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Current Challenges in Stability Issues for Numerical Differential Equations

Cetraro, Italy 2011

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Studies on Current Challenges in Stability Issues for Numerical Differential Equations

1 Introduction

This volume is the outgrowth of lectures presented during the CIME-EMS Summer School on Applied Mathematics, "Studies on Stability Issues for Numerical Differential Equations", held in Cetraro (Italy) in June 2011. The school was attended by about 50 participants, coming from Belgium, Canada, Germany, