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ABSTRACTS

Dynamic bifurcation for the numerical solution of the generalized Burgers equations

Boying Wu

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Abstract: This paper is focused on the stable of the zero solution and the bifurcation of the numerical equations of the generalized Burgers equation. The numerical equations are obtained by the central difference schemes and its multipliers are solved out by analyzing methods. It is shown that the origin is an asymptotically stable equilibrium point of the numerical equations of the generalized Burgers equation. Furthermore, it is proved that the numerical equations of the generalized Burgers equation undergoes a fold bifurcation at . Finally, some numerical simulations are shown to verify the analytical results.

Compact ADI Scheme with Extrapolation for 2D Parabolic Equations

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Abstract: A kind of compact alternating direction implicit (ADI) scheme for numerically solving a class of two-dimensional parabolic equations is proposed in this article. We demonstrate that the scheme is stable unconditionally, and the convergence order is in $O(\tau^2 + h^4)$ with respect to three different norms. Richardson extrapolation is designed for this scheme to improve the error accuracy, and sixth-order accurate approximation both in time and space is obtained when the time step is proportional to the spacial mesh parameter. We have successfully established error estimates and presented numerical experiments to show the high efficiency of the new scheme in this work.

Front-fixing Finite Element Methods for the American Option Pricing with Regime Switching

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Abstract: American option problems under regime switching model are considered in this talk. The conjectures in Yang, J. Sci. Comput. 44 (2010), 69-91 about the position of early exercise prices are proved, which generalize the results in Yi, Math. Methods in the Appl. Sci. 31 (2008), 1461-1477 by allowing the interest rates are different in two states. A front-fixing finite element method for the free boundary problems is proposed and implemented. Its stability is established under reasonable assumptions. Numerical results are given to examine the rate of convergence of our method, which is also compared with the usual finite element method.

Finite element analysis of electromagnetics in metamaterials

Yunqing Huang

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Abstract: In this talk we will report some recent advances in finite element analysis of electromagnetics in metamaterials. The stability properties, optimal error estimates and superconvergence are considered for various fully discrete schemes. Numerical tests are presented both for theoretical justification and some typical phenomenon such as cloaking, backward wave propagation etc.

Fractional Partial Differential Equations: Modeling and Computation

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Abstract: : The fractional calculus is almost as old as it's more familiar integer-order counterpart. The fractional partial differential equations are novel extensions of the traditional models, based on fractional calculus. They are now winning more and more scientific applications cross a variety of fields including control theory, biology, electrochemical processes, viscoelastic materials, polymer, finance, and etc. In this talk, we will explain a number of fractional models using the stochastic formulation of transport phenomena in terms of a random walk process. We will also present some efficient methods for the numerical solution of the time-space fractional diffusion equation. Particularly, we discuss the existence and uniqueness of the weak solution, and its spectral approximations based on the weak formulations. Finally, some interesting applications to viscoelastic materials, turbulence, and molecular biology will be addressed.

Compressible Wavelet Lattice Boltzmann Method and Applications

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Abstract: Lattice Boltzmann Method (LBM) is a novel numerical method for flows simulations. Compared with classic methods of Finite Difference Method, Finite Volume Method and Finite Element Method, LBM has numerous advantages, including inherent parallelization and simplicity of boundary condition treatment. LBM has been used to simulate incompressible flows since it was invented. To extend LBM to simulate compressible flows, there are two aspects of work to be done. First, it is to develop LB models for compressible flows. Second, it is to find feasible numerical methods. An improved lattice Boltzmann model is presented for compressible Navier-Stokes system with high Mach number. We start by constructing a simple Haar wavelet equilibrium function to replace the complicated Maxwellian function. The simple Haar wavelet function satisfies all needed relations to recover to Euler/Navier-Stokes equations. And we give its associated equilibrium distribution functions for compressible flows. And also, we explore relative boundary conditions and numerical methods and simulate compressible flows with developed models. Shock wave tubes and shock wave reflections are used to validate the new model. Numerical results indicate that the new LB model is successful with the simulation of compressible fluid.

Phase and Phase Transition of Soft Matter

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Abstract: Systems whose physical and mechanical energy scales are comparable to that of thermal energy at room temperature and are thus easily deformed by thermodynamic driving forces are considered soft matters. Examples include polymers, colloids, liquid crystals, gels, and a number of biological materials. Complex fluids refer to the subset of multi-component soft matters that can flow, and display non-Newtonian rheology. Soft matters and complex fluids are ubiquitous in nature and have a number of important industrial applications. What makes complex fluids interesting is that their properties can be quite different from those of liquids or crystals made up of small molecules. Soft matters exhibit many interesting behavior such as the appearance of partially ordered phases, defects or singularities, complex dynamics, etc, which makes them an ideal place for studying interesting physics. Equally importantly, the subject poses many new mathematical questions that are both fundamental and challenging. A brief account of my talk is as follows.

1. Modeling of soft matters

It is well-known that modeling is a complicated issue in the study of soft matters. The introduction of multiscale models, particularly Doi-Onsager type of kinetic models that explicitly takes into account the molecular structure, has drastically improved the situation. We have developed inhomogeneous Doi-Onsager models for liquid crystal systems. In addition, we have also established a systemic model which included isotropic phase, nematic phase, smectic phases and blue phases for liquid crystals.

2. Analysis issues

A fundamental assumption in the Onsager theory of liquid crystals is that minimizers of the Onsager model have axially symmetry. Establishing such axially symmetry has been an open problem in the mathematical theory of liquid crystals for a very long time. We were among the first groups to have independently proved that all minimizers of the Onsager model with Maier-Saupe potential are axially symmetric. We have also given a complete classification of the phase diagram. In addition, we have established a theory of small Deborah limit from inhomogeneous molecular models to the classical Ericksen-Leslie theory for liquid crystals.

3. Numerical methods of Quasicrystals

Quasicrystals (QCs), with long-range order and non-crystallographic symmetry, is one kind of fascinatingly ordered structures between period structures (crystals) and disordered structures. The discovery of QCs changes the traditional concept of classifying structures into: crystals and non-crystals, and gives a strong impact on materials science, solid state chemistry, condensed matter physics and soft matter, both on basic experimental and theoretical tools. QCs are a kind of whole-spatial structures. Traditionally the same dimensional numerical methods need period structures to approximate QCs. However, these methods can just compute few kinds of QCs, such as 12-fold QCs, because of the limitation of Simultaneous Diophantine Approximation. We provide a systematic numerical method to calculate all QCs where QCs could be treated as projections of a higher-dimensional space. We also present how to compute the energy density exactly without boundary effect. In addition, we take Lifshitz-Petrich model as an example to demonstrate our methods and show some numerical results.

