Contributed Session 7: Scientific Computation and Numerical Algorithms

Singular Bifurcations of Differential-Algebraic Equations

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Consider the differential-algebraic equation

$$\dot{x} = f(x,y), \;\; g(x,y) = 0, \tag{1}$$

where the constraint manifold $C := g^{-1}(0)$ is a smooth manifold and the singularity $S := \{(x,y) \in C : \det(g_y(x,y)) = 0\}$ is non-empty. The challenge is to obtain existence, uniqueness, multiplicity, regularity, invariant manifold and bifurcation results for (1) in a neighbourhood of points in S. Applications of DAEs in control theory and constrained mechanics are well-known, but there are many application areas where singularities are important but poorly understood, for instance, when posing similarity solutions in quasilinear PDEs such as degenerated diffusion equations or in parabolic PDE systems of diffusing and non-diffusing species.

We show how one can utilise Kronecker normal forms from the theory of matrix pencils to construct a Lyapunov-Schmidt reduction that reduces (1) near $(x,y) = (0,0)$ to an n-dimensional quasilinear normal form

$$\dot{u} = \mu + Au + O(2), \;\; s(u,v)\dot{v} = v + O(2), \tag{2}$$

where μ is a projection of $f(0,0), u \in \mathbb{R}^{n-1}, v \in \mathbb{R}$ and $s : \mathbb{R}^n \to \mathbb{R}$ satisfies $s^{-1}(0) = S$. We discuss the use of this and similar results to obtain bifurcations in both (1) and its discretisations.

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On the computation of magnetostatic systems and beyond, with applications to controlled fusion geometry

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The equations of magnetostatics describe interactions between a plasma in equilibrium between it pressure and a magnetic field. They are widely used in many large scale plasma physical simulations, like in thermonuclear fusion and in astrophysics. with a set of boundary conditions. Solving these boundary value problems still represents a formidable task.
In this communication we propose an iterative algorithm coupled with a discretization method for solving these equilibrium equations in three-dimensional domains. We will then present some results relevant to the application of those methods to the physics of controlled fusion plasma and compute some toroidal equilibrium configurations in the case of tokamak geometry . We then present some current extension of our spatial discretization to the magnetohydrodynamic equations, to achieve : conservation and divergence free constraint for the magnetic field as well as,positivity and small dissipation.

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Analysis of a dynamic Signorini's contact problem

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The purpose of this talk is to study the dynamic frictionless contact problem between an elastic body and a rigid foundation and to propose a numerical algorithm to solve it. In order to model the contact we consider Signorini conditions.
We present an existence result, whose proof is based on five fundamental steps: a discretization in time, using Newmark's method, which leads to a discretized problem with unique solution; the construction of functions approximating a solution of the problem; the treatment of the contact condition by means of a Lagrange multiplier whose orthogonality properties allow us to get a priori estimates; the convergence of said functions and, finally, the pass to the limit obtaining a weak solution of the continuous problem.
Then a numerical algorithm is proposed to approximate the solution of the contact problem. Such algorithm involves a contact multiplier, which is a fixed point of a nonlinear equation solved by using a generalized Newton method. The convergence of the method is studied numerically, and an academic test is used to validate the methodology.

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Mixing Properties of a non-Newtonian Fluid

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In this study, a detailed numerical analysis for the study dispersive mixing generated by the flow patterns of a non-Newtonian fluid in a square cavity was investigated. The Finite Difference Method has been applied to solve the non-linear governing vorticity coupled with the energy and concentration equations. Unsteady, laminar, and two dimensional flow of a non-Newtonian fluid was governed by the buoyancy parameters Grashof, Prandtl, Reynolds and Schmidt numbers. Mixing properties were investigated by simulating the dispersive mixing of a "coloured" fluid injected into the cavity while at rest. Therefore, the contributions of the flow structure, concentration distribution of the fluid behaviour were investigated. The calculations for temperature and concentration equations were carried out with different values of the Groshof and Schmidt numbers but obtained results were documented only for the concentration and streamlines structure. Further, Richardson extrapolation was used to obtain high-order accurate approximations.

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Use of a Computer Program in the solidification of a molten steel

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A computer program is developed to solve a moving boundary value problem arising in the solidification of molten steel. The numerical method is based on a front-tracking method using variable time step. Due to the presence of a moving boundary, the numerical solution of these problems is quite laborious. Analytical solutions, although very convenient, can only be applied to very specific cases. In situations where the thermal -physical properties depend on system variables or where the initial temperature distribution is not of a uniform type the analytical solutions are impossible. The computer approach offers a high degree of convenience, as it produces intermediate results while the calculations are being performed. The outcome of the solidification process is observed and the position of the moving boundary is given at each time step

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The application numerical methods for description phenomena in high current ontacts

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In the paper the mathematical model of high current contacts is presented. The model is described by partial differential equations. To solve these equations the diferent numerical methods are used. The transient and steady state is calculated. It give posiibility to simulate different time-space electromagnetic field distribution on the contacts surface. Such approach can be used to investigate proper contact's shapes in order to obtain demanded field distribution, what it is important in designing of contacts structure.

