Numerical Challenges in PDEs - IV
Program and Book of Abstracts

Campinas, January, 24th, 2020

About the event

This workshop is realized by LabMeC-FEC, Unicamp, with the participation of Prof. Mark Ainsworth of Brown University as a special guest, and of researchers and graduate students from Unicamp and other institutions.

Scientific Committee

- Denise de Siqueira - UTFPR-CT
- Maicon R. Correa - IMECC, Unicamp
- Philippe R. B. Devloo, FEC, Unicamp
- Sônia M. Gomes - IMECC, Unicamp

Sponsors

Schedule

January, 24th Morning	
9:00 - 9:10	Opening
9:10 - 10:00	Plenary lecture: Preconditioners for high order FEM mass matrix on triangles Prof. Mark Ainsworth - Brown University - Boston - USA
10:00 - 10:30	Coffee break (Poster session)
10:30 - 11:00	A unified form for programming p-adaptive function space - Phillipe R. B. Devloo - FEC - Unicamp- Campinas -SP
11:00 - 11:30	H(div)-conforming flux approximations based on general partitions and applications to Darcy's flows - Sônia Maria Gomes - IMEEC - Unicamp - Campinas -SP
11:30 - 12:00	On stabilized mixed formulations and hierarchical high order finite element spaces - Maicon R. Corrêa - IMEEC - Unicamp - Campinas -SP
January, 24th Afternoon	
13:30 - 14:00	Poster session
14:00 - 14:30	A posteriori error estimation for Multiscale Hybrid Mixed Method (MHM-Hdiv) Denise de Siqueira - UTFPR - Curitiba -PR
14:30 - 15:00	A Phase Field Model with Fractional Derivatives for Damage in Viscoelastic Materials Thais Clara da Costa Haveroth - IMEEC - Unicamp - Campinas -SP
14:30 - 15:00	A posteriori error estimation based on potential reconstruction by orthogonal projection - Paulo R. Bosing - UFFS - Chapecó - SC

Poster presentation	
10:00 - 10:30 13:30 - 14:00	- New H(div)-conforming multiscale hybrid-mixed methods for the elasticity problem on polygonal meshes: Agnaldo M. Farias - IFNMG - Salinas -MG - Development of high-order H(curl;Ω) - conforming approximation spaces for photonic waveguide analysis: Francisco T Orlandini - FEEC - Unicamp - Campinas -SP - On the application of the Primal Hybrid finite element method to heterogeneous elliptic problems: Giovanni Taraschi - IMECC - Unicamp - Campinas -SP - Development of a procedure for the solution of non-homogeneous partial differential equations using the Scaled Boundary Finite Element Method: Karolinne Oliveira Coelho - FEC - Unicamp - Campinas -SP - A CUDA accelerated numerical integration of elastoplastic finite elements residuals: Natália Ramos Vilas - FEC - Unicamp - Campinas -SP - Hybridized finite elements methods applied to hydro-mechanical problems: Pablo G. S. Carvalho - FEC - Unicamp - Campinas -SP - Automatic meshing for multiscale three-dimensional discrete fracture networks: Pedro Lima - FEC - Unicamp - Campinas -SP - On data adjustment of an elastoplastic constitutive model using optimization methods: Manouchehr Sanei - FEC - Unicamp - Campinas -SP - An iterative scheme for coupled poroelasto-plasticity and permeability: Manouchehr Sane - FEC - Unicamp - Campinas -SP

Plenary lecture

Preconditioners for high order FEM mass matrix on triangles - Mark Ainsworth

It is well-known that the stiffness matrix that arises in high order finite element discretisation of elliptic PDEs is generally ill-conditioned as the polynomial order p is increased.Although the mass matrix for low order (h-version) finite element approximation is well-conditioned, the mass matrix for the p-version is, like the stiffness matrix, generally ill-conditioned. For transient and singularly perturbed problems, it is necessary to invert the mass matrix, or a perturbation thereof, in order to carry out time stepping. We present an algorithm for preconditioning the two dimensional mass matrix which results in a preconditioned system whose condition number is independent of the polynomial order and the mesh size. Although the preconditioner is applicable to any choice of basis for the high order polynomials, we show that the preconditioner can be implemented efficiently in the case where a Bernstein polynomial basis is chosen. Numerical examples are presented illustrating the performance of the algorithm for a range of challenging applications. (This is joint work with Shuai Jiang, Brown University).