4. The physics of soft matters

One interesting feature of soft matters is that they may exhibit a variety of ordered phases like a complex solid. However, theoretical progress has been hindered by the lack of proper mathematical tools, even though physicists have long been interested in these phases and the transition between them. We have systematically developed a set of such tools and with them, we were able to establish a rather complete picture of the phase diagram of di-block and star-shaped tri-block copolymers and understand the complex phase transition process between these phases under the framework of self-consistent field theory.

An interpolating boundary element-free method (IBEFM) for linear problems

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Abstract: The moving least-squares (MLS) approximation is one of the most important methods to form the shape functions in meshless methods. The shape function of the MLS approximation does not satisfy the property of Kronecker function, then the boundary conditions in the meshless method based on the MLS approximation can be applied directly. The paper begins by discussing the interpolating moving least-squares (IMLS) method. The formulae of the IMLS method obtained by Lancaster are revised. On the basis of the boundary element-free method (BEFM), combining the boundary integral equation method with the IMLS method improved in this paper, the interpolating boundary element-free method (IBEFM) for two-dimensional potential and elasticity problems is presented, and the corresponding formulae of the IBEFM for two-dimensional potential and elasticity problems are obtained. In the IMLS method in this paper, the shape function satisfies the property of Kronecker function, and then in the IBEFM the boundary conditions can be applied directly and easily. The IBEFM is a direct meshless boundary integral equation method in which the basic unknown quantity is the real solution to the nodal variables. Thus it gives a greater computational precision. Numerical examples are presented to demonstrate the method.

Numerical realization of Max Noether's residual intersection theorem

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Abstract: The aim of this talk is to show numerical realization procedure for basic theorems of algebraic curves. A homotopy continuation method is introduced to compute out some elements of algebraic geometry such as intersection points (including multiplicity) between algebraic curves, singularities, genus of curves and the exact orders of a polynomial at the places of an algebraic curve with a finite center, etc. Moreover, as example, numerical procedure for determining whether three algebraic curves satisfy the conditions of Max Noether's residual intersection theorem is presented in the talk. The numerical experiments show that the proposed numerical procedures are well done accurately, effective and robust without using multiprecision arithmetic even if the coefficients of algebraic curves are inexact. The computational complexity of the numerical realization of Max Noether's residual intersection theorem is polynomial. Keywords: Algebraic Curve, Puiseux Expansion, Place, Homotopy Continuation, Multiple Root.

Optimal decay rates for a class of dissipative Mindlin-Timoshenko plates

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Abstract: In this talk we apply the theory of semigroup operators to obtain optimal polynomial decay rates for a class of 2D Mindlin-Timoshenko plates with a Kelvin-Voigt damping.

Post-Galerkin Methods Based on an Approximate Inertial Manifold

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Abstract: We consider the nonlinear elliptic boundary value problem

$$\begin{cases} -\Delta u + f(u) = 0 & \text{in } \Omega \subset \mathbb{R}, \\ u|_{\Gamma} = 0 & \text{on } \Gamma = \partial\Omega. \end{cases} \quad (1)$$

where Ω is a bounded domain in $\mathbb{R}^d$ with a smooth boundary Γ . Let $X = H_1^0(\Omega)$ be a Sobolev space and denote inner product and norm by $((,)) = (\nabla, \nabla)$, $||| |||^2 = ((,))$, respectively. Δ is the Laplace operator, and $f : \mathbb{R}^1 \rightarrow L^p(\Omega)$ is a Nemetsky operator. X_h is a finite element subspace defined on the grid with mesh size h .

The main results in this paper are the followings.

Theorem 1 Under some assumptions, there exists a mapping ϕ which is a Lipschitz continuous from X_h into $\hat{X}_h$,

$$\|\phi(w_1) - \phi(w_2)\| \leq l\|w_1 - w_2\|, \forall w_2, w_1 \in X_h \cap B_\rho,$$

and the solution u of (1) is at the neighborhood of the manifold $\mathcal{M}$ within thickness δ :

$$\text{dist}(u, \mathcal{M}) = \delta, \delta \leq ch^{2k+1+\alpha}.$$

where

$$\alpha = \begin{cases} 1/2, & d = 2, \\ 1/4, & d = 3. \end{cases}$$

Theorem 2 Under the same assumptions with theorem 1. The approximate solution based on the manifold $\mathcal{M} = \text{Graph}(\phi(u_h))$ possesses approximate property

$$\|u - (u_h + f(u_h))\| + h\|u - (u_h + \phi(u_h))\| \leq ch^{2k+2+\alpha}\|u\|_{k+1}.$$

Effective and True Condition Numbers of Linear Systems

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Abstract: For linear system $Ax = b$, the traditional condition number is the worst case for all b s and often overestimated in many problems. For a specific b , the effective condition number is a better upper bound for the relative error of x . But, it is also possible that this effective condition number is overestimated. In this talk, we study the true ratio of the relative error of x to the relative perturbation of b , called the true condition number. We obtain several new upper bounds and estimates for this true condition number. We also explore to change the system to an equivalent one by shifting b to minimize its effective condition number. Finally we apply all our results to functional approximation.

Soliton interactions in some semidiscrete integrable systems

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Abstract: In this talk, we will focus on the soliton interactions in some semidiscrete integrable systems. It will be shown that in some cases the solitary waves of the semidiscrete integrable systems can interact elastically. However, soliton interactions in the semidiscrete integrable systems possess different properties from the continuous solitons, for example, the shorter waves can travel faster than the taller ones. We also find that two stable solitary waves can be destroyed after interaction, and the elastic properties of collisions between two solitary waves are sensitively dependent on the choices of some parameters in solution. We therefore conclude that soliton interactions in semidiscrete integrable systems are richer than the ones in continuous soliton systems. The talk is based on the work cooperated with Tong Zhou.

Recent Advances in High Performance Algorithms for Computational Science and Engineering

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Abstract: In this talk we review some recent advances in high performance algorithms for relevant computational science and engineering applications. Of particular interest here are advanced nonlinear equation solvers, mesh generation and adaptive refinement and coarsening. We will discuss their implementation in high performance clusters and topics such as efficient data structures, partitioning strategies and related aspects. Multiphysics applications, as found in geoscience and offshore engineering will be used as demonstration problems.

Solitary waves in intricate river networks

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Abstract: Waves in intricate river networks is a problem with not much mathematical modeling. By intricate networks we mean channels that can have branching points (say as in a "Y" configuration) or sharp bends, such as 90 degrees corners. Solitary wave propagation in these domains has had very little attention.

In this talk both the mathematical and numerical modeling will be addressed for this problem.

