discussions and fostering a collaborative spirit within the scientific community.

1.2 Organizers

- Denise de Siqueira, UTFPR, PR
- Frederic Valentin, LNCC, RJ
- Sonia M. Gomes, Unicamp, SP

2 Program proposal

In this section we describe the plan of the mini-symposium, consisting of two sessions, of two hours each, and a plenary lecture. It is programed to occur on Thursday 19th and Friday 20th, September 2024.

2.1 Semi-plenary lecture of the CNMAC

 Blanca Ayuso de Dios - IMATI-CNR, Pavia Title: to be defined Abstract: to be defined

2.2 Plan of mini-symposium lectures

The following researchers have being contacted and declared interest in participating in the mini-symposium:

1. Amnon J Meir, Department of Mathematics, Southern Methodist University, US

https://www.smu.edu/dedman/academics/departments/math/people/faculty/ajmeir **Title:** On the Equations of Electroporoelasticity

Abstract: Complex physical phenomena and systems frequently involve multiple components, complex or coupled domains, complex physics or multi-physics, as well as multiple spacial and temporal scales. Such phenomena are often modeled by systems of coupled partial differential equations, or integro-partial differential equations, often nonlinear. One such phenomenon of interest is electroporoelasticity.

After introducing the equations of electroporoelasticity (the equations of poroelasticity coupled to Maxwell's equations) which naturally arise in geoscience, hydrology, and petroleum exploration, as well as various areas of science and technology, I will describe some recent results (well posedness), the numerical analysis of a finite-element based method for approximating solutions, and some interesting challenges.

2. Blanca Ayuso de Dios - University Milano-Biccoca, Italy https://orcid.org/0000-0003-4144-6984

Title: On the continuum limit of epidemic models on graphs **Abstract:** We consider an epidemic model defined on graphs and study the asymptotic behavior of the solutions as the number of vertices in the graph diverges. By relying on the theory of (graphons) we provide a characterization of the limit and establish convergence results. We also present approximation results for both deterministic and random discretizations. The analysis applies to dense and sparse graphs, including power-law networks. Extensive numerical results illustrate and assess the analytical findings. The results are based on joint work with Simone Dovetta (Politechnic of Torino) and Laura Spinolo (IMATI-CNR, Pavia).

3. Denise de Siqueira, UTFPR, PR

http://lattes.cnpq.br/8437756334087793

Title: Techniques for a posteriori error estimates inspired on the Prager-Synge Theorem

Abstract: A posteriori error estimation stands as a crucial technique for assessing and controlling errors in numerical simulations, providing a deeper understanding of solution accuracy and guiding adaptive mesh refinement. This talk explores the field of a posteriori error estimation, with particular emphasis on methods derived from the Prager-Synge theorem. The discussion covers recovery techniques and adaptive algorithms to derive error bounds and successful mesh refinement procedures. Numerical applications illustrate the effectiveness of these techniques in a variety of problems, including the Darcy problem, hybrid methods, and elasticity models.

4. Fabricio Simeoni de Sousa, USP/S. Carlos, SP http://lattes.cnpq.br/1361624597372651

Title: Development of efficient preconditioners based on multiscale domain decomposition methods for flows in porous media

Abstract:We present a new family of preconditioners for porous media flows based on the Multiscale Robin Coupled Method - MRCM. This domain decomposition method generalizes other discrete mixed multiscale methods by imposing Robin-type boundary conditions on the local problems. The MRCM is flexible and accurate, obtaining near-optimal scalability up to billions of unknowns in high-performance simulations, allowing the construction of efficient multiscale-based preconditioners for solving non-symmetric linear systems with Krylov subspace methods, such as GMRES.

5. Frederic Valentin, LNCC, RJ

http://lattes.cnpq.br/0635728154206559

Título: $H(div, \Omega)$ -optimality and fully computable a posteriori estimator for multiscale hybrid mixed methods

Abstract: The original Multiscale Hybrid-Mixed (MHM) method is a finite element method that naturally incorporates multiple scales while providing a primal solution with high-order accuracy. Local Neuman-type problems drive multi-scale basis functions and are embedded in the upscaling procedure, which are completely independent and therefore can be obtained naturally using parallel computing resources. In its one-level ver-

sion, the MHM method also provides an optimal convergent dual solution in natural norms (e.g. the velocity for Darcy model in space $H(div, \Omega)$). Unfortunately, the two-level MHM method loses this property when it adopts the computationally attractive option of maintaining the elliptical form of the local problems and approximating the basis functions using continuous piecewise polynomial interpolations. In the present work, we propose a new affordable local post-processing of the two-level MHM solution that releases a post-processed dual variable that recovers all the good properties of the one-level MHM solution. Furthermore, the postprocessed strategy leads to a fully computable a posteriori error estimator based on the equilibrated flux technique in the context of MHM methods. We conclude that the original two-level MHM method combined with the local post-processing and its associated a posteriori estimator becomes a competitive option for dealing with realistic multiscale problems when accuracy for both primal and dual variables on coarse meshes is required.

