Numerical methods for differential equations and applications

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In the contemporary language of mathematics, a special place is occupied by Numerical Analysis, thanks to the steadily developing interest for the interplay among abstract formalism, computations and simulation of real world phenomena. This research contribution means to offer an example of such conceptual interplay. In particular, main research activity of Ivonne Sgura in 2012 deals with the development and analysis of innovative techniques for the numerical approximation of differential equations in the following applicative areas of interest.

I) ELECTROCHEMISTRY

Keywords: electroplating, pattern formation in metal growth, green chemistry, Turing patterns, finite differences, ADI methods
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Metal plating is a well-assessed and widespread technology, ubiquitous in surface treatment technologies, exhibiting a wide-range of applications including, among others: energetics (fuel cells and batteries), chemical and biochemical sensors, electronic fabrication, corrosion and wear protection, surface decoration, preservation of metallic components, ranging from heritage to nuclear and aerospace. Curiously, in most cases, industrial success of electroplating is achieved at the cost of using extremely toxic and polluting additives in the related electrochemical process. The idea of this group is that this is essentially due to the poor fundamental knowledge of the physico-chemical basis of electrochemical metal growth and, in particular, of its dynamics. The present group aims to provide sustainable answers in this direction by using mathematical models for the description and prediction of morphogenesis in electrodeposition. For this reason, we have introduced a reaction-diffusion PDE system, accounting for the coupling between morphology and surface concentration of one chemical species adsorbed at the surface of the growing metal.

Papers [1,2] published in 2012 review the main results obtained in the last few years on these topics, focusing on the mathematical theoretical features in [1] and on electrochemical modelling assumptions in [2]. (For more detailed information on our previous results see other references in these papers). The PDE system proposed exhibits a surprisingly rich dynamic scenario, featuring: (i) existence of transition front waves moving with specific wave speeds; (ii) Turing instability and initiation of spatial patterns driven by diffusion; (iii) smoothing effects related to a forcing sinusoidal term.

In all cases, a numerical discretization for the electrochemical PDE system is needed to gain quantitative information on the evolution of the solution until its steady state is attained. In the papers [3,4], we introduce a new numerical approach based on high order finite differences in space and the Alternating Directions Implicit (ADI) method as time integrator for the approximation of the Turing patterns. Paper [3] presents a stability analysis for the proposed method and its application to the above unforced case (ii). The model is validated by comparing simulations with experiments on Cu film growth by electrodeposition. In paper [4] we apply the same approach to the forced PDE system for the approximation of oscillating Turing patterns, also when high forcing frequencies are considered. Our results give the mathematical and experimental evidences that the application of a small sinusoidal forcing term is able to drive the morphology of the growing film towards the industrially desirable surface finish in the way currently achieved only by non-green additives. An essay of these results is given in paper [5], an invited article by the Products Finishing Magazine, the largest in the U.S. that covers finishing and coatings.

II) NONLINEAR ELASTICITY AND BIOMECHANICS

Keywords: soft tissues, deformations of rubber-like and fiber-reinforced materials, non-smooth differential equations, multipoint BVPs, high order finite differences
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Rubber-like solids and biological soft tissues can both be efficiently modelled within the framework of finite elasticity, which can account for large deformations, physical nonlinearities, incompressibility. One of the most salient differences between elastomers and soft tissues is that at rest, elastomers are essentially isotropic whilst soft tissues are essentially anisotropic, because of the presence of collagen fibre bundles. In that respect, it is worthwhile to consider the effect of incorporating families of fibres into an isotropic matrix. Fibres introduce striking differences between the two classes of materials and the mathematical model describing material deformation can be differential equations with *non-smooth solutions*. In this case, general purpose numerical methods fail and instability phenomena appear in the numerical approximations. For this reason, in paper [6] a suitable numerical method based on finite differences is introduced to solve with high numerical accuracy Boundary Value Problems (BVPs) for Ordinary Differential Equations (ODEs) with singular solutions. In particular, we solve a biomechanical model describing the rectilinear shear deformation of a material reinforced by two families of fibres, that has a singularity in an unknown internal point of the domain.

The present research is part of a long-term project in this field including:

- participation to PRIN 2009 Project "Mathematics and Mechanics of Biological Assemblies and Soft Tissues" (MMBAST, www.dis.uniroma3.it/mmbast/PRIN2009/home.HTML) sponsored by Italian Minister of University and Research (principal investigator G. Saccomandi), aimed at developing novel and reliable mathematical models in biomechanics.

- Visiting Professor Fellowship by GNCS-INdAM (resp. I. Sgura) to support prof. Michel Destrade (Univ. Galway, Ireland) to visit the Department of Mathematics and Physics E. De Giorgi, research project "Numerical challenges in the modelling of soft solids: acoustic waves and instabilities". (Visit held in June 2012)

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2. Differential equations, Partial â€”Numerical solutions. I. Title. II. Title: Numerical methods. III.Â Preliminaries The first two chapters of this book are merely devoted to the numerical methods of solving the initial value problem associated to first-order ordinary differential equations. GENERALITIES, CONVENTIONS AND NOTATION Let f(x, y) be a real-valued function of two variables defined for the real x e [a, b] and all real y. Suppose that y is a real valued function defined on [a, b]. The equation y=A*,y) (i) is called an ordinary differential equation of the first order. Any real valued function y{x) which is differentiable and satisfies (1) for a < x < b is said to be a solution of Topics: Advanced introduction to applications and theory of numerical methods for solution of partial differential equations, especially of physically-arising partial differential equations, with emphasis on the fundamental ideas underlying various methods. Discretization methods, including finite difference & finite-volume schemes, spectral collocation, and Galerkin methods.Â Discussed application of spectral methods when the operator isn't diagonal as it is for Poisson, in particular for the example of the Schrodinger equation. You do spatial operations on f(x) and derivatives on ck, converting back-and-forth via FFTs, and thus can apply iterative methods in O(N log N) time. Numerical methods for ordinary differential equations are methods used to find numerical approximations to the solutions of ordinary differential equations (ODEs). Their use is also known as "numerical integration", although this term can also refer to the computation of integrals. Many differential equations cannot be solved using symbolic computation ("analysis"). For practical purposes, however â€“ such as in engineering â€“ a numeric approximation to the solution is often sufficient. The algorithms Numerical solution of ordinary differential equations. Kendall Atkinson, Weimin Han, David Stewart University of Iowa Iowa City, Iowa. A john wiley & sons, inc., publication.Â Numerical methods vary in their behavior, and the many different types of differ-ential equation problems affect the performance of numerical methods in a variety of ways. An excellent book for â€œreal worldâ€ examples of solving differential equations is that of Shampine, Gladwell, and Thompson [74]. The authors would like to thank Olaf Hansen, California State University at San Marcos, for his comments on reading an early version of the book. We also express our appreciation to John Wiley Publishers. Solving numerically differential equations is an art and partly a science. Every method has pro and cons. First choice: Euler explicit.Â In physics, how often do differential equations that can be solved analytically (as opposed to those requiring a numerical method) actually come up? In other words, are the analytical techniques taught in O.D.E. courses actually used in physics? Why are partial differential equations hard to solve? What content from calculus 1 and 2 should I review before taking differential equations?