Crank-Nicolson Scheme For The Oldroyd Model Of Order One

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Abstract: In this talk, we would like to analyze Crank-Nicolson scheme for the equations of motion arising in the Oldroyd model of order one with the forcing term independent of time or L^∞ in time. This model can be considered as an integral perturbation of Navier-Stokes equations. We would focus mainly on the difficulties due to the presence of the integral term. A priori error estimates in L^2 -norm are derived for the discrete problem which are optimal in nature.

On the existence of solutions to optimal control problems in time scales

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Abstract: We consider optimal control problems in time scales. Then we provide some properties for absolutely continuous functions in time scales. Then we consider a class of dynamical inclusions in time scales and extend to this class a convergence result of a sequence of almost inclusion trajectories to a limit which is actually a trajectory of the inclusion in question. We also introduce the so called Euler solution to dynamical systems in time scales and prove its existence.

A combination of the existence of Euler solutions with the compactness type result described above ensures the existence of an actual trajectory for the dynamical inclusion when the setvalued vector field is nonempty, compact, convex and has closed graph. Then, by making use of an extension of Filippovs Lemma and of compactness of trajectories for inclusions in time scale we prove the existence of optimal processes for control problems in time scales.

A semidefinite programming approximation for the problem of fitting positive exponential sums to empirical data.

Adalys Ivarez e Hugo Lara

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Abstract: In this work we deal with exponential sum models coming from data adquisition in empirical sciences. We present a two steps approach based on Tikhonov regularization and combinatorial optimization, to obtain stable parameter estimations which fit the data. We develop properties of the solutions, based on their optimality conditions. We also propose a semidefinite programming approximation for this combinatorial problem. Some numerical experiments are shown to illustrate our approach.

Investment Decisions under Uncertainty, Partial Differential Equations and Quantitative Finance

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Abstract: Industrial strategic decisions have evolved tremendously in the last decades towards a higher degree of quantitative analysis.

Such decisions require taking into account a large number of uncertain variables and volatile scenarios, much like financial market investments. Furthermore, they can be gauged and compared to portfolios of investments such as in stocks, derivatives and futures.

This revolution led to the development of a new field of managerial science known as Real Options. The use of Real Option techniques incorporates also the value of flexibility and gives a broader view of many business decisions that brings in techniques from quantitative finance and risk management. Such techniques are now part of the decision making process of many corporations and require a substantial amount of mathematical background. In particular, they require many tools from stochastic control and partial differential equations. In this talk we shall survey some basics of this approach as well as some applications in industrial problems.

Kohn-Sham equations and extrapolation methods for electronic structure calculations

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Abstract: Density Functional Theory (DFT) has been effectively employed for computing electronic structure of atoms and molecules. The most famous representative of this theory is the Kohn-Sham (KS) equation that consists in partitioning the total energy functional into kinetic energy, electrostatic energy, external potential energy and the exchange-correlation energy functional which exact form is unknown so far. In this talk we present the KS equation and we give an overview of the main methods employed to solve it and how we can enhance performance by applying the DIIS (Direct Inversion in the Iterative Subspace) extrapolation scheme.

Numerical Analysis for incompressible quasi-Newtonian flows with dual-mixed formulations via FEM-BEM coupling¹

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Abstract: We analyze the coupling of the dual-mixed finite element method with the boundary integral equation method, to solve problems concerned with incompressible quasi-Newtonian flows. We consider two cases as model examples, which are the exterior Stokes problem and a transmission problem between a linear Stokes flow with a quasi-Newtonian flow with mixed boundary conditions. The result is a mixed scheme for both, the exterior Stokes problem and the quasi-Newtonian problem. The approach is based on the introduction of both the flux and the strain tensor as further unknowns, which yields a two-fold saddle point operator equation as the resulting variational formulation. In both cases, we derive existence and uniqueness of solution for the continuous and discrete formulations and provide the associated error analysis. In particular, the corresponding Galerkin scheme is defined by using piecewise constant functions and Raviart-Thomas spaces of lowest order. Most of our analysis makes use of an extension of the classical Babuska-Brezzi theory to a class of nonlinear saddle-point problems. Also, we develop a-posteriori error estimates (of Bank-Weiser type) and propose a reliable adaptive algorithm to compute the finite elements solutions. Finally, several numerical results are provided, which support the theoretical results.

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Oscillations in the Biotic Pyrite Iron Cycle by Acidithiobacillus Ferrooxidans Bacteria

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Abstract: Motivated by the report of oscillatory behavior in pH and bacteria in acid mine drainage literature, we model the biotic pyrite iron cycle (a set of chemical reactions that releases acidic products into the environment) catalyzed by bacteria *Acidithiobacillus Ferrooxidans* with the aim of explaining why such a periodic behavior.

These microorganisms utilize those chemical reaction products to survive in that acidic medium by generating ATP and water in their cytoplasm. A non-dimensional analysis of the corresponding dynamical model shows the existence of, under certain circumstances, up to four non-trivial steady states. The stability of the equilibrium solutions is determined by using Routh-Hurwitz conditions. Two Hopf bifurcation values are found for the bacteria metabolism parameter.

Their stability and those of the associated periodic orbits are found numerically by utilizing parameter values given in the literature. Furthermore, we found values of the bifurcation parameter that exhibit SNP, homoclinic and doubling period bifurcations as well as stable chaotic behaviour. The coexistence under certain conditions of two stable steady states leads to the possibility of reducing the amount of sulphuric acid generated by the biotic iron cycle.

Mathematical analysis and simulation of cancer treatment models

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Abstract: Cancer is considered a serious public health problem worldwide. Following information given by the World Health Organization [6], 7.6 million people worldwide died from cancer in 2008, approximately 70% of cancer deaths occur in low- and middle-income countries and 30% of cancers could be prevented. One of the most applied type of cancer treatment is the antineoplastic chemotherapy, which has different features in order to eliminate tumour cells: the administration of one or more cycle-nonspecific or cycle-specific drug, joint application (or not) with other treatments and it is usually administered periodically, i.e., in cycles.

We present two mathematical models for cancer chemotherapy and surgery. The first one is a mathematical model to analyze the chemotherapeutic schedules taking into account both the competition between tumour and normal cells and the effect of angiogenic process in the carrying capacity of tumour cells associated with the vascular endothelial cells. We focus our research on antiangiogenic schedule (metronomic chemotherapy) (Hanahan *et al.* [1]). In order to get closer to clinical practice, we use some experimental data for numerical simulations. Moreover, according to the model, metronomic chemotherapy, compared to the conventional treatment, leads to a more effective action in the reduction of the tumour and provides the patient an increased survival (Rodrigues *et al.* [5]).

The second proposed model investigates treatments for large human tumours considering surgery and the cell-kill hypothesis proposed by Norton & Simon [3]. We use some biological and pharmacological data in the numerical approach, the administration of drug is in cycles (periodic infusion) and the surgery is performed instantaneously on the tumour cells population (Kohandel *et al.* [2]). An analysis of stability considering only chemotherapy with a continuously drug administration is presented. In according to Norton & Simon [3], our results indicate that chemotherapy is less efficient in treating tumours that have reached a plateau level of growing and then the sequencing chemotherapy-surgery can provide a better outcome.

