

NUMERICAL CHALLENGES IN PDE 2016 - PART I

- **Date:** 02/09/2016
- **Venue:**
 - 9:00-12:10 Auditório do IMECC, R. Sérgio Buarque de Holanda, 651
 - 14:00-16:10 Auditório do Laboratório de Computação Científica e Visualização Galileu, R. Josias Willard Gibbs s/n

PROGRAM

- **9:00-9:10 Opening section**
- **9:10-10:00 Plenary talk**
 - Prof. Jay Gopalakrishnan, Portland State University, USA
Implementation of DPG methods in the NGSolve package
- **10:00-10:40 Poster section and coffee break**
 - Felipe A. G. da Silva (Doutorado em Matemática Aplicada, Unicamp), Maicon R. Correa e Eduardo C. Abreu (IMECC, Unicamp)
A study of high order discontinuous Galerkin methods for hyperbolic problems
 - Juan C. Rodríguez (Doutorado em Matemática Aplicada, Unicamp) e Maicon R. Correa (IMECC, Unicamp)
Hierarchical High Order Finite Element Spaces for Stabilized Mixed Formulations of Tracer Flow Problem in Porous Media
 - Margui A. R. Pinedo (Doutorado em Matemática Aplicada, Unicamp), Maicon R. Correa e Sônia M. Gomes (IMECC, Unicamp)
Hybrid-Mixed Finite Element Methods for a Non-Linear Elliptic Problem
 - Tatiana A. Suárez (Mestrado em Geofísica, USP) e Fernando B. Ribeiro (IAG, USP)
A Solução de Alguns Problemas de Transferência de Calor na Presença de Mudança de Estado: o Efeito do Calor Latente e da Segregação de Cristais
 - Benedito S. Abreu (Doutorado em Matemática Aplicada, Unicamp) e Maicon R. Correa (IMECC, Unicamp)
A General Flux Based FEM for Reaction-Diffusion Problems
- **10:40-12:10 Oral presentations**
 - Philippe R. B. Devloo (FEC, Unicamp)
NeoPZ: An Object Oriented Finite Element Framework
 - Gujji M. M. Reddy (ICMC, USP – São Carlos)
Ritz-Volterra reconstructions and a posteriori error analysis of finite element method for parabolic integro-differential equations
 - Thiago D. Santos (Doutorado em Engenharia Civil, Unicamp), Mathieu Morlighem (UCI, USA), Hélène Serouss, Eric Larour (JPL/Caltech, USA), P. R. B. Devloo (FEC, Unicamp) e J. C. Simões (UFRGS)
h-Adaptivity Applied to Ice Sheet Simulation
- **12:10-14:00 Lunch break**

- **14:00-15:30 Oral presentations**

- Sônia M. Gomes (IMECC, Unicamp)
New Approximation Space Configurations for Mixed Finite Element Formulations
- J. L. Boldrini (IMECC, Unicamp), Eduardo A. Moraes (Mestrado em Engenharia Mecânica, Unicamp), L. R. Chiarelli, F. G. Fumes e M. L. Bittencourt (FEM, Unicamp)
A Thermodynamic Consistent Non-isothermal Phase Field Model for Structural Damage and Fatigue
- Pablo G. S. Carvalho (Mestrado em Engenharia Civil, Unicamp) e P. R. B. Devloo (FEC, Unicamp)
Stokes Flow Computational Modeling and Comparative Study Between Approximation Spaces

- **15:30-16:10** Poster section and coffee break

ABSTRACTS OF THE CONTRIBUTIONS

Implementation of DPG methods in the NGSolve package

Jay Gopalakrishnan, Portland University, USA

Abstract

I will discuss ways to implement discontinuous Petrov Galerkin methods using a python interface to the C++ codebase in NGSolve package.

NeoPZ: An Object Oriented Finite Element Framework

Philippe R B Devloo, FEC-Unicamp

This talk gives an overview of the features of the object oriented programming environment NeoPZ. The objective of NeoPZ is to offer the scientific community advanced finite element algorithms in a coherent framework. It hopes to foster the advancement of finite element research by making complex algorithms accessible through a simple class interface. It organized by modules that can, theoretically, be used independently.

