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February 25–28, 2019, Petrópolis, Brazil

H(DIV) FINITE ELEMENTS BASED ON NON-AFFINE MESHES FOR THREE DIMENSIONAL MIXED FORMULATIONS OF FLOW PROBLEMS WITH ARBITRARY HIGH ORDER FLUX DIVERGENCE ACCURACY

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Keywords: *Mixed finite element formulation, non-affine meshes, enhanced accuracy.*

H(div)-conforming finite element approximation spaces are usually formed by locally backtracking vector polynomial spaces defined on the master element by the Piola transformation. The main focus of the present work is to study the effect of using non-affine elements on the accuracy of three dimensional flux approximations based on such spaces. For instance, instead of order $k+1$ for flux and flux divergence obtained with Raviart-Thomas or Ndlec spaces with normal fluxes of degree k, based on affine hexahedra or triangular prisms, reduced orders k for flux and $k-1$ for flux divergence may occur for distorted elements. To improve this scenario, a hierarchy of enriched flux approximations is considered, with increasing orders of divergence accuracy, holding for general space stable configurations. The original vector polynomial space is required to be expressed by a decomposition in terms of edge and internal shape functions. The enriched versions are defined by adding internal shape functions of the original family of spaces up to higher degree level $k+n$, $n>0$, while keeping fixed the original border fluxes of degree k. This procedure gives approximations with the same original flux accuracy, but with enhanced divergence order $k+n+1$, in the affine case, or $k+n-1$ for elements mapped by general multilinear mappings. The loss of convergence in the flux variable due to quadrilateral face distortions cannot be corrected by including higher order internal functions. Application of these enriched flux spaces to the mixed finite element formulation of a Darcy's model problem is discussed. The computational cost of matrix assembly increases with

n, but the global condensed systems to be solved have same dimension and structure of the original scheme.

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February 25–28, 2019, Petrópolis, Brazil

CONSERVATIVE FINITE VOLUME LAGRANGIAN-EULERIAN FRAMEWORK FOR APPROXIMATING HYPERBOLIC MODELS WITH SOURCE TERMS

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Keywords: *Lagrangian-Eulerian, Balance Laws, Hyperbolic Conservation Laws*

We present a simple numerical method based on a Lagrangian-Eulerian framework for approximate solutions of nonlinear balance law problems. This framework has been used for dealing with the dynamic forward tracking of the delicate well-balancing between the first-order hyperbolic flux and the source term. The mass conservation takes place in a local space-time control volume, and this region is used a novel approach to define naturally a balance law. This balance law is the central idea to build a efficient numerical method to approximate solution to balance law problems. We do not use approximate or exact Riemann solvers nor nonlinear reconstructions and we do not use upwind source term discretizations either. We present numerical solutions to nontrivial partial differential equations of several types, both hyperbolic conservation laws and balance laws. Verification of the technique is also made by comparison with analytical solutions when they are available. We present our latest results in applying the weak asymptotic solutions technique to this framework.

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(WCMNA) February 25–28, 2019, Petrópolis, Brazil

A New Pairing Function for Mesh Multiplication in Large Scale Simulations

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Abstract. Often unstructured grid methods, such as finite elements, are used in high fidelity simulations. In these methods, solution accuracy is associated with the interpolation order and to the grid size. Unstructured parallel mesh refinement is computationally expensive due to subdomains interface communication. In [3] we propose a fast tetrahedral mesh multiplication technique, based on a uniform tetrahedral mesh refinement scheme applying edge bisection recursively (also called Bey's refinement [1]). The method is very fast and does not require any communication among processes since we apply a particular pairing function to create unique indexes for globally shared mesh entities.

Classical pairing functions, such as the Cantor and Szudzik functions, may be used to create these new indexes. Although Cantor and Szudzik functions supply a straightforward way for building new indexes, they have limitations when used in a computer program. For practical purposes in large-scale simulations, a proper pairing function should be capable of mapping the largest possible index values within the range of the output number representation. Now, we check this assumption for Cantor's pairing function. Let's consider the pair $\langle 65535; 65535\rangle$, of the largest unsigned 16-bit integers. It returns 8589803520 when paired by Cantor's function, which is a number greater than the largest unsigned 32-bits integer (2^{32}) and, consequently, limits its use for our purposes.

In this work we explore mesh properties and graph theory ([2]) to define a pairing function that associates each pair of integers (i, j) with a single value $f(i, j)$ of order n(number of vertexes of the mesh), which we will call *economic pairing*. Therefore, the *economic pairing* maps the largest index values possible within the range of the output number representation. We will show several examples to demonstrate the efficiency of the new *economic pairing* function.

Keywords: Mesh refinement, edge-based data structures, pairing functions

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Workshop on Computational Modeling and Numerical Analysis (WCMNA)
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MIXED FEM BASED ON MAPPING METHOD FOR A SINGULAR PROBLEM

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Keywords: *Mixed finite elements, hp adaptivity, curved and anisotropic meshes, quarter-point elements, boundary point singularity.*

The mapping-based method [3] can be interpreted as a reformulation of the original problem in a parametric space, where the singularity is smoothed and therefore, the classical finite element methods are able to solve with the desired precision. The aim of this work is use this kind of method to solve a problem whose singularity is of square root type and a quarter point type mapping, introduced in [1] and [2], is applied.