Oral presentations

A unified form for programming p-adaptive function spaces - Philippe R. B. Devloo

In this contribution we show how a geometric map and function space can be created fro the complete family of element topologies can be developed based on static template classes. The fundamental class is the definition of the topology of the element. From this class both a static geometry and shape function class are derived. The fundamental concept is that lll element topologies are constructed as the union of open sets of points (called sides). This framework allows eventually to implement shape functions for all element topologies within a unique templated function of approximately 25 lines of code.

H(div)-conforming flux approximations based on general partitions and applications to Darcys flows - Sônia Maria Gomes

The importance of $\mathbf{H}$(div)-conforming approximations is well recognized for conservative mixed formulations of multiphysics systems. There exists in the literature a variety of such approximation spaces, which are usually restricted to standard element geometries. We describe the principles in the construction of more general $\mathbf{H}$(div)-conforming contexts, the partitions allowing non-convex polygonal/polyhedral local subdomains. Given a finite dimensional normal flux space Λ_c, piecewise defined over a partition of the mesh skeleton, the approximation spaces keep fixed the face flux components constrained by Λ_c, but the internal flux components and the potential approximations inside the subdomains may be enriched in different extents: with respect to internal mesh size, internal polynomial degree, or both. Some recent applications of these constrained space configurations are discussed for the mixed formulation of Darcy's flows [1, 2, 3, 4], an unified error analysis holding for them.

References

[1] PR Devloo, O Durn, SM Gomes, N Shauer, Mixed finite element approximations based on 3D hp-adaptive curved meshes with two types of H(div)-conforming spaces, IJNME 113 (7) (2018), 1045-1060.

[2] PR Devloo, O Durn, Farias, SM Gomes, H(div) finite elements based on non-affine meshes for three dimensional mixed formulations of flow problems with arbitrary high order accuracy of the divergence of the flux, ¡hal-01880382¿, 2018.

[3] PR Devloo, O Durán, SMGomes, M Ainsworth, High-order composite finite element exact sequences based on tetrahedral-hexahedral-prismatic-pyramidal partitions, CMAME 355 (2019) 952-975.

[4] O Durán, PR Devloo, SM Gomes, F Valentin, A multiscale hybrid method for Darcy's problems using mixed finite element local solvers, CMAME 354 (2019) 213-244.

On stabilized mixed formulations and hierarchical high order finite element spaces - Maicon R. Corrêa

The development of accurate and stable mixed finite element methods for elliptic problems is related to the choice of the main unknowns of the problem and of the respective finite dimensional subspaces for their approximation. Some classical examples of unknowns/problems are the displacement and the stress tensor in the linear elasticity, the flux and the pressure in the Darcy problem and the velocity and the pressure in the Stokes problem. The chosen finite element subspaces must be compatible, in the sense that they must satisfy compatibility conditions, such as the inf-sup condition, in order to provide stable numerical solutions. To overcome the compatibility conditions, several stabilized mixed finite element methods have been developed, allowing to the use of originally unstable spaces. In this work, we present a high-order finite element methodology to solve the Darcy problem based on the combination of stabilized mixed finite element methods with a hierarchical methodology for the construction of finite dimensional subspaces. The chosen stabilized methods are free of mesh dependent stabilization parameters and allow for the use of different high order finite element approximations for the flux and the pressure variables. The results obtained with discretizations based on quadrilateral elements are compared with the ones given by classical mixed formulation with Raviart-Thomas elements.

A posteriori error estimation for Multiscale Hybrid Mixed Method (MHM-Hdiv) - Denise de Siqueira

A posteriori error estimates are fundamental for efficient error control of the numerical simulations. Usually, they are based on local error indicators defined in terms of the computed approximations, which can be used to error control and to modify the discretization with adaptive mesh adaptivity in order to get a desired accuracy with reduced computational effort.