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A p -order homogeneous like-distance in convex programming

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Abstract: We consider a p -order homogeneous like-distance with $p \geq 1$ associated with ϕ -divergences in the context of proximal point methods. By using Fenchel duality theory, this approach leads in the primal space to a multiplier method involving rational powers in the multipliers. Dual and primal convergence results are shown, in particular, all limit points of the sequences generated by the proximal point method and by the multiplier method are optimal solutions of problems dual and primal respectively.

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On the study of fuzzy preconditioners for Maxwell equations

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Abstract: This work deals with the theoretical study of electromagnetic scattering phenomena by the boundary integral equation methods in combination with other numerical schemes. Specifically deals with the mathematical study of a fuzzy Calderon multiplicative preconditioner for the dielectric Maxwell equations based on a preconditioning technique introduced by Snorre H. Christiansen for the EFIE case. We introduce a new robust preconditioner which is invertible at resonant frequencies and working in a wide range of frequencies. Moreover we prove that the associated operators satisfy a uniform discrete Inf-Sup conditions in the chosen discrete spaces

Global Convergence for a derivative-free trust region method with models based in polynomial interpolation

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Abstract: We present a derivative-free trust region method for solving unconstrained optimization problems. In each iteration we minimize a quadratic model function in a region around the current point, where the model is trustworthy. We utilize polynomial interpolation to build the model.

The main result is to establish a theoretical foundation for using interpolant models as approximations of the true objective function in a derivative-free optimization algorithm. To ensure global convergence of an optimization algorithm that uses a model of the objective function it is typically necessary to guarantee a certain quality of this model. In the case of polynomial interpolation, unlike the Taylor expansion, the error bounds depend not only on the center of the expansion and on the function that is being approximated but also on the set of interpolation points. In order to maintain the quality of the interpolation model it is necessary to understand and maintain the quality of the interpolation set.

We will examine some constants that characterize the quality of an interpolation set, and under certain conditions establish the error bound between a polynomial interpolant and the true function. Thus, we show that polynomial interpolation models are good approximations for the function to be optimized. Then we can conclude the global convergence to the algorithm and present some computational results.

On the complexity of steepest descent algorithms for minimizing quadratic functions

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Abstract: In this talk we intend to discuss the following question: How fast can a steepest descent algorithm be for minimizing a quadratic function? We do not tackle the general case of convex differentiable functions, which is more difficult, but we intend to obtain guidelines on how algorithms should be analysed. The difference between steepest descent methods lies exclusively on the choice of step length at each iteration.

We examine patterns in the distribution of step lengths in steepest descent algorithms for minimizing a convex quadratic function. We show how a large number of short steps are needed, and how these relate to the much smaller number of large steps. We note that the order in which the step lengths is used is irrelevant, and show a worst case example with a small number of variables. We also conceive a brute force algorithm which is in a certain way optimal, and compare it with known algorithms (i.e., with other choices of step lengths).

Numerical results of viscoelastic flows in a cross-slot geometry by using a dumbbell model

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Abstract: Our research team have studied a wide range of problems involving viscoelastic free surface flows. The technique employed is well known by many researchers from this area, which is a finite difference method on a staggered grid and the fluid is modelled by a Marker-and-Cell approach ([2]). This methodology have been capable of simulating many problems involving unsteady and steady viscoelastic free surface flows, such as, jet buckling, dieswell, impacting drop and fountain flow (see, as example,[3, 6]).

In this work, we are specially concerned with confined flows of viscoelastic fluids in a planar cross-slot geometry. This problem is very important to investigate purely elastic instabilities of viscoelastic flows because Newtonian fluids at the same condition remain perfectly steady. Several researchers have been studying this problem (or similar) in 2D and 3D dimensions ([1, 4, 5]). Poole, Alves and Oliveira [4] successfully used a numerical technique with a simple viscoelastic constitutive equation (UCM) to model this steady asymmetry under creeping-flow conditions ($Re = 0$). Recently, Rocha, Poole, Alves and Oliveira [5] extended previous studies in infinitely extensionable models (UCM and Oldroyd-B fluids) to finite extendable non-linear elastic models (FENE-P and FENE-CR models). They provided quantitative data of benchmark quality for flows in two geometries, a planar cross-slot geometry and rounded-corner geometry, by exploring the effects of finite extensibility (L^2), Weissenberg number (Wi) and concentration of polymer solution (β).

In the present work, we claim to get a good agreement between our results with Rocha et al. [5] ones. Moreover, predictions for fully developed flow of FENE-CR fluid with Newtonian solvent into a channel is also presented in this work. We compare the exact solution with numerical results to validate our methodology for FENE-CR fluids.

To develop our numerical methodology, we consider incompressible, isothermal and laminar flows described by the mass conservation equation, the equation of motion and constitutive FENE-CR equation in the conservation and dimensionless form as follow,

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \frac{\beta}{Re} \nabla^2 \mathbf{u} + \nabla \cdot \mathbf{T}, \quad (3)$$

$$\frac{\partial \mathbf{A}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{A}) - [\mathbf{A} \cdot \nabla \mathbf{u} + (\nabla \mathbf{u})^T \cdot \mathbf{A}] = -\frac{1}{Wi} f(tr(\mathbf{A})) [\mathbf{A} - \mathbf{I}], \quad (4)$$

$$\mathbf{T} = \frac{(1 - \beta)}{Re Wi} f(tr(\mathbf{A})) [\mathbf{A} - \mathbf{I}], \quad (5)$$

where t is the time, $\mathbf{u}$ is the velocity vector, p is the pressure, $\mathbf{T}$ represents the viscoelastic contribution tensor linked to configuration tensor $\mathbf{A}$ for FENE-CR model. The relevant numbers Re and Wi are the Reynolds and the Weissenberg numbers, respectively. The amount of Newtonian solvent is controlled by the constant non-dimensional β .

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Conservation laws for evolution equations

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Abstract: In [6] Nail Ibragimov proved a new result connecting symmetries and conservation laws. The so-called Ibragimov's theorem on conservation laws provides a nonlocal conservation law for any differential equation admitting Lie symmetries. In [7] Ibragimov introduced the concept of nonlinearly self-adjoint differential equations, generalizing the concept of self-adjoint equations [6] and weak self-adjoint equations [5]. These concepts allow one to construct local conservation laws for such equations using the conservation theorem established in [6]. In [1, 2, 3, 4] classes of evolution equations of first, third, fourth and fifth order are considered from the point of view of the new developments introduced in [6, 7]. In this work we find the nonlinearly self-adjoint subclasses of evolution equations up to fifth-order and we show how to construct local conservation laws for these equations.

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PERFORMANCE STUDY OF ITERATIVE METHODS FOR SEISMIC TOMOGRAPHY

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Abstract:

We study the relative performance of some iterative methods for linear systems in the solution of discrete ill-posed problems arising from seismic tomography. We consider the standard conjugate gradient (CG) method and some of their variants, namely the conjugate gradient method for the normal equations (CGNR, [6]), the conjugate gradient methods suggested by Polak and Ribière (CGPR) and by Fletcher and Reeves (CGFR) [4]. The forward modeling was performed by acoustic ray tracing [1] which provides the distances (tomography matrix G) travelled by each ray in each element of the 2-D medium. The traveltimes are computed by multiplying the matrix G by the vector of true slowness s (the reciprocal of true velocities and then each component is randomly perturbed). The inversion input in the matrix G and the vector of traveltimes t , and for the inverse procedure we use the CG algorithms above listed. Furthermore, each inverse problem originates the travel time, the coefficients of the model and the vagarosity of the matter [5]. We consider the model proposed by [5] which is described as a non symmetric anticlinal with tectonic origin. Such situation has great relevance in oil exploration, since it has structural traps with folds that could accumulate hydrocarbons. The reservoir is represented by a porous sandstone (1,500 m/s) and the sealing by a impermeable shale (2,500 m/s). The model was discretized in 800 blocks, where each block is a $10\ m \times 10\ m$ square. For the simulations we considered 30 sources in one borehole and 30 receivers in the other, in such a way that we have 900 rays or 900 equations. We employ the classical Tikhonov regularization of the resulting perturbed linear system, computing the regularization parameter λ with the aid of the package Regularization Tools [3]. For a tolerance of 10^{-10} for the residual norm and the regularization parameter just mentioned, the inversion algorithm produced a reconstructed model that correctly approximates the true one. Afterwards, we kept fixed these parameters and compared the number of iterations for convergence of each method. For the current model, the curves of the residual norm versus number of iterations for the iterative methods were similar to each other. Ongoing work comprises a collection of models for which we can estimate a performance profile [2] for each variant of the CG method.

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Methodologies and Applications of Level-Set Methods with Radial Basis Functions

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Abstract: The Level-Set Method is a well-established tool for tracking time-dependent moving-boundaries. Its applications are mainly found on image and video segmentation, data classification and tracking of free boundaries in fluid flow simulation. The present work considers formulations of level-set method based on a mesh-free approach – Radial Basis Function (RBF) Interpolants – as well as their applications and computational aspects. Primarily, it focuses on approaches for image segmentation and for tracking of free boundaries, where important properties and results are shown. Possible future directions to Level-Set Method with Radial Basis Functions are also exposed.

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A study on the Halley's method using L-BFGS method.

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Abstract: We consider the system of type $F(x) = 0$, where $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is an application twice differentiable. Many optimization problems can be solved by finding solutions of a system (usually nonlinear) of equations. The methods utilized to solve numerically those systems are iterative in nature. From an initial guess they generate a sequence of iterates that converges to a solution of the system. Among these algorithms Newton's method is broadly utilized, and under certain assumptions, it has quadratic convergence. Nevertheless, the evaluation of the inverse of the Jacobian turns Newton's method fairly expensive computationally. In order to circumvent this problem, quasi Newton methods are widely used in practice, but for large problems the approximation for the Hessian holds a large memory space. Quasi Newton methods with limited memory have also been studied, in particular L-BFGS method, where the Hessian matrix is approximated without performing a matrix multiplication. Furthermore, we mention tensor methods, in particular Halley's method. This method belongs to a class of algorithms with cubic convergence, which by considering its degree of accuracy is better than Newton's method. We propose in this paper a study on the Halley's method using L-BFGS method.

A new iterative method for computing the pseudo inverse, using the Penrose equations

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Abstract: Given an arbitrary matrix A , we define the pseudo inverse of A , the unique matrix X satisfying the Penrose equations

$$AXA = A; \tag{6}$$

$$XAX = X; \tag{7}$$

$$(AX)^* = AX; \tag{8}$$

$$(XA)^* = XA. \tag{9}$$

we denote the pseudo inverse of A by $A^\dagger$.

There are several iterative methods for approximating the pseudo inverse $A^\dagger$ of a matrix A based on the Penrose equations, for example, the famous Newtons method, proposed et al. [3], and generalized et al. [1], defined by

$$X_0 = \alpha A^*, \quad X_{k+1} = X_k(2I - AX_k) \quad (10)$$

Another recent iterative method based on the Penrose equations was proposed by Petković et al. [2], and is given by

$$X_0 = \beta A^*, \quad X_{k+1} = (1 + \beta)X_k - \beta X_k A X_k \quad (11)$$

In this work, we proposed another iterative method, in this case based on the four Penrose equations. Using the equations (6)-(9) we have

$$\begin{aligned} X &= XAX = XAXAX = X(AX)^2 = X[(AX)^2]^* \\ &= XX^*A^*X^*A^* = XX^*(XA)^*A^* = XX^*XAA^* \end{aligned}$$

thus $X = XX^*XAA^*$. Now, consider $\beta \in \mathbb{R}$ then

$$X = X - \beta(XX^*XAA^* - X) = X - \beta XX^*XAA^* + \beta X = X[(1 + \beta)I - \beta X^*XAA^*]$$

and this suggests the iteration $X_{k+1} = X_k[(1 + \beta)I - \beta X_k^*X_kAA^*]$.

Let A be a matrix in $C^{m \times n}$, and take β a positive number, we define the follow iterative method

$$X_0 = \beta A^*, \quad X_{k+1} = X_k[(1 + \beta)I - \beta X_k^*X_kAA^*] \quad (12)$$

The follow theorems about the above method is showed

Theorem 1 If $0 < \beta < \min\{\frac{2}{\rho(A^*A)}, \frac{1}{3}\}$, then the iterative method (12) converges to pseudo inverse of matrix A .

Theorem 2 The error matrix $E_k = X_k - A^\dagger$ satisfy the follow recurrence relation

$$E_{k+1} = (1 - 2\beta)E_k - 3\beta E_k A E_k - \beta E_k A E_k A E_k. \quad (13)$$

Wich proves that the iterative method converges, and it has a error with first-order, second-order and third-order terms. The follow lemma show important informations, necessary to establish a convergence criterion.

Lemma 1 Consider $t_k = \|E_k A\|_2$, $e_k = \|E_k\|_2$ and $r_k = \|E_{k+1} - E_k\|$, then we have

$$\lim_{k \rightarrow \infty} \frac{t_{k+1}}{t_k} = \lim_{k \rightarrow \infty} \frac{e_{k+1}}{e_k} = \lim_{k \rightarrow \infty} \frac{r_{k+1}}{r_k} = 1 - 2\beta$$

Then, if we consider a tolerance tol , using that $r_k = E_{k+1} - E_k = X_{k+1} - X_k$, we can use as a convergence criterion $|r_k - (1 - 2\beta)r_{k-1}| < r_{k-1}tol$.

We provided some numerical examples, and comparisons with the method (11) that belongs the same class of methods.

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Filter Algorithms Globally Convergent: theory, implementation and application

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Abstract: We discuss in this work methods used to solve nonlinear programming problems in which one wishes to minimize a function into a particular region of the multidimensional space. To solve these problems we can use iterative algorithms that generate a sequence of points, which we hope to converge to a stationary point. A way to induce the convergence is to make use of the filter criterion to verify if a trial point should be accepted as the next iterate. To be accepted by the filter, the point should provide a decrease in the objective function or in the infeasibility measure considered, when compared to the current point. The point can be tested by two kinds of filter criteria, original or slanting, that are defined according to the rule that measures the reduction in the objective function value. In this work we present a general filter algorithm, globally convergent, which does not depend neither on the particular method used to calculate the step nor on the filter criterion adopted. The convergence is guaranteed under the assumption that the step satisfies an efficiency condition which establishes that near a feasible non-stationary point the decrease in the objective function is relatively large. We showed that such condition is satisfied for at least two methods used in the calculation of the step, one of them is based on Sequential Quadratic Programming (SQP) and the other is based on Inexact Restoration (IR), for both filter criteria. For the former method, we presented a general proof that the efficiency condition of the step is satisfied, being valid both for the original and for the slanting filter criterion. The general filter algorithm, as well as the internal algorithms used to determine the step were implemented in MATLAB and numerical experiments were performed with problems from the CUTer collection. These tests have not presented significant numerical differences between the filter criteria, however, the SQP algorithm was more robust than IR and also more efficient when it comes to the number of functions and gradients evaluations. Furthermore, we also analyze the applicability of the studied algorithms to practical problems. For this purpose, we consider an optimization problem that arises in structural reliability analysis when it is desired to determine the failure probability of a structure. Numerical tests were performed with some particular problems of the structural reliability and the results indicated that our general filter algorithm can be used in this context.

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Quasi Projection Analysis of Galerkin Method For a Nonlinear Parabolic Equation

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Abstract:

consider the following nonlinear parabolic problem :

$$\frac{\partial u}{\partial t} - \operatorname{div} A(u, \nabla u) + f(u, \nabla u) = 0, \quad (x, t) \in \Omega \times J \quad (14)$$

with initial and homogenous Dirichlet boundary conditions

$$u(x, 0) = u_0(x), \quad x \in \Omega; \quad (15)$$

$$u(x, t) = 0, \quad x \in \partial\Omega, \quad t \in J, \quad (16)$$

where Ω is a bounded domain in R^n with boundary $\partial\Omega$ and $J = (0, t]$. The function A and f are respectively, vector and scalar valued defined $\Omega \times R$. For our use assume the following condition:

- (i) The problem (1.1)-(1.3) has a unique solution with bounded gradients $|\nabla u|, |\nabla u_t|$.
- (ii) The function A and f are sufficiently smooth and bounded.
- (iii) The matrix $\frac{\partial A}{\partial \xi} = [\frac{\partial A_i}{\partial \xi_j}]$, where $\xi = (\xi_1, \xi_2, \dots, \xi_n)$ and $\xi_j = \frac{\partial u}{\partial x_j}$ is uniformly positive definite.

Earlier, already demonstrated the superconvergence phenomena associated with a linear parabolic equation using quasi-projection technique. Later generalized these results to a quasilinear parabolic equation of the form $c(x, t, u)u_t - \operatorname{div}[a(x, t, u)\nabla u + b(x, t, u)] + f(x, u, t) = 0$.

In this present work knot superconvergence of semidiscrete Galerkin approximation is established to the solution of (1.1) – (1.3) in a single space variable. The convergence at the knot points are shown to be order $h^{2r-1/2}$. In addition, an optimal L^∞ estimate is also derived

Interior-Point Method for Hydrothermal Dispatch Problem

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Abstract: This paper presents a model for the optimization of the hydrothermal dispatch [1] which is modeled as a nonlinear, nonconvex problem involving both equality and inequality constraints and bounded variables. The model's goal is the minimization of the costs of electricity generation, which can be summarized as the costs of thermal generation and the costs incurred by energy deficits. The methodology proposed to solve this problem is the Interior-Point method [2] which is widely used in several classes of problems, combined with ideas of the well-known Gauss-Newton method [2] in nonlinear programming. The combination of the aforementioned techniques together with the Interior-Point method presents good computational performance and satisfactory results when applied to the hydrothermal dispatch problem for a test system based on the Brazilian Interconnected System.

Key words: Hydrothermal dispatch, nonlinear programming, Interior-Point method.

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Global Convergence of a Derivative Free Method for Unconstrained Optimization

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Abstract:

Many industrial and engineering applications need to solve optimization problems in which the derivatives of the objective function are not available. Nevertheless, they try to avoid unnecessary evaluations in the objective function. The absence of computable derivatives prohibit the use of Taylor models largely used in optimization with derivatives. In general, this kind of problem without derivatives is not easy, since we attempt to obtain a minimum point with less information. The optimization without derivatives is well described in the work of Conn, Scheinberg, and Vicente [2].

The purpose of this paper is to analyze the problem of minimization without derivatives based on the method proposed by Powell in [3]. This proposal studies a method of unconstrained minimization that does not use the derivatives of the objective function and it also prevents excessive evaluations of this function. More formally, it solves the problem

$$\begin{array}{ll} \text{minimize} & F(x) \\ \text{subject to} & x \in \mathbb{R}^n, \end{array}$$

where the objective function $F : \mathbb{R}^n \rightarrow \mathbb{R}$ is twice differentiable (the differentiability of F is required for theoretical purposes).

The method proposed by Powell in [3] is based on the trust region method [1]. In general, such methods use a approximation of the objective function to obtain a sufficient reduction of F within a closed set. Generally, this approximation is a quadratic polynomial and it is obtained by using a Taylor approximation with derivatives. As the approach discussed in this paper does not use derivatives, the approximations are constructed using a quadratic polynomial interpolation. Each iteration of the method considers a affine linear set with $(n + 1)$ points. For one iteration to another at most one point of the interpolating set is changed. Moreover, only one objective function value is computed by iteration.