In [2] a special mapping was defined in order for the calculation of stress intensity factors of elastic fracture mechanics. The main idea is to use the 8-noded isoparametric element by placing the mid-side node near the singuarity at the quarter point node. In order to improve the results a colapsed quarter point mapping is introduced where the nodes on the one side is colapsed on the singular point, Figure 1.

For the simulations two mesh scenarios (Figure 2) are considered, by fixing some macro quarter point elements at the coarse level, and subdividing them by mapping uniformly refined square meshes on the master element by their corresponding geometric transforms. For eight-noded coarse quadrilateral quarter-point elements, placing two mid-side nodes near the singular vertex, radial singularity is exactly captured along element edges, and their refinements reveal shape regular curved meshes. For an improved version, using collapsed quadrilateral quarter-point elements obtained by reducing one of the quadrilateral element edges to the singular point, the radial singularity is captured inside the coarse macro elements as well.

Their uniform refinement generates anisotropic meshes, grading towards the singular point. The obtained results show a superior advantage of convergence acceleration of the approximate solution when compared to usual techniques of h, p and hp-refinements

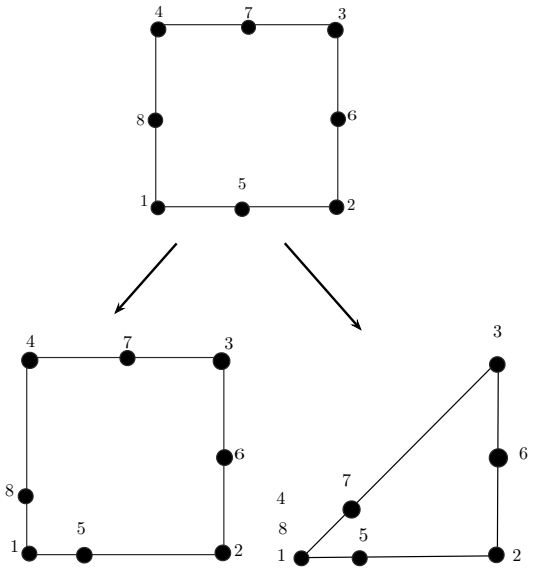
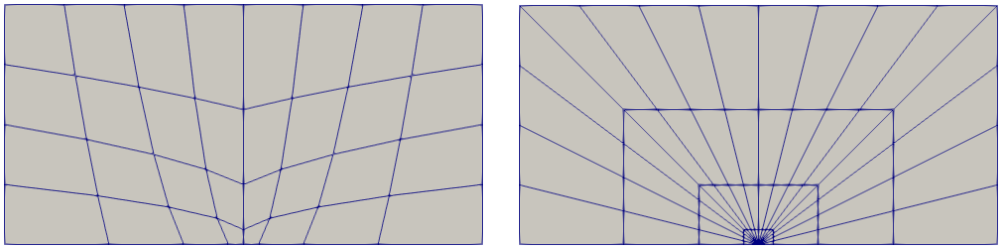


Figure 1: Mid-side mapping on top, quater point mapping down left and colapsed mapping down rigth



(a) quarter point mesh (b) colapsed quarter point mesh

Figure 2: Mesh scenarios

adaptive. In particular, with the use of collapsed elements, it was possible to obtain an accuracy equivalent to that applied to smooth problems in uniform meshes.

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GAUSS-LEGENDRE QUADRATURE OVER TRIANGLES: A PRACTICAL APPROACH

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Keywords: *Quadrature Guass-Legendre, Single and double integral, Finete element, Algorithm, Matlab, Numerical solution.*

It is presented the 1D Gauss-Legendre quadrature and it is extended to 2D triangular domain. The main objective of the present paper is to develop a practical and simple algorithm for numerical integration over triangular domain by using the well-established Gauss-Legendre quadrature. It is also demonstrated the effectiveness of the above algorithm by applying it to some typical integrals as shown in this work.

The main contribution of the present work is bring a straight algorithm presentation of the required calculation for points and weights coefficients needed in the Gauss-Legendre quadrature for 1D and 2D integrations over triangular elements.

The triangular elements used to discretise 2D domains with either straight sides or curved sides are very widely used in finite element analysis [01][02].The basic problem of integrating a function of two variables over the domain of the triangle were first given by Hammer et al. [03]. As stated before by use of a simple but straightforward algorithms, Gaussian-Legendre points and corresponding weights are calculated and presented for clarity and reference, its is done for 1D domain and easily extended for 2D triangular domains. The integral formulas presented in this work are based on the sampling points and weight coefficients of Gauss-Legendre quadrature formulas. Such approach enables one to obtain formulas of very high degree of precision, as Gauss-Legendre quadrature rules of high order are well discussed [04][05][06].

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GOAL ORIENTED DYNAMIC MESH ADAPTATION FOR SPACE-TIME DISCONTINUOUS GALERKIN FINITE ELEMENT DISCRETIZATION OF LINEAR PARABOLIC PROBLEMS

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Keywords: *goal oriented error estimation, high-order discontinuous Galerkin, mesh adaptation, parabolic equations.*

Adaptive techniques based on a goal oriented a posteriori error estimation are widely used in the finite element space-time discretizations of parabolic problems for improving the reliability of the goal functional approximation [3]. The evaluation of the global error estimator and error localization in time and space is based on the approximation of the exact solution to an appropriate dual problem using discretization of high order in time and space.