6. Jefferson W. D. Fernandes, UFMG, MG

http://lattes.cnpq.br/7825614402843839

Title: Improving Multiscale Hybrid Method high-contrast flows with the Steklov eigenvalue problem

Abstract: Porous media flows play a crucial role in various engineering and environmental contexts, exhibiting inherent multiscale and highcontrast characteristics due to the presence of heterogeneous materials or diverse loads. Standard numerical methods often struggle to maintain accuracy under such conditions. To enhance simulation performance, a multiscale approach becomes imperative, requiring effective techniques to incorporate minor scale effects on larger ones. However, in most multiscale methods an expressive reduction in flux complexity between macro domains is performed, leading to potential drawbacks in robustness and precision. This research addresses this challenge by proposing an eigenvector/eigenvalue analysis of boundary fluxes and selectively enriching them using a Steklov analysis. The numerical approximation yields values on the domain boundary, harmonically extended to the interior. Then, this analysis is taken into account to examine flux patterns in each subdomain through the associated Steklov problem, using it as an indicator to enrich the MHM approximation space. The effectiveness of these strategies is evaluated in the context of a Darcy flow problem within a maze-like domain, featuring a single connection between the inlet and outlet domain.

7. Johnny Guzman - Brown University, US

https://applied math.brown.edu/people/johnny-guzman

Title: Finite Element Exterior Calculus (FEEC) with smoother spaces **Abstract:** FEEC is now a well developed field of numerical analysis. It borrows from and makes connections with several other areas in mathematics (e.g. algebraic topology, geometric integration). A central topic in FEEC are Whitney forms which were originally developed by H. Whitney to prove de Rham's Theorem. In fact, Whitney forms were later, independently, discovered in two and three dimensions by J.-C. Nedelec and since then have been used in a wide variety of applications: electro-magnetism, solid mechanics, etc. Whitney orms form a discrete de Rham complex of a simplicial decomposition. The regularity of this complex is in some sense minimal, whereas in some applications forms with more regularity are more natural. In recent years with collaborators, borrowing ideas from the spline community we have developed forms that are smoother that also fit into discrete de Rham complexes. This led us to tackle two questions that were unresolved in our community: 1) Develop a discrete elasticity sequence on a simplicial triangulation in three dimensions and 2) justify why Lagrange elements on special meshes work for Maxwell eigenvalue problems.

8. Philippe R. B. Devloo - UNICAMP- FECFAU, SP http://lattes.cnpq.br/6051486998967925

Título: Iterative methods to solve saddle point problems

Resumo: Saddle point problems frequently appear in many mathematical and engineering applications. Most sets of partial differential equations with constraints give rise to saddle point linear systems. This is the case, for instance, when one uses mixed finite element formulations to solve fluid flows and/or elasticity problems under full incompressibility. Many direct and iterative methods have been proposed to overcome the challenges of saddle point problems due to indefiniteness and often poor spectral properties, such as the Schur complement and the Uzawa's method. However, each method rely on the sub-block matrices properties in order to ensure stability and convergence. In the context of mixed finite element for incompressible flows using stable H(div)-L2 spaces for velocity and pressure, respectively, we have been developing iterative methods that can effectively solve a saddle point problem by introducing a small compressibility to the original matrix allowing for the static condensation of pressures. The resulting matrix is symmetric positive-definite, which allows the usage of Cholesky decomposition or CG-like iterative solvers to compute the incremental solution for the velocities unknowns. The pressure correction was shown to be proportional to the unbalanced force caused by the compressibility perturbation, and can be explicitly updated during the iterative process once the velocity increment is obtained.

9. Sônia M. Gomes - UNICAMP-IMECC, SP

Title: Analysis of a two-scale stress-displacement mixed finite element method for elasticity problems

Abstract:We consider two-scale stress-displacement mixed finite element elasticity models using H(div)-conforming tensor approximations for the stress variable, whilst displacement and rotation fields represent multipliers to impose divergence and symmetry constraints. The discretization is based on general polyhedral meshes with flat faces in a global-local context. There are primary variables at the coarser level, solving normal stress trace (traction), piecewise defined over a partition of the mesh skeleton (faces), and piecewise polyhedral rigid motions. The fine details of the solution (secondary variables) are obtained by completely independent local formulations based on tetrahedral sub-partitions in each polyhedral sub-domain, the traction variable playing the role of boundary data. As compared to the traction accuracy, internal variables may be enriched with respect to internal mesh size, internal polynomial degree, or both. The sub-partitions do not have to match across subdomain interfaces, but a mild compatibility constraint is required. Stability and error estimates are proved for the method using a variety of two-scale space configurations associated to known stable single-scale space settings. Enhanced accuracy rates for displacement and super-convergent divergence of the stress can be obtained. Stress, rotation, and stress symmetry errors keep the same accuracy order determined by the traction discretization. Efficient computational implementation based on static condensation and numerical simulation results are presented to attest convergence properties of the method.