In this work we propose a posteriori error estimation to a multiscale hybrid method using mixed finite element local solvers introduced in [3]. The procedure is based on potential and flux reconstruction explored by [1] and [2]. The main idea is to use a mixed formulation based on constrained flux approximations to reconstruct the primal and/or dual solution applying a smoothing procedure on the interface of the macro partition of the domain and solving a local projection problem with smooth boundary condition. Some numerical experiments are presented in order to illustrate the efficiency of the proposal.

References

[1] M. Ainsworth, A framework for obtaining guaranteed error bounds for finite element approximations. J. of Comp. and App. Math. 234 (2010) 2618-2632.

[2] G. V. Pencheva, M. Vohralik, M. F.. Weeler andT. Wildey. Robust a posteriori error control and adaptivity for multiscale, multinumerics, and mortar coupling. SIAM J. Numer. Anal. (2013) 51 (1): 526-554.

[3] O. Durán, P. R. B. Devloo, S. M. Gomes and F. Valentin, A multiscale hybrid method for Darcy's problems using mixed finite element local solvers Comp. Meth. in App. Mech.Enging. (354), (2019), 213-244.

A Phase Field Model with Fractional Derivatives for Damage in Viscoelastic Materials - Tais C. da Costa Haveroth

We present a framework based on phase field and fractional derivatives to describe damage in materials with viscoelastic behavior. The model is thermodynamically consistent and the damage is considered as a dynamical phase field variable. The viscoelastic material modeling is included by using a suitable free-energy potential and pseudo-potentials of dissipation. The freeenergy potential allows the consideration of finite strains and includes the degradation function in the formulation. We propose and test a new degradation function that properly couple the stress response and the damage evolution for viscoelastic materials, in particular for polymeric materials. On the other hand, the definition of a viscoelastic pseudo-potential of dissipation leads to a constitutive stress/strain relation in terms of fractional derivatives. The developed model produces a set of equations for the evolution of motion, damage and temperature that is numerically solved by using a semi-implicit scheme. The model proposed is tested for some examples to predict failure for viscoelastic materials.

A posteriori error estimation based on potential reconstruction by orthogonal projection - Paulo R. Bosing

For the Poisson equation we introduce a new definition for the reconstruction potential based on orthogonal projection with respect to the $L^2(\Omega)$-inner product. Using the orthogonal projection properties and the classic Prager-Synge theorem [1] we obtain a completely determinate a posteriori error estimates for the gradient of the error in the scenario of continuous space. These preliminar results are used as a guide to obtain more applicable and practical a posteriori error estimates for the potential and for the flux.

Using the abstract energy norm a posteriori error estimates, proved in Theorem 4.1 of [3], we demonstrate a variation of the Theorem 6.10 of [2]. These allow to establish the new results of a posteriori error estimates for the potential. On the other side, using our definition for the reconstruction potential and the general abstract estimates proved in Theorem 3.1 of [2], we prove the a posteriori error estimates for the flux.

We highlight that in both case the error is bounded by three terms which are free of undetermined constant, are locally efficient, and are responsible for measuring the following quantities: (i) how near the gradient of the numerical solution is of the gradient of the reconstruction potential; (ii) how near the gradient of the reconstruction potential is of the flux reconstruction; (iii) the oscillation between f and their L^2-projection.

References

[1] F. Bertrand and D. Boffi. The Prager-Synge theorem in reconstruction based a posteriori error estimation, 2019.

[2] M. Vohralk, Unified primal formulation-based a priori and a posteriori error analysis of mixed finite element methods. Math. Comput. 79(272) (2010) 2001-2032.