There are several possibilities for compute such approximation. However, in each of them the dual parabolic problem has to be solved backwards in time that pose additional implementation challenges and computational costs. For example, the dual problem can be solved using the same discretization order in time and space as the primal parabolic problem. Then local higher-order space-time interpolation is used for approximation of the dual solution. For parabolic problem these local methods can be comparably accurate [2],[3].

In this work we aim at an posteriori error estimator and adaptive goal-oriented algorithm for efficient approximation of a goal functional evaluated at solution of parabolic equations discretized by the discontinuous in time and space Galerkin finite element method $dG(k)dG(l)$. We derive an exact error representation in goal functional using continuous dual problem formulation and error representation in space introduced in [1]. For asses local and global error estimate the dual problem is approximated on the same time-space mesh using continuous in time $cG(\hat{k})dG(\hat{l})$ method with $\hat{k} > k$ and $\hat{l} > l$. For improving quality of the dual approximation in space the discrete dual solution is postprocessed using Oswald interpolation operator. Note that owing to easy local implementation of high-order dG approximation the computational effort to solve the dual problem with

higher order approximation increase insignificantly and produce accurate asymptotically exact error estimate. The estimate is decomposed in time and space component and then used in dynamical mesh adaptation algorithm. Presented numerical results confirm asymptotical exactness of the error estimate. Dynamical mesh adaptation algorithm is numerically tested and validated for two-dimensional linear parabolic problems.

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A COMPARATIVE STUDY OF NUMERICAL SCHEMES FOR SOLVING NAVIER STOKES EQUATIONS USING FLOW PROBLEMS BENCHMARKS

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Keywords: *Navier-Stokes, Benchmark, FEniCS*

Numerical algorithms for the computation of fluid flow still remains an active area of research and there is a large literature on discretization schemes. This work aims to solve Navier-Stokes equations by using the FEniCS, a flexible platform of public domain which has different finite element methods implemented in Python. A comparative study of projection (Chorin and IPCS) and stabilized (SUPG/PSPG) methods are presented to solve Navier-Stokes equations. In order to do this, incompressible flow problems benchmarks are adopted, namely: Bidimensional Cavity, Pressure Driven Channel, Flow around a Cylinder, Taylor-Green Vortex. The results obtained in this study demonstrate that the methods simulated by using FEniCS environment were appropriate for solving Navier-Stokes equations.

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A RUNGE-KUTTA DISCONTINUOUS GALERKIN METHOD FOR HYPERBOLIC CONSERVATION LAWS ON QUADRILATERAL MESHES

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Keywords: *Hyperbolic problems, Discontinuous Galerkin, Semi-discrete formulations, Runge-Kutta time discretizations, Gradient Reconstruction, Slope Limiters.*

In this work we present a Discontinuous Galerkin method for the numerical approximation of bidimensional scalar hyperbolic conservation laws on general quadrilateral meshes. The good local stability properties of Total Variation Runge-Kutta (TVDRK) methods are combined with stable numerical flux functions and with the gradient reconstruction technique in order to construct stabilization strategies for the proposed Discontinuous Galerkin method, allowing to the correct resolution of abrupt gradients and discontinuous solutions, without spurious oscillations in the numerical solutions. The gradient reconstruction technique is used in a simple fashion avoiding unnecessary limiting of directional derivatives linked to transport problems, with linear and non-linear fluxes.

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ADAPTIVITY SCHEMES FOR SPINODAL DECOMPOSITION SIMULATIONS USING THE CAHN-HILLIARD EQUATION

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Keywords: *Cahn-Hilliard equation, Spatial adaptivity, Temporal adaptivity.*

Spinodal decomposition is a process where a mixture of solids or liquids is submitted to a rapid unmixing from one thermodynamic state into two coexisting phases. This phenomenon occurs when the mixture is above a critical temperature and is submitted to deep quenching, that is, a sudden cooling, reaching a given temperature lesser than the critical temperature, when both phases can coexist. This phenomenon can be modelled by the phase-field technique, where the phases are separated by a finite width interface, where surface tension effects are the main driving forces.

The Cahn-Hilliard equation is one of the most used equations to simulate the spinodal decomposition over a binary mixture and has been widely explored in the past decades. However, numerically solving the Cahn-Hilliard equation is not a trivial task since it contains a nonlinear term and the bilaplacian operator in its formulation. When used to simulate a spinodal decomposition, the Cahn-Hilliard equation reveals significant complexities related to the space and time discretization, leading to simulations with high computational cost. In this study, we propose a space-time adaptivity scheme to reduce the computational cost without compromising the accuracy of the simulations.

The space adaptivity scheme consists on considering the flux jump of the phase field as the error indicator, previously assessed by Stogner et al. (2008), and refining the elements marked with the bisection mesh refinement procedure. The time marching scheme with variable time step (time-adaptivity) relies on linear feedback control theory, where a higher order extrapolation method uses an error estimate from a lower order integration method, as presented in Vignal et al. (2017) and in Söderlind (2002) for the time step controllers.

The finite element method is employed to discretize in space the Cahn-Hilliard equation. Since the Cahn-Hilliard equation is a fourth-order partial differential equation, the use of C^1-continuous elements are required. Nevertheless, the use of a splitting technique, through a mixed formulation, enables the use of C^0-continuous elements at the cost of an extra degree of freedom per node, since the chemical potential is now a solved field. For time integration, a method with unconditional energy-stability property is used to evaluate the evolution of the concentration field. We compare both spatial and temporal errors for all simulations - fixed and adaptive - and conclude that it is possible to optimize the performance of the Cahn-Hilliard simulations without compromising the accuracy of the solutions with the present scheme.