The method has three types of iterations: *alpha alternative*, *beta alternative* and *trust region*. The alpha and beta alternative iterations aim to improve the distribution of interpolation points, so that they remain affine linearly. The iterations of trust region aim to minimize the quadratic model within a certain region in the hope that most of this reduction may be inherited by the objective function. These iterations of trust region are based on quadratic polynomial interpolation with complete freedom in determining the Hessian of the model, provided that they are symmetrical and bounded.

The purposes of our work are to explain a method in an algorithmic way that meets the requirements of the method proposed by Powell in [3] and to prove its the global convergence. Various properties of the algorithm and the interpolation sets were obtained. Then, we proved that all the points of accumulation of any sequence generated by the algorithm are stationary.

Key words: trust region methods, convergence theory, derivative free optimization, unconstrained minimization.

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Estimation of Monetary Policy Preferences: a Genetic Algorithm Approach

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Abstract: Since June 1999, Brazil has adopted the inflation targeting regime as its monetary policy guideline. In this regime, the central bank announces to the public a mid-term target for inflation and undertakes to act so that the actual inflation moves towards that goal. The main instrument for achieving this is the SELIC interest rate, adjusted at regular meetings of the Monetary Policy Committee (Copom) [1].

While monetary policy arises from a complex procedure involving a large amount of subjective evaluations, it is possible to model the decision making process as an optimal control problem. This is done by assuming that the Central Bank's goal is to minimize the expected value of the following quadratic loss function:

$$V = \sum_{t=0}^{\infty} \delta^t (\lambda_{\pi} \pi_t^2 + \lambda_h h_t^2 + \lambda_i (i_t - i_{t-1})^2), \quad (17)$$

restricted by a linear model that represents the connections between the main macroeconomic variables:

$$\pi_{t+1} = \alpha(L)\pi_t + \beta(L)\pi_t^e + \gamma(L)h_t + \delta(L)\Delta c_t + \varepsilon_{\pi,t+1}, \quad (18)$$

$$h_{t+1} = \eta(L)h_t + \theta(L)(i_t - \pi_t^e) + \kappa(L)c_t + \varepsilon_{h,t+1}, \quad (19)$$

$$\pi_{t+1}^e = \lambda(L)\pi_t^e + \nu(L)\pi_t + \xi(L)\Delta c_t + \tau(L)\Delta i_t + \varepsilon_{\pi^e,t+1}, \quad (20)$$

$$c_{t+1} = \rho(L)c_t + \mu(L)\pi_t + \phi(L)\pi_t^e + \psi(L)\Delta i_t + \varepsilon_{c,t+1}, \quad (21)$$

where: $\alpha(L), \beta(L), \text{etc.}$, are polynomials in the lag operator L defined by $Lx_t = x_{t-1}$; π_t is the natural logarithm of the inflation rate (IPCA) accumulated in twelve months in period t : $\ln(1 + IPCA_t/100)$; π_t^e corresponds to the natural logarithm of the expected inflation rate for the next 12 months in period t : $\ln(1 + IPCA_t^e/100)$; h_t is the natural logarithm of the output gap (difference between the conducted GDP and potential GDP) in period t : $\ln(1 + Gap_t)$; c_t is the natural logarithm of real effective exchange rate in period t : $\ln(Exchange_t)$, where $\Delta c_t = c_t - c_{t-1}$; i_t is the logarithm of the Selic rate set by Copom in force at end of period t : $\ln(1 + SELIC_t/100)$, with $\Delta i_t = i_t - i_{t-1}$; and ε_t represents the random shocks occurring in period t .

Considering this approach, the monetary policy is posed as a linear-quadratic regulator problem (LQR), where the Central Bank preferences can be associated with the weights that define the loss function, that is $\delta, \lambda_{\pi}, \lambda_h$ e λ_i . According to Dennis [2], knowledge of these preferences, besides contributing to the understanding of monetary policy actions, allows for a comparison of the goals of Central Bank in different intervals of time. So, in this framework, there are extensive literatures devoted to estimating this monetary policy preferences. However, most of these studies have focused on the preferences of the Federal Reserve and Central Banks from European countries (e.g. [2, 3]).

With regard to the monetary policy in Brazil, only Aragn and Portugal [4] have presented estimates for the preferences of the Central Bank of Brazil. These authors applied a grid-search method to calibrate the loss function of the central bank, choosing the weights such that the solution of the corresponding optimal control problem resulted in the best fit between the real monetary policy and the simulated optimal monetary policy.

Motivated by the scarcity of studies of this kind on Brazilian monetary policy, the present work aims at estimating the preferences of the Central Bank of Brazil. For this, the calibration strategy is also used. However, instead of applying the usual grid-search method, a genetic algorithm with real coding is proposed to estimate the preferences.

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Optimal Design of an Ammonia Synthesis Reactor*

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Abstract: Ammonia is one of the most important chemicals produced in the world and it is used in the manufacture of fertilizers, explosives, pharmaceuticals, fibers, plastics, paper, etc. Due to its broad applicability, modeling and simulation of process have received considerable attention among the process industries. Ammonia is produced from the reaction of hydrogen and nitrogen at high temperature and high pressures along with catalyst. Its production depends on temperature of feed gas at the top of the reactor (top temperature), the partial pressures of the reactants and the reactor length. The optimal design problem requires obtaining the optimal reactor length with maximum economic returns subject to a number of equality constraints involving solution of coupled differential equations. In this work new results are obtained for the reactor length and optimal cost.

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An Approach to the Problem of Covering Solids by Spheres of Different Diameters

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Abstract: Given a solid and a set of spheres available to take part in its covering, we seek good positionings of the center of these spheres in order to meet the following objective: maximize the covered volume while minimizing the number of spheres used in the covering and also minimizing the overlap between the spheres. Solving this problem is not so easy as describing it. Such a problem is classified as NP-hard and is commonly formulated as a non-convex mixed-integer non-linear problem (non-convex MINLP). We then propose a mathematical programming formulation for the problem of covering a solid by a finite number of spheres of different size.

A Modified Nonlinear Spectral Galerkin Method for the Equations of Motion Arising in the Kelvin-Voigt Fluids

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Abstract: In this work, a variant of nonlinear Galerkin method is proposed and analysed for equations of motions arising in a Kelvin-Voigt model of viscoelastic fluids. Some new a priori bounds are obtained for the exact solution when the forcing function is independent of time or belongs to L^1 in time. As a consequence, existence of a global attractor is shown. For the spectral Galerkin scheme, existence of a unique discrete solution to the semidiscrete scheme is proved and again existence of a discrete global attractor is established. Further, optimal error estimate in $L^1(L^2)$ and $L^1(H_0^1)$ -norms are proved. Finally, a modified nonlinear Galerkin method is developed and optimal error bounds are derived.