- Geometric map
- Approximation space
- Variational statement or weak form
- Linear Algebra
- Finite element tools

Examples of applications shall be presented in order to illustrate the efficiency of different finite element formulations implemented using the NeoPZ tools.

Ritz–Volterra reconstructions and a posteriori error analysis of finite element method for parabolic integro-differential equations

Gujji M M Reddy

Abstract: Parabolic integro-differential equations (PIDE) arise in various physical applications. Despite being so rich in the *a priori* analysis and in spite of the importance of these equations in the modelling of several physical phenomena, the topic of *a posteriori* error analysis for such kind of equations remains unexplored. Since PIDE may be thought of as a perturbation of the purely parabolic problem, therefore, it is natural to see whether the *a posteriori* error analysis of parabolic problems can be extended to PIDE. An attempt has been made to generalize the results of purely parabolic problems to PIDE. *A posteriori* error estimates for both semidiscrete and implicit fully discrete backward Euler method for linear parabolic integro-differential equations are obtained in a bounded convex polygonal or polyhedral domain. A novel space-time reconstruction operator is introduced, which is a generalization of the elliptic reconstruction operator [SIAM J. Numer. Anal. , 41, pp. 1585–1594, (2003)], and we call it as Ritz–Volterra reconstruction operator. The Ritz–Volterra reconstruction operator is used a crucial way to derive optimal order *a posteriori* error estimates in the $L^\infty(L^2)$ and $L^2(H^1)$ -norms.

h-Adaptivity Applied to Ice Sheet Simulation

Thiago Dias dos Santos
Mathieu Morlighem
Hélène Seroussi
Eric Larour
Jefferson Cardia Simões
Philippe Remy Bernard Devloo

This work proposes to make contributions in ice sheet modeling. Ice sheets have received attention by national and international scientific community in recent decades because of its potential contribution to sea level rise. This work aims to contribute in ice sheet modeling by applying *h*-adaptive refinement and goal-oriented error estimates with the ISSM software (Ice Sheet System Model). ISSM is developed by Jet Propulsion Laboratory at the California Institute of Technology (JPL/Caltech) and by the University of California at Irvine (UCI). The algorithm of *h*-adaptive refinement is based on the finite element library NeoPZ, developed by the Computational Mechanics Laboratory at UNICAMP. The set of partial differential equations of ice sheet evolution and the numerical scheme to solve them are presented. Numerical experiments based on the Marine Ice-Sheet Model Intercomparison Project (MISOMIP) are simulated using ISSM and NeoPZ. Results using *h*-adaptive refinement show reduction of the numerical error and computational cost.

New space configurations for mixed finite element formulations

Sônia M. Gomes - IMECC, Unicamp

This talk is concerned with recent progresses in the design of advanced finite element methods for mixed formulations. There are different possibilities of choosing balanced pairs of approximation spaces for dual (flux) and primal (pressure) variables to be used in discrete versions of the mixed finite element method for elliptic problems arising in fluid simulations. Three cases shall be discussed for 3D formulations based on tetrahedral, hexahedral and prismatic meshes [1]. The principle guiding the constructions of the approximation spaces is the property that the divergence of the dual space and the primal approximation space should coincide, while keeping the same order of accuracy for the flux variable and varying the accuracy order of the primal variable. Some cases correspond to the classic spaces of Raviart-Thomas, Brezzi-Douglas-Marini, Brezzi-Douglas-Fortin-Marini or Nédélec types. A new kind of approximation is proposed by further incrementing the order of some internal flux functions, and matching primal functions at the border fluxes. A summarized description shall be presented of the construction of hierarchical shape functions for the $H(\text{div})$ -conforming spaces for the flux approximations and of an unified error analysis for all these three kinds of space families, and element geometries. Numerical results shall be presented illustrating the optimal convergence rates and the effects of static condensation in the reduction of the dimension of linear global systems to be solved.

References

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A Thermodynamic Consistent Non-isothermal Phase Field Model for Structural Damage and Fatigue

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Abstract

We present a general thermodynamic consistent non-isothermal model for the evolution of damage, fatigue and fracture in materials under the hypothesis of small deformation. The approach is based on the principle of virtual power (PVP), the balance of energy and the second law of thermodynamics in the form of the generalized Clausius-Duhem inequality for the entropy. In addition to the usual physical fields, the model uses the phase field approach to describe the evolution of both damage and fatigue. The kinematic descriptor (phase field) for damage is considered a continuous dynamical variable whose evolution equation is obtained by the PVP. The kinematic descriptor (another phase field) for fatigue is a continuous internal variable whose evolution equation is considered as a constitutive relation to be determined in a thermodynamically consistent way. The behaviour of particular material classes can be specified by their corresponding free-energy potential (which gives the reversible parts of the involved thermodynamic forces) and their associated pseudo-potential of dissipation (which gives the irreversible parts of the involved thermodynamic forces). To exemplify our general model, we present the case of an isotropic linear elastic material with viscous dissipation and constant specific heat. The corresponding case of irreversible damage is also presented by using penalisation. The presented damage and fatigue phase field approach is a framework from which other methods in the literature may be recovered. The model is approximated by a nodal high-order finite element method with explicit fourth-order Runge-Kutta time integration. Results for one-dimensional examples are presented and conclusions are addressed.

Abstract

Stokes flow computational modeling and comparative study between approximation spaces

Pablo Giovanni Silva Carvalho and Philippe R. B. Devloo

The present work proposes a numerical analysis adapted to different approximation spaces for Stokes flow problems. A computational method based on a mathematical formulation will be constructed for continuous Finite Element Method (FEM) and compared to H(Div) and Discontinuous Galerkin Method (DGM). In order to obtain a numerical simulation compatible with imposed conditions, a computational code will be implemented in NeoPZ, an object oriented environment for scientific programming. This approach will make possible a comparative study between approximation spaces, verifying orders, errors and rates of convergence; identifying best performance. This work will also be motivated to describe the motion of a viscous fluid. In this direction, a computational modeling of Stokes flow through a porous domain will be simulated to enable further analysis of self-compacting concrete (SCC) flow around reinforcing bars. Results can be compared to a homogenization technique representing reinforcing bars domain by the Darcy law and interface coupled with Stokes flow theory. The aim of this work is to understand a relevant and applicable Stokes flow problem, verifying performance of approximation spaces and mathematical optimization.

A study of high order discontinuous Galerkin methods for hyperbolic problems

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Keywords: Hyperbolic differential equations , Galerkin methods , Semi-discrete scheme, Runge-Kutta formulas, High order central schemes.

ABSTRACT

The focus of this work is the computational study of some Discontinuous Galerkin methods for numerical approximation of first order hyperbolic differential problems, focusing on explicit schemes with discretization based on Runge-Kutta type methods in time, in problems with linear and nonlinear fluxes. Specifically, the good local stability properties of Runge-Kutta methods are combined with stable numerical flux functions and slope limiters in order to propose new higher-order Discontinuous Galerkin methods that achieve high resolution of abrupt gradients and discontinuous solutions, without spurious oscillations in numerical solutions.

References

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Hierarchical High Order Finite Element Spaces for Stabilized Mixed Formulations of Tracer Flow Problem in Porous Media

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Abstract

The development of mathematical and computational models for flow simulation in porous media is of interest in various areas of Applied and Engineering Sciences. As an example of a problem in this area, the process of injecting a tracer compound that allows to track the temporal and spatial evolution the flow in interior reservoirs informing the preferred direction. The behavior of the velocity $\mathbf{u}(\mathbf{x})$ and the pressure $p(\mathbf{x})$ is modeled by a elliptical system obtained from the Darcy and conservation mass laws, given by

$$\mathbf{u} = -\mathbf{K}\nabla p \quad \text{in } \Omega \quad (\text{Darcy's Law}) \quad (1)$$

$$\text{div } \mathbf{u} = f \quad \text{in } \Omega \quad (\text{Mass Conservation}) \quad (2)$$

$$\mathbf{u} \cdot \mathbf{n} = \bar{h} \quad \text{on } \partial\Omega, \quad (\text{Boundary Condition}) \quad (3)$$

let Ω be an open bounded domain in \mathbb{R}^n , with continuous Lipschitz boundary $\partial\Omega$, and external unit normal vector \mathbf{n} , representing a rigid porous media saturated with an incompressible fluid. The variable $\mathbf{u}(\mathbf{x})$, called Darcy's velocity, represents the average fluid velocity in the porous media, related with the gradient of the hydraulic pressure $p(\mathbf{x})$ through the tensor \mathbf{K} , representing the permeability of the porous matrix divided by the fluid viscosity (that will be simply named as permeability). The source term f must satisfy