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NUMERICAL ANALYSIS OF A MILTISCALE FINITE ELEMENT METHOD FOR APPROXIMATING THE CANCER CELL PROLIFERATION IN THE COLON

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Keywords: *Multiscale Modelling, Colorectal Cancer, Homogenization.*

The human colon is prone to develop a cancer due to its cell renovation that consists in a large number of cell divisions per day located in small cavities of the colon epithelium, called crypts. The colon epithelium is filled by millions of crypts, and it is known that mutations in the cell proliferation process (inside the crypts) can lead to the carcinogenesis. The colonic cell proliferation can be modeled by using multiscales [3]. In particular, we can use a reference crypt, as a micro-scale domain, that is periodically distributed in a macroscale domain that is a portion of the colon epithelium. The relative multiscale solution will depend then on the micro domain crypt structure chosed. Differently to [3], we consider here a more realistic crypt structure, and present the associated coupled multiscale model that describes the evolution of a compartment of abnormal cells set located inside the crypts. The final model results in a coupled PDE system formed by an elliptic and parabolic equations whose unknowns are the proliferative cell density and the exerted cell pressure.

Another novelty of this work is the introducion of a new stable and convergent finite difference method that solves the coupled PDE problem and that is equivalent to a finite element method using quadrilateral elements [2]. This method despite to be centered in space and backward in time, is proved to be second order in a H^1 discrete norm. We then extend this method to solve the multiscale problem by using an HMM-FEM method [1], which provide good approximations with no large computational effort. Finally, we prove that the numerical multiscale solution converges with known rates using the L^2 and H^1 norms.

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PROJECTION IN NEGATIVE NORMS AND THE REGULARIZATION OF ROUGH LINEAR FUNCTIONALS

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Keywords: *Rough linear functionals, Negative norms, Projection, Regularization.*

Rough linear functionals (such as Dirac Delta distributions) often appear on the right-hand side of variational formulations of PDEs. As they live in negative Sobolev spaces, they dramatically affect adaptive finite element procedures to approximate the solution of a given PDE. To overcome this drawback, we propose an alternative that, in a first step, computes a projection of the rough functional over piecewise polynomial spaces, up to a desired precision in a negative norm sense. The projection (being L^p-regular) is then used as the right-hand side of a regularized problem for which adaptive Galerkin methods performs better. An error analysis of the proposed methodology will be shown, together with numerical experiments.

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Workshop on Computational Modeling and Numerical Analysis (WCMNA)
February 25–28, 2019, Petrópolis, Brazil

THE DYNAMIC DIFFUSION METHOD FOR ADVECTION-DIFFUSION-REACTION PROBLEMS

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Keywords: *Multiscale Finite Element Formulation, Dynamic Diffusion Method, Bubble Functions, Advection-Diffusion-Reaction Equations.*

- We present here the Dynamic Diffusion (DD) method introduced in [1, 2]. This method is based on a two-scale finite element formulation since it decomposes the velocity field in coarse and subgrid scales. The latter is used to determine the smallest amount of artificial diffusion to minimize the subgrid-scale kinetic energy. This is done locally and dynamically, by imposing some constraints on the resolved scale solution, yielding a parameter-free consistent method. The subgrid scale space is defined by using bubble functions, whose degrees of freedom are locally eliminated in favor of the degrees of freedom that live on the resolved scales. Therefore, the DD method emerges naturally from the solution decomposition into two scales as well as the decomposition of the velocity field. More importantly, it yields a parameter-free method, overcoming the main drawback of common stabilized methods. While the use of bubble functions to span the subgrid approximate space enables solution enrichment, it also provides simplicity to the model solution.

A complete convergence analysis of this methodology is under development but it is already possible to demonstrate that the DD method has optimal convergence rates, according to those presented by classical stabilized methods such as SUPG, CAU and so on. These convergence rates are also verified by numerical experiments that are studied for convection-diffusion-reaction problems. In addition, we observe that DD method is robust for a wide scope of application problems. Overall, this proposed DD scheme has good stability properties for transport problems both in the case of dominant advection and in the case of dominant reaction.

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Workshop on Computational Modeling and Numerical Analysis (WCMNA)
February 25–28, 2019, Petrópolis, Brazil

NUMERICAL SIMULATIONS WITH PROPER GENERALIZED DECOMPOSITION AND DISCONTINUOUS GALERKIN METHOD

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Keywords: *Proper Generalized Decomposition, Discontinuous Galerkin, coefficients and boundary conditions as parameters.*

Traditional computational tools used in a real word numerical simulation of complex multiscale and/or multi-parameter engineering problems suffer the so-called curse of dimensionality. In such a case the number of degrees of freedom grows exponentially with respect to dimension and number of parameters in the problem in consideration. That implies the necessity of developing model reduction techniques for reduce the complexity of problem. One of such model, called Proper Generalized Decomposition (PGD) method, have been introduced for a priori construction of approximations of the solution of problems in low rank order tensor space, see e.g.[1, 2]. The idea of PGD method is to construct an approximation of the solution under the form of a low rank separated representation which dimensionality grows only linearly with the dimension of problem. The main difference of PGD solver is the possibility of adding model parameters such as material properties, geometrical parameters, etc, as extra-coordinates of the problem. In this work we develop PGD technique for the Discontinuous Galerkin approximation of parametrized elliptic and parabolic problems considering equation coefficients and boundary (initial) conditions as parameters. Presented numerical results illustrate the precision and convergence of the method, as well as its potential in solving complex multidimensional problems with parameters as extra-coordinates.

