
Applied Math and Computational Science across the Americas
Mathématiques appliquées et modélisation numérique à travers l'Amérique
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GUSTAVO BUSCAGLIA, ICMC, University of São Paulo, Brazil
Domain decomposition with Robin interface conditions for reservoir simulation

A multiscale method for the porous-media flow equations is proposed. It is based on a domain-decomposition procedure in which the subdomains are coupled by Robin boundary conditions. There appear two independent spaces on the skeleton of the decomposition, corresponding to interface pressures and fluxes, that can be chosen with great flexibility to accommodate local features of the permeability field. Experiments will be presented comparing the proposed method to existing ones in the simulation of realistic flow in high-contrast channelized porous formations.

Joint work with Rafael T. Guiraldello, Fabrício S. Sousa, and Roberto F. Ausas (ICMC, University of São Paulo, Brazil), and Felipe Pereira (The University of Texas at Dallas, USA).

JOSE CASTILLO, San Diego State University
High Order Compact Mimetic Differences and Discrete Energy Decay in 2D Wave Motions

Mimetic Difference Operators Div, Grad and Curl, have been constructed to provide a high order of accuracy in numerical schemes that mimic the properties of their corresponding continuum operators; hence they would be faithful to the physics. However; this faithfulness of the discrete basic operators might not be enough if the numerical difference scheme introduces some numerical energy increase, which would obviously result in a potentially unstable performance. We present a high order compact mimetic scheme for 2-D wave motions and show that the energy of the system is also conserved in the discrete sense.

MIGUEL DUMETT, San Diego State University
A high-order accurate mimetic discretization of the Eikonal equation with Soner boundary conditions

High-order accurate Castillo-Grone mimetic gradients are for adapted for solving the Eikonal equation with Soner boundary conditions. An iterative method based on the linearization of a variational formulation is proposed. The method reduces at each step the absolute error (infinity norm). The accuracy of the solution is several orders of magnitude much better than the accuracy than the one achieved by Sethian's first-order Fast Marching method (see the attached figure).

Joint work with Jorge Eliecer Ospino Portillo.

MIGUEL DUMETT, San Diego State University, USA
L1 Norm Regularization of the Kirchhoff Standard Migrated Image

The composition of the Kirchhoff Forward Modeling operator and its transpose, the Kirchhoff Migration operator, applied on a seismic reflectivity map can be inverted by modern optimization techniques, in particular an L1 regularized least squares procedure that achieves a sharper image and better amplitudes than the Classical Standard Migration. Future developments are considered.

JUAN CARLOS CABRAL FIGUEREDO, National University of Asuncion, Paraguay
On adaptive control strategy for restarting GMRES

The Generalized Minimal Residual method (GMRES) is normally used for the solution of large, sparse and nonsymmetric linear systems arising from science and engineering problems. In practice, the restarted GMRES method, denoted as GMRES(m), is used to reduced storage and orthogonalization costs. However, if an inappropriate m is chosen, the method may present stagnation or slow convergence.

This talk has two parts. In the first part, we discuss advances in the control theory for accelerating the convergence of GMRES(m). This new method modifies adaptively the dimension of the Krylov subspace using control techniques. In the second part, we discuss techniques used to overcome stagnation in GMRES(m). The techniques are based on the modification of the structure of the search subspace. In particular, we discuss conditions for characterizing the stagnation of the restarted GMRES method, and we show several alternatives to avoid such stagnation using adaptive control for switching conveniently the enrichment between several possible options obtained from the literature. Results of our implemented techniques, solving problems with real data, are presented and show that the adaptive method is more robust than classical ones.

This work is a joint work with Christian Schaerer supported by POS-007 and 14-INV-186.

JUAN CARLOS GALVIS, UNIVERSIDAD NACIONAL DE COLOMBIA

Numerical methods for high-contrast multiscale problems

In this talk, we review the design and analysis of robust domain decomposition and multiscale finite element algorithms for high-contrast multiscale problems. In particular, we review the construction of coarse spaces using spectral information of local bilinear forms. We present some applications to linear and nonlinear problems including a novel conservative discretization for two-phase flow in ahigh-contrast multiscale porous media.

SILVIA JIMENEZ-BOLANOS, Colgate University

Navier Slip Condition for Viscous Fluids on a Rough Boundary

In this talk, using homogenization methods and boundary layer techniques, I will derive asymptotically the effective Navier slip boundary condition, as a first-order corrector, to the no-slip condition on the interface between a fluid and a rough surface. The method used provides a formula to calculate the slip length for various geometries. I will also show some computations done, using FreeFem++, which agree with experimental data.

OSNI MARQUES, Lawrence Berkeley National Laboratory, USA

Nonlinear Eigensolver based on Padé Approximants

In this presentation, we discuss a strategy for finding nontrivial solutions (λ, x) for a class of nonlinear eigenvalue problems of the form $F(\lambda)x = 0$. Specifically, we focus on problems related to the modeling of waveguide-loaded accelerator cavities through a finite element discretization of Maxwell's equation, where some of the matrices involved exhibit low-rank properties. We use rational functions to approximate the nonlinear terms of the problem, together with Padé approximants. This allows a linearization of the original problem, through a generalized eigenvalue of dimension larger than the original problem. We show the impact of the degree of the Padé approximants in the linearization process and convergence, and alternatives for solving the resulting linearized problem.

CARLOS E. MEJÍA, Universidad Nacional de Colombia, Medellín

Finite difference methods for fractional advection dispersion equations

In recent years, fractional differential equation (FDE) models have been proposed in many fields such as fluid dynamics, geology, finance, biology and so on. Simultaneously reliable numerical methods for FDEs are in great demand and this talk is a contribution on this direction. We focus our attention on time fractional advection dispersion equations (TFADE) as potential tools for the prediction of the environmental consequences of groundwater contamination. For an initial boundary value problem for a linear two dimensional TFADE with variable coefficients, we consider a new implicit, consistent, unconditionally stable and convergent finite difference method of solution. Additionally, we develop a stable method of solution for an inverse problem based on a linear one dimensional TFADE. We offer illustrative numerical experiments and some insight on our current research on FDEs with time and/or space fractional derivatives.

SUELY OLIVEIRA, The University of Iowa
Parallel Computing Large-scale Data Problems

Large data problems appear in different applications. For example, LiDAR measurements for terrain in geoinformatics and data warehouses for weather modeling. Knowledge of diverse areas of computer science plays a significant role in data science. My research has shifted from scientific computing to data sciences, including the creation of a certificate in Large Data Analysis involving Computer Science, Statistics and Mathematics Departments at the University of Iowa. In the capstone course for this new certificate, we work on various projects involving different types of data sets, parallel algorithms with MapReduce and other parallel paradigms such message passing and GPUs. One type of application I will cover in this talk is classification with a large number of data points and a moderate number of features. It is an improvement on standard soft-margin SVM algorithms. The new algorithm is very fast in terms of numbers of iterations, and relatively easy to parallelize in distributed memory clusters.

SANDRA AUGUSTA SANTOS, UNICAMP
On the rank-sparsity decomposition problem

The rank-sparsity decomposition problem is motivated by the need to extract, from data collected by a large-scale sensor network, a (sparse) model, partially hidden, and a small number of sources of noise (low rank). This type of problem has inherent interest from the applications perspective, arising in a number of settings such as the statistical model selection, the rigidity of a matrix, and the system identification, to name a few. It has also a clean description as a type of nonlinear discrete-optimization problem for which powerful methods to address large-scale problems are of great interest, being currently under investigation. In this presentation, the advances derived from the cooperation agreement FAPESP-University of Michigan, in collaboration with prof. Jon Lee (UM), prof. Marcia Fampa (UFRJ) and the PhD student Ivan Nascimento (IMECC-Unicamp) will be reported.

MARCUS SARKIS, Worcester Polytechnic Institute
On an adaptive finite element phase-field dynamic fracture model

Abstract: In this talk we describe an efficient finite element treatment of a variational, time-discrete model for dynamic brittle fracture. We start by providing an overview of an existing dynamic fracture model that stems from Griffith's theory and based on the Ambrosio-Tortorelli crack regularization. We propose an efficient numerical scheme based on the bilinear finite elements. For the temporal discretization of the wave equations of motion, we use generalized alpha-time integration algorithm, which is implicit and unconditionally stable. To accommodate the crack irreversibility, we use a primal-dual active set strategy, which can be identified as a semi-smooth Newton's method. It is well known that to resolve the crack-path accurately, the mesh near the crack needs to be very fine, so it is common to use adaptive meshes. We propose a simple, robust, local mesh-refinement criterion to reduce the computational cost. We show that the phase-field based variational approach and adaptive finite-elements provides an efficient procedure for simulating the complex crack propagation including crack-branching.