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the compatibility condition $\int_{\Omega} f d\Omega = \int_{\partial\Omega} \bar{h} ds$. Beyond the elliptic system, a convection-diffusion equation with convection dominate, express the conservation of mass the tracer like

$$\phi \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = 0 \quad \text{in } \Omega \times (0, T], \quad (4)$$

where $c(\mathbf{x}, t)$ is the concentration of fluid injected, ϕ porosity of media and $T > 0$ with initial and boundary conditions

$$c(\mathbf{x}, 0) = c_0 \quad \text{in } \Omega \quad \text{and} \quad c(\mathbf{x}, t) = g \quad \text{in } \partial\Omega \times (0, T]. \quad (5)$$

The construction of mixed finite element methods involves the simultaneous approximation of the velocity and the pressure, thus requiring compatible finite element subspaces of $H(\text{div}, \Omega)$ and $L^2(\Omega)$, in the sense that they must satisfy a compatibility condition, or inf-sup condition, in order to provide stable numerical solutions for the Darcy system. This compatibility requirement reduces the flexibility in constructing such subspaces. *Galerkin Least Squares* (GLS) method is an alternative stable procedure to avoid this kind of delicate balance. It consists in augmenting the dual mixed formulation with weighted residual terms of $H^1(\Omega)$ type for the pressure and of $H(\text{div}, \Omega)$ type for the velocity [1]. In this work, we present a study of convergence of this method applied to the problem of Darcy (1)-(3) in a homogeneous media using hierarchical $H(\text{div}, \Omega)$ -conforms subspaces for the velocity [2], that guarantee the continuity of the normal component of the flow at the interfaces of the elements, and $H^1(\Omega)$ continuous subspaces for the pressure. For the transport problem is considered a finite volumes method of type *upwind*, using the linearization of the gradient reconstruction solution to obtain a better approach [3].

References

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HYBRID-MIXED FINITE ELEMENT METHODS FOR A NON-LINEAR ELLIPTIC PROBLEM

MARGUI R. PINEDO, MAICON R. CORREA, AND SONIA M. GÔMES

ABSTRACT. In this work we present an iterative type algorithm to get numerical solutions of the nonlinear elliptic problem given by

$$\begin{aligned}\alpha(\mathbf{x}, p)p - \operatorname{div}(K(\mathbf{x}, p)\nabla p) &= f \quad \text{in } \Omega, \\ p &= 0 \quad \text{on } \partial\Omega.\end{aligned}$$

by using hybrid-mixed finite element methods in quadrilateral meshes, with compatible spaces such as those based on RT (Raviart-Thomas) [4], BDM (Brezzi-Douglas-Marini) [2] and ABF (Arnold-Boffi-Falk) [1] families. We compare some properties of these spaces, in linear and non-linear versions of the studied problem, and by numerical experiments we check the accuracy and the quality of the approximations of the scalar variable, the flux and its divergence on affine and non-affine quadrilateral meshes.

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A solução de alguns problemas de transferência de calor na presença de mudança de estado: o efeito da liberação de calor latente e da segregação de cristais

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Abstract

A maioria dos corpos ígneos são formados através de injeções repetidas de magma, ou de rocha total ou parcialmente fundida, ao longo do tempo. O magma injetado tem diferentes propriedades físicas e químicas dependendo do ambiente onde é gerado. O seu resfriamento produz uma grande variedade de rochas da crosta continental. Neste estudo, se apresenta a evolução térmica de um corpo intrusivo formado por múltiplas injeções de basalto na crosta superior. No processo de resfriamento do magma e de formação de rochas ígneas, a composição e a fração do líquido remanescente se altera com o tempo e varia com as diferentes injeções de magma, dependendo da sua temperatura e da sua profundidade. A liberação de calor latente e sensível esquenta progressivamente a rocha encaixante permitindo que ela se funda, contribuindo para a alteração da composição química do líquido residual, líquido ainda presente no processo de resfriamento, e da distribuição de temperatura da crosta.