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RBF-FD APPROXIMATIONS BASED ON POLYHARMONIC SPLINES BASIS WITH SUPPLEMENTARY POLYNOMIALS APPLIED IN THE SIMULATION OF INCOMPRESSIBLE VISCOUS FLOWS AROUND A CIRCULAR CYLINDER

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Keywords: *Radial Basis Function generated Finite Differential, polyharmonic splines basis, supplementary polynomials, circular cylinder.*

The Radial Basis Function generated Finite Differential (RBF-FD) is a meshless method that has highlighted in the last decades by its flexibility in the numerical approximation of PDEs, ease of computational implementation and in the approach of complex geometries. It has already been successfully applied to various engineering problems such as heat transfer, electrostatics, vibration, seismic modeling, and in particular, fluid dynamics problems [1]. In this work, we present applications of RBF-FD with polyharmonic splines basis (PHS) with supplementary polynomials [2], RBF(PHS)-FD for short, using the vorticity and stream-function formulation in the simulation of incompressible viscous flows around a circular cylinder for number of Reynolds less than 49 and Reynolds 100 [3]. We discretize the domain in non-uniform point cloud. The replacement of the stream-function on the cylinder surface is done using the mean of the up and down cylinder flow calculations. For the calculation of the flows we use a velocity interpolation with the RBF-FD itself. Results are discussed and compared with the literature.

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ISOGEOMETRIC RESIDUAL MINIMIZATION (IGRM)

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Keywords: *Isogeometric analysis, Residual minimization, Iterative solvers*

In this talk, we propose the Isogeometric Residual Minimization (iGRM) with direction splitting. The method mixes the benefits resulting from isogeometric analysis [1], residual minimization, and alternating direction solver [2]. Namely, we utilize tensor product B-spline basis functions, and an alternating direction methods [3,4]. We apply a stabilized method based on residual minimization. We propose a preconditioned conjugate gradients method with a linear computational cost resulting from a Kronecker product structure of the system of linear equations. We test our method on two-dimensional simulations of advection-diffusion problems, including the problem with the manufactured solution, the Eriksson-Johnson problem, and a rotating flow problem. We compare our method to the Streamline Upwind Petrov-Galerkin stabilization method. The resulting method is not restricted to a Kronecker product structure of the diffusion or advection data.
Acknowledgement. National Science Centre, Poland, grant no. 2017/26/M/ST1/00281.

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HYBRIDIZABLE DISCONTINUOUS GALERKIN METHOD IN CURVED DOMAINS VIA EXTENSIONS FROM SUBDOMAINS

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Keywords: *Hybridizable discontinuous Galerkin, curved domains, unfitted methods, high order.*

We propose and analyze a method to numerically solve partial differential equations in domains not necessarily polyhedral. The domain is approximated by a polyhedral computational subdomain where a high order hybridizable discontinuous Galerkin (HDG) method is employed. The boundary data is transferred to the computational boundary using a technique developed in [2] that allows us to obtain a high order approximation, even though the computational domain does not exactly fit the actual domain. It consists of integrating the approximation of the gradient of the solution along transferring paths connecting the computational boundary and the true boundary.

During the last decade, the method has been extended and analyzed in a variety of context: convection diffusion [3], elliptic interface problems [5], Stokes equations [4, 7], Oseen problem [8] and Grad-Shafranov equation [6]. In the case of Stokes and Oseen problems, we first seek for a discrete pressure having zero-mean in the computational domain and then the zero-mean condition in the entire domain is recovered by a post-process that involves an extrapolation of the discrete pressure.

In this presentation, we will explain how to obtain the numerical method when applied to Stokes equations. We show the method is well-posed under assumptions related to the distance between the computational domain and the true boundary and provide the error estimates showing that the method is optimal. In addition, we will numerically explore the capabilities of this technique when applied to steady state incompressible Navier-Stokes equations.

The development of this technique has been possible thanks to the collaboration with Bernardo Cockburn (University of Minnesota), Weifeng Qiu (City University of Honk

Kong), Tonatiuh Sánchez–Vizuet (New York University) and Ricardo Oyarzúa (Universidad del Bío–Bío); and also to the contribution of my students Patrick Vega, Felipe Vargas and Paulo Zúñiga. I would like also to acknowledge the financial support of Conicyt-Chile through Fondecyt Project No. 1160320, Project AFB170001 of the PIA Program: Concurso Apoyo a Centros Cientificos y Tecnologicos de Excelencia con Financiamiento Basal.

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NUMERICAL AND COMPUTATIONAL ANALYSIS OF TIME-DEPENDENT ADVECTION - DIFFUSION - REACTION EQUATION WITH ANISOTROPIC DIFFUSION, IN ATMOSPHERIC POLLUTION

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Keywords: *pollutant dispersion, advection - diffusion - reaction equation, anisotropic diffusion, SUPG.*

In this work we solve the time-dependent advection - reaction - diffusion equation with anisotropic diffusion. This problem has been widely addressed in the stationary case by considering different types of modern stabilization techniques. However, when real phenomena are considered an implementation in order to have an acceptable computational cost is needed; for this reason, the use of standard SUPG (Stream Upwind Petrov Galerkin) method for the space discretization and Euler scheme for the time discretization are satisfactory. In order to find an approximate solution for the problem, we compare the strategy of temporal-spatial or spatial-temporal solution with different stabilization parameters (see [3]). Due to the importance of the choice of the stabilization parameter in the stabilized methods, we present numerical tests to compare the parameters behavior and choose the most adequate to be considered in the applications. Finally, we present an example to describe the odor dispersion behavior in a real world scenario.