A description in the phase, time, and parameter spaces about periodic orbits with high stability

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Abstract: It is known that dynamic systems develop stable periodic behavior. This stability can be characterized by the time the system takes to converge to its asymptotic regime. In some cases, the flow around the stable periodic orbit converge very fast to the orbit when compared with other stable periodic orbits with equivalent topology. We call such orbits as high stable periodic orbits. Under perturbation, the dynamic converge quickly to this attractor, playing an important role in systems where the regular stability is required. We present a study in the 2D-parameter space where two continuous sets, with this behavior of high stability, intersect at a point transforming drastically the surrounding parameter space, i.e., a large domain of periodicity behavior is created around the intersection point. We show scaling laws that organize this phenomenon in the phase, time, and parameter spaces.

Expansion Planning Problem of an Electrical Network with Reliability

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Abstract: The problem of expansion of the electric distribution system is a complex one and is more difficult if the reliability is integrated in the decision of planning of the future network. This work considers the expansion planning problem of an electrical network of a primary system distribution, it considers radial networks and all the energy are supplied by substations. The objective is to describe the problem, present the mathematical formulation and a methodology that permits to integrate reliability criteria in the model based on Bhowmik. The problem consist in determine the capacity, the number and the location of the substations, also the topology in terms of connections of the feeders such that the installation and losses cost are minimized. The electric restrictions such that the first and second Kirchhoff's law are attained. The problem is formulated as a model of multi-objective mixed integer programming (MIP), which belongs to a class of NP complete. The model applies to a primary network of a existing distribution and operating in good condition which is known forecasts of load increase of demand for different periods of the planning horizon. Assumes prior knowledge of the branches that can be added to the network with the options of gauges and the definition of what nodes are capable of installing the distribution substation. The proposal to use an exact method to solve such a model has been successful when applied to small networks, but proved to be restrictive in the application in real networks due to their size and characteristics of non-linear inherent power network. To overcome this difficulty, it was used a two stage methodology to find solutions good enough for the problem under discussion. The resolution of the model using this methodology adapted to consider reliability in the problem of expansion and associated with the technique presented in the study allowed the creation of multi-stage planning for the expansion of the real networks.

An Implicit Technique for Solving Low Reynolds Number Moving Free Surface Flows: The XPP model.

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Abstract: In this presentation we shall describe the development of an implicit finite difference method for solving transient three-dimensional incompressible free surface flows, modeled by the XPP model. To reduce the CPU time of explicit low-Reynolds number calculations, we have combined a projection method with an implicit technique for treating the pressure on the free surface. The projection method is employed to uncouple the velocity and the pressure fields, allowing each variable to be solved separately. We employ the normal stress condition on the free surface to derive an implicit technique for calculating the pressure at the free surface. Numerical results demonstrate that this modification is essential for the construction of methods that are more stable than those provided by discretizing the free surface explicitly. In addition, we show that the proposed method can be applied to viscoelastic fluids. Numerical results include the simulation of jet buckling and extrudate swell for Reynolds numbers in the range $[0.01, 0.5]$.

A Numerical Study of the Log Conformation Representation

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Abstract: This work aims to study in detail, by means of a simple equation, the statement that the numerical instability associated with a high Weissenberg number in equations with source term can be solved by a change of variable, called Logarithmic Conformation Representation. It is considered the linear advection equation with appropriated source term. Besides the convective balance required by the CFL condition, one must take into account an elastic balance imposed by the source term. That has been reported as cause of the High Weissenberg Number Problem (HWNP). Still, for better understanding, we introduce another change of variable, called Root Conformation Representation. So, some important aspects of numerical treatment are explored, as well as comparisons with the exact solution of the simple problem considered, in analogy to what happens in the simulation of visco-elastic fluid flows, in which the higher We , the more intense are the elastic interactions imposed by the source term.

Considering the FOU discretization of the convective term and the explicit Euler transient term, we saw that by including a source term in the linear advection equation it is also inserted a restriction of stability on the spatial mesh, and that such restriction is influenced by the Weissenberg number. Thus, the higher We , the much more restrictive should be the space step. This characterizes the HWNP, but can be improved when logarithmic representation is used. Numerical simulations performed provides a good understanding of the scene that occurs in HWNP, leaving the concern that the solution of complex problems can have results "far" from the true solution, ie, the mesh size used nowadays should perhaps be much more refined than what happens in practice.

CFD Simulation of Conservation Equations Using the Topus Scheme

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Abstract: This work reports experiments on the use of an advection bounded upwinding scheme, namely TOPUS, for flows of practical interest. The numerical results are compared with analytical, numerical and experimental data and show good agreement with them. The TOPUS scheme showed to be a powerful and generic scheme for complex flow phenomena.

Adaptive Numerical Simulation of a Non-Evaporating Spray in a Turbulent Jet

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Abstract: This work presents a numerical methodology to simulate a three-dimensional turbulent non-evaporating spray jet. The carrier phase is considered in an Eulerian framework, while the dispersed phase is tracked in a Lagrangian framework. The interactions between the two phases are considered to be a two-way coupling. The numerical method combines an adaptive mesh refinement technique, an implicit-explicit time stepping strategy, a linear multilevel-multigrid for carrier phase and the Modified Euler method for dispersed phase. Mathematically, the carrier phase is modelled by the non-steady Navier-Stokes equations for a three-dimensional incompressible flow whose material properties vary. The turbulence is modelled using large eddy simulation. The dispersed phase is modelled by a ODE system (velocity and position) for each droplet. The Navier-Stokes solver is based on an increment pressure projection method. The dynamic adaptive mesh form a level hierarchy composed by a set of nested, cartesian grid patches (block-structured grid). Refinement criteria are sharp gradients, regions of vorticity shedding, droplet positions, and localized small length scale features of the flow. Information on how often the adaptive grid changes, on the number of computational cells in use, on the stability properties, size of the integration time step, and diameter/velocity distribution of droplets is gathered and shows the capabilities and the potential of the numerical methodology in use.

An Adaptive Uzawa Method for the Steady Stokes Equations[†]

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Abstract: The present work is motivated by the study of incompressible flows at low Reynolds numbers. In the limit, as the Reynolds number approaches to zero, the dynamics of the system is modeled by the steady Stokes equations. An adaptive version of Uzawa Method is proposed to solve those equations with Dirichlet boundary conditions on locally refined grids. Adaptive mesh refinements increase locally the resolution of the method to improve accuracy at low computational cost. A finite difference approach is used for the discretization of the fluid velocity in a staggered fashion and Uzawa Method is employed to handle the pressure-velocity coupling in primitive variables. To solve the resulting set of algebraic equations, the matrix representing the discretization on the adaptive grid is built and the related linear system solved by PETSc (Portable, Extensible Toolkit for Scientific Computation, www.mcs.anl.gov/petsc) library. Several methods are tested for their performance, including the biconjugate gradient and GMRES methods, with suitable preconditioners. The parallel capabilities are investigated.

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