O trabalho consistiu na solução da equação de condução de calor, levando em consideração mudança de fase e liberação de calor latente em um intervalo finito de temperaturas, ou seja, em uma situação diferente do problema clássico de Stefan. A equação de condução de calor foi resolvida em uma única direção, usando o método das diferenças finitas, na formulação implícita. O modelo consiste em uma camada horizontal com condutividade e difusividade térmicas constantes, na qual são introduzidas, em sequência, uma série de lâminas de rocha inicialmente fundidas, cuja temperatura inicial é a temperatura de solidificação ou, liquidus do sistema rocha-magma. Liquidus é a temperatura a partir da qual a mudança de fase se inicia. As propriedades térmicas do magma são diferentes da rocha do modelo inicial. No contato entre a rocha encaixante e o volume de rocha fundida foi imposta uma condição de contorno do tipo de Neumann. A temperatura foi fixada na superfície do modelo e o fluxo de calor foi fixado na base do modelo.

A duração total do processo de resfriamento é de 3.2 Ma (milhões de anos), com tempo de 10^4 anos entre duas injeções consecutivas de magma. Cada injeção tem uma espessura de 50 m que corresponde a um acréscimo de basalto a uma taxa de 5mm/ano . As frações de fusão variam com a profundidade de 0,09 a 0,43 que correspondem à composição de diferentes tipos de rocha da crosta. A quantidade de água na cristalização contida no basalto não altera consideravelmente os resultados deste estudo.

A FLUX-BASED FEM FOR REACTION-DIFFUSION PROBLEMS.

BENEDITO S. ABREU ^{*} & MAICON R. CORREA [†]

1 Overview/Summary

The stationary diffusion-reaction linear problem arises in many situations, for example when modelling a reacting flow in a porous medium. Such a problem, in simple terms, may be mathematically described by the following boundary value problem

$$\begin{cases} \alpha(\mathbf{x})p - \operatorname{div}(K(\mathbf{x})\nabla p) &= f, & x \in \Omega \\ p &= p_D, & x \in \Gamma_D, \\ -(K(\mathbf{x})\nabla p) \cdot \mathbf{n} &= 0, & x \in \Gamma_N, \end{cases} \quad (1.1)$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$. Moreover $p : \Omega \rightarrow \mathbb{R}$ represents the scalar field (pressure, for instance), with $\alpha(\mathbf{x}) \geq \alpha_{\min} > 0$ and $K(\mathbf{x}) \geq K_{\min} > 0$. In order to obtain a good approximation to the vector field related to the unknown p (usually the Darcy's velocity), a common approach consists in deploying the mixed dual finite element formulation whereby both the unknowns are computed within specific spaces. In this manner, we start by writing the previous equation as a first order system

$$\alpha(\mathbf{x})p + \operatorname{div} \mathbf{u} = f, \quad \mathbf{u} = -K(\mathbf{x})\nabla p, \quad \mathbf{x} \in \Omega, \quad (1.2)$$

where $\mathbf{u} : \Omega \rightarrow \mathbb{R}^2$ is the Darcy's velocity. In turn, the variables \mathbf{u} and p for the latter are respectively approximated into $H(\operatorname{div}, \Omega)$ and $L^2(\Omega)$ subspaces, leading to a bigger linear system. Furthermore, a compatibility condition (inf-sup condition) between these subspaces is required [1].

On the other hand, on account of particular features in this problem, the penalty method suggests us merely to eliminate the scalar unknown obtaining thus an uncoupled scheme involving only the vector unknown. Proceeding this way, we can thereby recover the scalar field by postprocessing the vector solution. The postprocessing stage can be performed using parallelism and thus reducing the overall computational cost.

In this work we consider a version of the mixed finite element method applied to stationary reaction-diffusion problems whereby the scalar field is recovered by local postprocessing of the vector field (the primary unknown). Numerical results for the Raviart-Thomas[3] and Arnold-Boffi-Falk[2] families of mixed finite elements, as well as an enriched combination, are addressed on quadrilateral meshes deploying static condensation. Results concerning accuracy on affine and general quadrilateral meshes are shown. An extension of this scheme to the case involving advection is pursued (ongoing).

References

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