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A RECURSIVE PARALLEL IMPLEMENTATION OF THE MULTISCALE MIXED METHOD FOR INCOMPRESSIBLE TWO-PHASE FLOW

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Keywords: *Multiscale Methods, Darcy's equation, two-phase incompressible flow, Parallelism.*

We are interested in the numerical approximation of partial differential equations of elliptic-parabolic nature, in the context of incompressible two-phase flow problems in heterogeneous porous media. Numerical solutions of elliptic boundary value problems with high contrast and discontinuous coefficients are often expensive and time consuming, so efficient numerical methods are necessary. Indeed, methods that can take advantage of CPU-GPU clusters are of particular interest because GPUs have larger computational power than CPUs alone. In this work, we focus on the multiscale mixed method MuMM introduced in [1] (see also [2] where the variational formulation of [1] was presented), that is based on a non-overlapping iterative domain decomposition procedure with Robin interface conditions. Local multiscale basis functions are calculated in each subdomain to represent the discrete solutions that can be efficiently computed in CPU-GPU clusters. The method presented here uses a new technique to cluster multiscale basis functions associated with nearest neighbor subdomains, leading to a small (and local) linear system for the interface between the subdomains. The global solution is obtained by recursively applying the MuMM to all pairs of subdomains until the union of subdomains reach the whole domain. The resulting interface linear systems are easily handled by Schur decomposition along with a LU factorization. The novelty of this method is that it does not use an iterative procedure to compute the global solution and shows excellent parallel performance.

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A POSTERIORI ERROR ANALYSIS OF HDG METHODS IN FLUID MECHANICS

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Keywords: *Brinkman equations, Oseen Brinkman equations, hybridizable discontinuous Galerkin method, a posteriori error analysis.*

We introduce an analyze a posteriori error estimators, of the residual type, for a hybridizable discontinuous Galerkin (HDG) method applied to two problems arising from fluid mechanics. The first one is a gradient-velocity-pressure formulation of the Brinkman problem, where, in order to derive our estimator, we use the Oswald interpolant and a suitable constructed postprocessed approximation of the velocity. The second problem is a gradient-velocity-pressure formulation of Oseen equations. In this case, in addition to the properties of the Oswald interpolant, we employ a weighted function technique to control the L^2-error of the velocity. For both cases we establish reliability and local efficiency of the estimator for the L^2-error of the velocity gradient and the pressure and the H^1-error of the velocity, with constants written explicitly in terms of the physical parameters. Numerical experiments validate the quality of the adaptive scheme.

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A VARIATIONAL MULTISCALE METHOD FOR SOLVING INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

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Keywords: *Finite element method, Multiscale formulation, Navier-Stokes equation, Incompressible flow problems.*

In this work we present a variational multiscale (VMS) finite element method for solving the incompressible Navier-Stokes equations. The proposed method consists of a decomposition for both the velocity and the pressure fields into coarse/resolved scales and fine/unresolved scales together with the addition of a residual-based nonlinear operator to the enriched Galerkin formulation, following a similar strategy of the method presented in [1] for scalar advection-diffusion equation. This choice of decomposition is shown to be favorable for simulating flows at high Reynolds number. This operator introduces an artificial viscosity only on the unresolved mesh scales of the discretization. This is done dynamically at element level, by imposing some constraints on the resolved scale solution, yielding a parameter-free consistent method as given in [2]. In order to reduce the computational cost typical of two-scale methods, the subgrid scale space is defined using bubble functions whose degrees of freedom are locally eliminated in favor of the degrees of freedom that live on the resolved scales.
To improve the convergence of the nonlinear process, we use a dynamic damping factor presented by [3] in which is often essential for the convergence of the iterative process and for the reduction of the number of iterations. Accuracy comparisons with the streamline-upwind/Petrov-Galerkin (SUPG) formulation combined with the pressure stabilizing/ Petrov-Galerkin (PSPG) and least-squares on incompressibility constraint method are conducted based on 2D steady state driven cavity flow with high Reynolds number.

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AN EVALUATION OF THE USE OF THE REVERSE CUTHILL-MCKEE METHOD ALONG WITH PSEUDOPERIPHERAL VERTEX FINDERS

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Keywords: *Reverse Cuthill-McKee method, pseudoperipheral vertex finder, sparse matrices.*

The solution of several problems is reduced to the solution of large-scale sparse linear systems. Specifically, many problems in engineering and science involve the analysis and solution of large and complex problems defined by a set of linear equations in the form $Ax = b$, where $A = [aij]$ is an $n \times n$ large-scale sparse matrix, b is a known n-vector, and x is the unknown n-vector solution.

A low-cost solution using a linear system solver demands to order appropriately the variables of the sparse linear system. Consequently, linear system solvers can be computed after a matrix reordering to reduce the computational time of the solution. Thus, reducing profile of sparse matrices can be an important task in solving large-scale sparse linear systems, if the original matrix is not ordered appropriately.

When using iterative methods for solving linear systems, the cost of the transference of data to and from memory is related to the number of non-null coefficients in the lines of the matrix system A. Cache hit rates are increased if the non-null coefficients in each line lie in the same level of the memory hierarchy.