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Error estimation of a class of quadratic immersed finite element methods for elliptic interface problems

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In this paper, we carry out error estimation of a class of immersed finite element (IFE) methods for elliptic interface problems with both perfect and imperfect interface jump conditions. A key feature of these methods is that their partitions can be independent of the location of the interface. These quadratic IFE spaces reduce to the standard quadratic finite element space when the interface is not in the interior of any element. More importantly, we demonstrate that these IFE spaces have the optimal (slightly lower order in one case) approximation capability expected from a finite element space using quadratic polynomials.

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Numerical solution of a non-local elliptic problem modelling a thermistor with a finite element and a finite volume method

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In this work we consider the non-local elliptic problem :

$$w'' + \lambda \frac{f(w)}{\left(\int_{-1}^{1} f(w)dx\right)^2} = 0, \quad -1 < x < 1, \qquad (1)$$

$$\mathcal{B}_{\pm}(w) = w'(x) \pm aw(x) = 0, \quad x = \pm 1,$$

where $w = w(x) = w(x;\lambda)$, $\lambda > 0$ and f is a function with the properties $f(s) > 0$, $f'(s) < 0$, $f''(s) > 0$ for $s > 0$, $\int_0^\infty f(s)ds < \infty$. The solution of the equation represents the steady state of the thermistor device. The problem for a critical value of the parameter λ, λ^* has a unique solution, for $\lambda < \lambda^*$ at least two solutions and for $\lambda > \lambda^*$ has no solution. We apply a finite element and a finite volume method based on piecewise quadratic functions in order to find a numerical solution of the problem for the case that $\lambda < \lambda^*$ and for the stable branch of the bifurcation diagram. A comparison of these two methods is made regarding their order of convergence for $f = f(s) = e^{-s}$ and $f(s) = (1+s)^{-p}$ for $p = 2$, and for Robin boundary conditions. Also for the same problem but with Dirichlet boundary conditions, a situation where the solution is unique for $\lambda \leq \lambda^*$, an additional comparison is presented.

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Study of an axisymetric Problem in a complex geometry

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Many problems in physics and mechanics have been treated by axisymetric techniques in simple geometries. In this paper, we study problems in more complicated geometries. In most cases, these problems can also be treated by axisymetric techniques. These geometries can be: -A cylinder with small deformation on one side. -A domain wich is the union of reservoirs in 3-D of cylindrical pipes. In this case, we make use of finite element method for the reservoirs and spectral methods for the pipes. Here, we study the first geometry, and the idea is to find a conforming transformation between the domain and the real cylinder, then we use the asymptotic developpement for the solutions by taking in account the side that has been perturbed. We make use of analytical results from [1] and [2]. Numerical results are also presented for this case . Key-Words: Spectral Methods, Fluid Mechanics, Complex Geometries References:

[1] Jie Shen- Efficient Spectral-Galerkin Methods IV. Spherical Geometries, SIAM J.Sci. Comput. Vol. 20, No. 4, pp. 1438–1455, 1999.
[2] F.Z. Nouri & K. Amoura, Study of the axisymetric Laplace's Problem in a complex geometry, presented aux journees mathematiques Algeriennes Francaises (JMAF), Constantine (Novembre 2005).

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An Automated Method for the Analysis of a Multi-Parameter Family of Dynamical Systems

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We introduce an automated, computer-assisted method for the analysis of a multi-parameter family of discrete dynamical systems.

As an example application we analyze asymptotic dynamics of the nonlinear density-dependent Leslie population model, which yields a $2d$-paramter nonlinear system on $\mathbf{R}^d$. In particular, we use a computer program to construct a set of parameters for which the dynamical system exhibits multiple basins of attraction and, as a result, more than one asymptotic behavior of the population is possible.

We conduct rigorous numerical computations with the use of interval arithmetic and combinatorial methods based on cubical outer approximations of the map, and therefore we are able to actually prove some properties of the dynamical system, unlike it is usually done with numerical simulations.

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Nonlinear dynamics of systems confined to the Nosé - Hoover thermostat

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The subject of the talk is intimately related to the problem of computer modelling Gibbs' distribution using the Molecular Dynamics method. Due to the shortage of computer memory there is a need for constructing mechanical systems that could serve as the Gibbs thermostat. The Berendsen and the Nosé - Hoover thermostats are among the most employed. The Nosé - Hoover (N&H) model is also very interesting from the point of view of nonlinear physics, and it is worth noting that the ensemble of harmonic oscillators confined to the N&H thermostat is of primary importance for understanding the problem of equilibrium dynamics.

To study the dynamics of the ensemble both the analytical (averaging), and the computer (simulation and visualization) methods were employed, and it was found that the dynamics is specified by a characteristic frequency $\Omega_\alpha \sim \sqrt{\alpha}$, where α is the dissipative parameter of the thermostat. For sufficiently small α, Ω_α determines oscillations round the stationary solution corresponding to the quasi-thermodynamical equilibrium of the system. This regime is also characterized by the presence of parametric resonance. For values of Ω_α which lie inside or above the frequency band of the oscillators, the motion of the ensemble could become chaotic. The obtained results may be useful for the needs of molecular dynamics, especially for low temperature problems where the harmonic approximation is justifiable.

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