Joint work with Christopher Larsen and S. M. Mallikarjunaiah

DANIEL SZYLD, Temple University
Asynchronous Optimized Schwarz, Theory and Experiments

Asynchronous methods refer to parallel iterative procedures where each process performs its task without waiting for other processes to be completed, i.e., with whatever information it has locally available and with no synchronizations with other processes. In this talk, an asynchronous version of the optimized Schwarz method is presented for the solution of differential equations on a parallel computational environment. In a one-way subdivision of the computational domain, with overlap, the method is shown to converge when the optimal artificial interface conditions are used. Convergence is also proved under very mild conditions on the size of the subdomains, when approximate (non-optimal) interface conditions are utilized. A different result for bounded rectangular domains is also shown. Numerical results are presented on large three-dimensional problems illustrating the efficiency of the proposed asynchronous parallel implementation of the method. The main application shown is the calculation of the gravitational potential in the area around the Chicxulub crater, in Yucatan, where an asteroid is believed to have landed 66 million years ago contributing to the extinction of the dinosaurs. (Joint work with José Garay, Temple University; Fréderic Magoulés and Cedric Venet, CentraleSupelec, Châtenay Malabry, France)

CRISTINA TURNER, Universidad Nacional de Córdoba
Adjoint method for a tumour invasion PDE-constrained optimization problem using FEM

In this talk we present a method for estimating unknown parameters that appear on a non-linear reaction-diffusion model of cancer invasion. This model considers that tumor-induced alteration of micro-enviromental pH provides a mechanism for cancer invasion. A coupled system reaction-diffusion describing this model is given by three partial differential equations for the non dimensional spatial distribution and temporal evolution of the density of normal tissue, the neoplastic tissue growth and the excess concentration of $H+$ ions. Each of the model parameters has a corresponding biological interpretation. For instance, the growth rate of neoplastic tissue, the diffusion coefficient. After solving the forward problem properly, we use the model for the estimation of parameters by fitting the numerical solution with real data, obtained via in vitro experiments and medical imaging. We define an appropriate functional to compare both the real data and the numerical solution. We use the adjoint method for the minimization of this functional and Finite element method to solve both the direct and inverse problem, computing the posterior error in both problem. Moreover, we show some ideas about the possibilities of a therapeutic methodology in order to treat the tumor.

FRÉDÉRIC VALENTIN, LNCC - National Laboratory for Scientific Computation
Multiscale Hybrid-Mixed Method for Fluids

This work presents a family of finite element methods for multiscale fluid problems, named Multiscale Hybrid-Mixed (MHM) methods. The MHM method is a consequence of a hybridization procedure which characterizes the unknowns as a direct sum of a "coarse" solution and the solutions to problems with Neumann boundary conditions driven by the multipliers. As a result, the MHM method becomes a strategy that naturally incorporates multiple scales while providing solutions with high-order precision for the primal and dual variables. The completely independent local problems are embedded in the upscaling procedure, and computational approximations may be naturally obtained in a parallel computing environment. Well-posedness and best approximation results for the one- and two-level versions of the MHM method show that the method is optimal convergent and achieves super-convergence for the velocity field with respect to the mesh parameter. Interesting, the numerical velocity field turns out to be locally conservative. Also, a face-based a posteriori estimator is shown to be locally efficient and reliable with respect to the natural norms. The general framework and some recent results are illustrated for the Stokes and Brinkman equations, and validated through a large varieties of numerical results for highly heterogeneous coefficient problems.

References

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PAULA VASQUEZ, University of South Carolina
Dynamical modeling of the yeast genome

A genome is a complete copy of the entire set of genetic material that makeup a specific organism. Progress in live-cell microscopy had made clear that the genome is far from being a static information warehouse. Rather, it is a mechanically active entity that is constantly altering its shape. Chromosome motion can be described from polymer physics principles. Considering the organization of these long macromolecules and their constant exposure to random forces, understanding the mechanisms that alter their behavior requires integrating cell biology with physical principles that govern fluctuating chains. This talk focuses in applications of polymer theory to the studies of nuclear organization and function in yeast cells.