This work focuses on the problem of efficiently converting a sparse matrix into a band matrix. Such a conversion is often the first step of many linear algebraic algorithms that deal with large-scale sparse linear matrices. Specifically, this work considers the well-known Reverse Cuthill-Mckee method [1]. Thus, this paper evaluates several algorithms for finding pseudo-peripheral vertices along with variants of Kaveh's B and D algorithms [3]. Additionally, this experiment evaluates the use of the Reverse Cuthill-Mckee method without the use of an algorithm for the identification of a pseudo-peripheral vertex. Extensive experiments among these pseudoperipheral vertex finders applied to a large set of standard benchmark matrices show that the George-Liu algorithm [2] remains in the

state of the practice to provide pseudoperipheral vertices to the Reverse Cuthill-McKee method.

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H(DIV)-CONFORMING APPROXIMATIONS ON PYRAMIDS FOR MIXED METHODS BASED ON HYBRID MESHES

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Keywords: *Mixed finite elements, Hierarchical shape functions, Projection-based interpolants, 3D Hybrid meshes, Pyramids.*

Development of H(div)-conforming approximation spaces for flux approximations based on pyramids are particularly challenging. Unlike other usual three dimensional geometric cases, the pyramid has four faces converging to a point at its tip, requiring special care for the definition of flux values there. Rational functions have been used for the construction of high order pyramid vector shape functions, as proposed in [3], and references there in. However, in the context of mixed methods, there is the additional difficulty of verifying the conformity of the spaces formed by the divergence of the vector functions and the scalar functions used for the potential variable, which is not a trivial task when rational polynomials are used. Instead, following the principles used in [1] for H^1-conforming pyramidal elements, and in [2] for a lowest-order composite finite element exact sequence on pyramids, an alternative approach is considered, by dividing each pyramid into two or four internal tetrahedra, and using there available piecewise polynomials vector basis functions for tetrahedra. The normal components associated with the faces of internal tetrahedral elements are restraint to quadrilateral shape functions intersecting them on the quadrilateral face of the pyramid, which might be shared by a neighboring hexahedron. Mixed formulation for Poisson problems are considered for approximations based on hybrid meshes formed by tetrahedra and hexahedra, with pyramids making the transition between both geometry. An error analysis is outlined by taking into account local projections commuting the de Rham diagram, which present a general form for all element geometry and different space configurations. Results of simulations for some test problems verify the performance of the new developed techniques.

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H(DIV)-CONFORMING SPACES BASED ON GENERAL MESHES WITH INTERFACE CONSTRAINTS FOR MULTISCALE MIXED SIMULATIONS

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Keywords: *Multiscale Mixed finite elements, Hybridization, Enhanced local accuracy.*

Multiscaled Hybrid Mixed (MHM) method [1] is considered for the soimulation of Darcy's flows with strongly varying solutions. It follows the divide-and-conquer principle, for which the solutions are characterized in terms of boundary value problems locally set on each macrodomain, which are assembled by using transmission conditions throughout the mesh skeleton, normal fluxes (multiplier) making the interelement connection. The multiplier and coarse piecewise constant potential approximations in each subdomain are computed in an upscaling stage. Then, small details are resolved by local problems, using fine representations inside the subdomains, setting the multiplier as Neumann boundary conditions (downscaling). A recent MHM-H(div) variant adopts mixed finite elements at the dowscaling stage, instead of continuous finite elements used in all previous publications of the MHM method. The MHM-H(div) method can be interpreted as a mixed formulation based on constrained space configurations. Error estimations shall be derived for a class of such two-scale constrained space configurations for MHM-H(div) method applied to Darcy's flows, and results of some verification tests shall be presented. These results are part of the article [2].

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ENRICHED MIXED FINITE ELEMENT METHODS FOR LINEAR ELASTICITY WITH WEAK SYMMETRY

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Keywords: *Mixed finite element method, Linear elasticity, Weak stress symmetry, Enhanced accuracy, Hybrid formulation*

Finite element spaces for the mixed approximation of linear elasticity problems with weak stress symmetry are derived. The approximations are based on the application of enriched versions of classic Poisson-compatible spaces, for stress and displacement variables, and/or enriched Stokes-compatible space configurations, for the choice of rotation spaces used to weakly enforce stress symmetry. Accordingly, the stress space has to be adapted to maintain stability. Such enrichment procedures are done via space increments with extra bubble functions, which have their support on a single element (in the case of H^1-conforming approximations) or with vanishing normal components on element edges (in the case of $H(\mathrm{div})$-conforming spaces). The advantage of using bubbles in the enrichment process relies on the fact that all extra degrees of freedom can be condensed, in a way that the number of equations to be solved and the matrix structure are not affected. Enhanced approximations are observed when using the resulting enriched space configurations, which may have different orders of accuracy for the different variables. We show results of a

general error analysis that identifies the contribution of each kind of bubble increment on the accuracy of the variables, individually. The use of enriched Poisson spaces improves the rates of convergence of the displacement and/or of the divergence of the stress field. Stokes enrichment contributes to equilibrate the accuracy of weak enforcement of stress symmetry with the stress approximation itself, reaching the maximum rate given by the normal traces (which are not affected by this kind of enrichment).