[3] M. Vohralk, Guaranteed and fully robust a posteriori error estimates for conforming discretizations of diffusion problems with

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Poster session

New H(div)-conforming multiscale hybrid-mixed methods for the elasticity problem on polygonal meshes - Agnaldo M. Farias

Extending the one-scale results obtained in [1], we propose new two-wcale discretizations based on macro partitions, the global system solving normal stress (multiplier) over the mesh skeleton, and piecewise constant displacements. Using the multiplier as Neumann boundary conditions, higher resolution local solvers give details for internal stress tensors, displacement components with vanishing mean values, and rotation (to weakly enforce symmetry). Different choices to approximate local problems are discussed, based on locally stable pairs of finite elements defined on affine second-level meshes. Those choices generate a family of multiscale finite element methods for which stability and convergence are proved in a unified framework. For instance, L^2- error analysis reveals multiplier, stress tensor and rotation with the same accuracy order, but super convergence for stress divergence and enhanced displacement approximations occur. Numerical verifications assess theoretical results and highlight the high precision of the new methods on coarse meshes for multilayered heterogeneous material problems. More details can be found in [2].

References

[1] P. R. B. Devloo, S. M. Gomes, T. Quinelato and S. Tian, Enriched two dimensional mixed finite element models for linear elasticity with weak stress symmetry, hal-01928789 2018, Comput. Math. Appl., to appear.

[2] P. R. B. Devloo, A. M. Farias, S. M. Gomes, W. Pereira, A. J. B. dos Santos and F. Valentin, New H(div)-conforming multiscale hybrid-mixed methods for the elasticity problem on polygonal meshes, $< hal - 02415020 >$.

Development of high-order H(curl;Ω) - conforming approximation spaces for photonic waveguide analysis - Francisco T Orlandini

High precision approximation of dispersion parameters is a major concern in the design of photonic waveguides and the Computational Electromagnetics (CE) community has sought many different numerical techniques in order to achieve this requirement. In the present work, a high-order Finite Element Method (FEM) scheme is introduced, presenting high convergence rates and being able to deal with waveguides with curved cross-section and lossy inhomogeneous media with transverse anisotropy. The H(curl; Ω)-conforming elements used in the scheme are a hierarchical construction of the Nédélec elements of the first kind, implemented in the NeoPZ framework. The importance of using non-linear mapped elements when using high-order elements is discussed and real-world scenario results are presented. Finally, the hierarchical construction of the elements is explored in an example of how hp-adaptive finite elements can significantly reduce the number of equations while still achieving high precision results.

On the application of the Primal Hybrid finite element method to heterogeneous elliptic problems - Giovanni Taraschi

In this work we study the application of the Primal Hybrid finite element method of [1] to anisotropic and heterogeneous 2nd order elliptic problems and propose the use of local post-processing to evaluate the flux from the approximated Lagrange multipliers. As shown in [1], within the primal hybrid formulation of the Poisson problem, the Lagrange multipliers are equivalent to the normal flow at the boundaries of each element and are continuous between two neighboring elements. Thus the post-processing technique leads to a global $H(\text{div})$ flux. In order to check the accuracy of the methodology, we present some preliminary numerical experiments comparing the results with those obtained from the Classical H_1 Galerkin method.

For the numerical tests we chose a boundary value problem from [2]. This problem has a discontinuous analytical solution for the flow, making the approximation for the flux more challenging. Although both the Classical Galerkin and the Primal Hybrid method achieve the same convergence rates, for the primal scalar variable, the proposed post processing technique leads to vector fields with continuous normal component, what does not hold in the classical Galerkin approximation.

References

[1] Raviart, P.A., Thomas, J.M., *Primal hybrid finite element methods for 2nd order elliptic equations.*. Mathematics of computation, Vol 31. p391-413. (1977).

[2] Crumpton, P.I., Shaw, G.J., Ware, A.F., *Discretisation and multigrid solution of elliptic equations with mixed derivative terms and strongly discontinuous coefficients*. Journal of Computational Physics, Volume 116. p343–358. (1995).

Error estimation based on enrichment of mixed finite element spaces - Gustavo Alcalá Baptistela

In the context of finite element methods for partial differential equations, it is possible to consider a priori and a posteriori error analyses. A priori error estimates give bounds to approximation errors of the variables involved depending on regularity assumptions on the exact solution and on the approximation solution. A posteriori error estimates is based only in the approximate solution and the data of the problem, therefore, this approach is useful for efficient error control of the numerical simulations, in practical problems where the real solution is unknown. The purpose here is to derive an efficient and robust a posteriori error estimations for the enriched mixed methods.The general methodology is based on potential and flux reconstruction. The proposed scheme for potential reconstruction follows three main steps: solution of the problem using an enriched space configuration for flux and potential variables (no post processing is required), smoothing of the potential variable and solution of local Dirichlet problem.

Development of a procedure for the solution of non-homogeneous partial differential equations using the Scaled Boundary Finite Element Method - Karolinne Oliveira Coelho

The Scaled Boundary Finite Element Method (SBFEM) is a finite element approximation technique in which the shape functions are constructed based on a semi-analytical approach. Due to its features, this method is particularly efficient to approximate problems with strong internal singularities, for instance, fracture mechanics simulation. In this study, a novel procedure to construct bubble functions is proposed to approximate non-homogeneous partial differential equations using the scaled boundary finite element method (SBFEM). The main advantage of such an approach is the orthogonality between the bubbles and SBFEM approximation functions. Two numerical tests, a Steklov and an Elasticity problem, are accomplished. Optimal rates of convergence are obtained even for the problem with square-root singularity. For the Elasticity problem, the novel bubble approach leads to lower error values than the traditional SBFEM.

A CUDA accelerated numerical integration of elastoplastic finite elements residuals - Natália Ramos Vilas Boas

Finite Element Method (FEM) is a numerical technique to approximate partial differential equations. It has been widely used to approximate solutions of physical problems in different fields of research. The numerical simulation challenging engineering problems with small error require fine meshes and leads to high computational cost. To overcome this difficulty parallel computing is becoming a mainstream tool. Among the techniques available to improve the performance of this type of computational application is the execution of the algorithm using Graphics Processing Unit (GPU) programming. Although GPU was originally developed for graphics processing, it has been used in the last years as a general purpose machine with high parallelism power through the availability of libraries such as CUDA or OpenGL. The purpose of this research is to develop an efficient algorithm for the evaluation of the finite element residual and Jacobian matrix. We target the particular variational formulation of an elastoplastic problem with associative plasticity but will try to show that the approach can be extended to other fields and problems. The presented strategy for the calculation of the residual and tangent matrix rely on several computational ingredients such as gathering and scattering operations, sparse matrix multiplications, and a parallel coloring procedure for assembly process. The verification of the nonlinear approximated solution includes comparison with regular CPU implementation in terms of numerical results and execution efficiency. For residual computations of elasto-plasticity, the GPU outperforms the CPU by a factor of up to 10.

Hybridized finite elements methods applied to hydro-mechanical problems - Pablo G. S. Carvalho

The present work presents the study of hybrid element formulations of some relevant fluid and geomechanical problems in the context of recent demands of the Petroleum industry. The analyzed methods allow the use of numerical techniques, such as static condensation, in order to obtain considerable improvements in performance. A special focus is given to the multiscale hybrid-mixed (MHM) method, a numerical technique targeted to approximate systems of differential equations with strongly varying solutions. This is extended here to the Stokes equation. In this regard, a new hybrid formulation is proposed: the Stokes tensor is decomposed into tangential traction, adding conditions on faces driven by Lagrange multipliers. For incompressible fluids and H(div)-conforming formulation, this method naturally gives exact divergence-free velocity fields, with local conservation at any scale, leading to accurate results with a very reduced number of global equations; properties that few schemes can achieve. All the methods are implemented using an object-oriented computational environment.

Automatic meshing for multiscale three-dimensional discrete fracture networks - Pedro Lima

Multi-scale finite element methods require special types of meshes, specifically, those that relate coarse elements to sub-meshes of finner elements. The geometric description of a Discrete Fracture Network

(DFN) in this context, involves the ability of inserting multiple fractures in a pre-defined coarse mesh, while building a sub-mesh around these fractures and tracking fine/coarse element relations. Main steps involve: locating intersections and refining elements at those points, building a data structure that associates each element of a fracture surface to the coarse volume that encloses it, and then generate a sub-mesh of fine elements around the fractures to fill these coarse elements, without altering originally defined nodes in the coarse mesh. This work presents an approach for automatic finite element meshing of fractured reservoirs suited to Multiscale Hybrid-Mixed methods (MHM) [1]. The code is written in C++ and largely relies on two finite element libraries: NeoPZ [3] and Gmsh [2]. Starting with a coarse mesh, fractures are entered as 3D polygons, built from their corner points, and inserted one-by-one. Intersections with one-dimensional elements are computed first and subsequently used to define the intersection with two-dimensional elements (faces). Triangles that result from refining faces to conform to the intersecting fractures are checked for quality, and those with bad aspect ratio (given a tolerance) are coalesced, as fracture surface nodes are snapped into previously defined nodes. The resulting faces are utilized to define volume shells that can be tetrahedralized using Constrained Delaunay algorithms available in the Gmsh library. Element connectivity, transformations between parametric domains of fine/coarse elements, and all other relevant finite element computations are implemented using NeoPZ. Results show that the proposed technique can efficiently construct adequate 3D meshes. While relying on neighborhood information and consistent element topologies available from NeoPZ's geometric meshes, enables optimization of multiple algorithms of geometric search that would, otherwise, require a considerable amount of floating-point operations.

References

[1] Devloo, P., Teng, W. and Zhang, C. *Multiscale hybrid-mixed finite element method for flow simulation in fractured porous media.* CMES, Vol 119. p145-163. (2019)

[2] Geuzaine, C. and Remacle, J.-F. *Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities.* Int. J. Num. Meth. Engng., Volume 79. (2009)

[3] Devloo,P. *PZ: An Obj.orient. environment for sci.progr.* (1997)**doi:**10.1016/S0045-7825(97)00097-2

On data adjustment of an elastoplastic constitutive model using optimization methods - Manouchehr Sanei

The role of geomechanics in the oil industry is important to understand the productivity of a reservoir during its life cycle, including drilling, completion, and production. To consider the geomechanical behavior, it is essential to understand the mechanical properties of the reservoir rock. This behavior may be different under loading and unloading due to permanent elastoplastic deformation. Therefore, the mechanical behavior of the rock is simulated using an elastoplastic constitutive model. The constitutive model can rather complex using a large number of parameters which may be difficult to be evaluated. This contribution proposes a methodology for determining these parameters using an engineering point of view. A data adjustment of an elastoplastic constitutive model from the laboratory test data is developed. The experimental data were obtained using three types of loading conditions, e.g., triaxial, oedometric, and hydrostatic. The experiments were run at Cenpes/Petrobras, Brazil. The data adjustment of elastoplastic model parameters is done using an optimization method which minimizes the difference between measurement data and numerical results by using a properly defined object function. The minimization of the object function is obtained by using optimization methods (e.g. e.g. Newton, Quasi-Newton, Gradient descent method or others). To show the accuracy of the procedure, numerical results from elastoplastic models are compared with measured test data.

An iterative scheme for coupled poroelasto-plasticity and permeability - Manouchehr Sanei

The drilling of reservoir usually leads to change of pore pressure around the wellbore which causes the stress redistribution. For instance, an increase in effective stress will lead to reservoir rock compaction. Such reservoir compaction can cause irreversible (plastic) deformation in reservoir rock which constrains fluid flow and influence to the porosity and permeability. For understanding drilling in petroleum industry, it is necessary to analyze poroelasto-plastic in hydrocarbon reservoirs. This study implements an iterative scheme for coupled poroelasto-plasticity and permeability in hydrocarbon reservoirs by using of the fixed stress split scheme. The elastoplastic deformation analysis includes the linear component based on Biots theory and the nonlinear component based on the Mohr-Coulomb plasticity model. The fluid flow formulation in this coupling is defined by Darcy's law including nonlinear permeability based on Petunin model. The numerical approximation is implemented using continuous Galerkin finite element for rock deformation and mixed finite element approximation for pore pressure. Several numerical simulations are performed and for selected cases, the results are compared with semi-analytical solutions obtained by an explicit Runge-Kutta solver.