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HYDRODYNAMICS STABILITY ANALYSIS OF A COMPRESSIBLE VISCOUS FLOW BY DENSITY VARIATIONS ALONG DEFORMING DOMAINS

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Keywords: *Navier-Stokes Equations, Newtonian Fluid, Elastic Boundaries, Peristaltic Transport.*

It is well known the importance of peristaltic transport of a compressible viscous fluid in a pipe with elastic boundary, as a model of blood transport in arteries. In fact, peristaltic transport is a natural mechanism of pumping most physiological fluids induced by a progressive wave of area contraction or expansion along the length of the boundary of a fluid filled distensible tube. We study the influence of small density variations along the fluid flow on the stability of model solutions. Assuming a particular relation between pressure and density, we obtain a nonlinear parabolic partial differential equation governing the density. We discuss about the appearance and interpretation of instabilities.

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A GRAPHIC TOOL FOR STRUCTURAL ANALYSIS OF LINEAR ELEMENT MODELS WITH AN OOP APPROACH

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Keywords: *Matrix structural analysis, Object-oriented programming, Graphic tool, Educational software.*

This work describes the implementation of a program to perform linear-elastic analysis of two and three-dimensional linear element (reticulated) models, such as frames, trusses, and grillages, using the direct stiffness method, a conventional displacement-based procedure of the finite element method. The LESM (Linear Elements Structural Model) program was designed as a complementary tool for undergraduate and graduate structural analysis courses at PUC-Rio, focusing on the development of didactic algorithms to perform each step of the analysis, allowing any user to implement new procedures with relative simplicity.

To achieve this goal, the MATLAB platform with an OOP paradigm proved to be an appropriate approach. The OOP paradigm provides an intrinsic incremental nature of the development of a structural analysis system, as new features can be easily incorporated in the system. Moreover, the use of OOP leads to a more close integration between the matrix structural analysis theory and the computer implementation, improving the program understandability and easing the system documentation [1].

One contribution of this work is the proposed OOP class organization. Dealing with different types of reticulated structure models in a generic fashion led to the definition of an important class of the LESM program: the Analysis Model class, responsible for generically handling the different aspects of 2D and 3D trusses, 2D and 3D frames, and grillage models.

The two most common theories for the idealization of bending behavior of beam elements are considered: Euler-Bernoulli and Timoshenko's theories. Another contribution of this

work is the unification of these two theories of beam elements. Following the developments of [2], all expressions for shape functions, stiffness coefficients and fixed-end-forces are similar for both theories. The only difference resides on a traditional Timoshenko parameter that relates bending rigidity with shear rigidity.

Another important component is the open source code documentation of LESM, which is based on formal software engineering design: the Unified Modelling Language (UML) pattern.

Furthermore, a graphical user interface of simple usage and multiple functionalities combined with computer graphics techniques and computational geometry methods in MATLAB was developed for practical use of the program. An important feature of the user interface is the mouse interaction with canvas to draw model topology, pick objects, and manipulate camera visualization. The program handles mouse interactions by creating objects of inherited subclasses from a generic superclass that manages mouse events [3].

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February 25–28, 2019, Petrópolis, Brazil

NEW RESULTS ON THE MHM FOR LINEAR ELASTICITY

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Keywords: *Multiscale, Finite Element, Elasticity, Superconvergence, Non-conforming, High-order.*

Numerical simulations of three-dimensional wave propagation in highly heterogeneous media is a challenging problem due to their computational cost. When modeling elastic media, it is even worse due to the vector nature of the main unknowns. In today's scenario of increasing computing power, the machines provide good environments to obtain solutions to tough problems. To this end, numerical algorithms should make good use of these new architectures, characterized by a large number of interconnected computing nodes with multiple processing units of different types. In this context, the "divide and conquer" philosophy emerges as a natural candidate to drive the development of trivial parallel algorithms. Multiscale finite elements have this concept embedded in their own definitions. In a broad sense, they are built to be precise on coarse meshes by upscaling, into their basis functions, missing unresolved structures present in the domain, physical data or the solution itself. These so-called multiscale basis functions are computed from independent element-wise local problems.

Recently, the classical hybridization procedure [2] has been used to devise a new family of high-order multiscale finite element methods, the Multiscale Hybrid-Mixed (MHM) methods. Starting from a (rough) partition $\mathcal{P}$ of the domain Ω, these methods compute a set of independent local solutions, that composes the multiscale basis functions, and use them to assemble a global problem on the partition skeleton. Numerical approximations for both primal and dual unknowns are then obtained from a simple post-processing step that combines global degrees of freedom and local solutions. In terms of practical use, some of the good features of the MHM methods are (1) formulation is free of artificial numerical parameters, (2) global problem is very similar between different methods, even when changing the PDE, (3) local problems associated to the same element differ one-another only on source term and boundary conditions (4) local problems are defined on a

continuous formulation, so that one can use different numerical methods to obtain local solutions.

In [1], an MHM method was developed for the linear elasticity model. The analysis of the MHM method on two- and three-dimensional conforming simplicial meshes showed the method is well-posed and achieves superconvergence when using the standard Galerkin method at the local level. In this work, we show the extension of the method in [1] to non-conforming polytopal meshes with new superconvergent error estimates in the $H^1(\mathcal{P})$ and $L^2(\Omega)$ norms for the displacement field. The new theory also enables the use of high-order discontinuous interpolations in the partition skeleton. Numerical results validate the theory, show the good approximation for the post-processed stress field, and convergence results by a skeleton-based refinement. Finally, we show a multiscale three-dimensional test and compare the results, in terms of performance, with the standard Galerkin method.

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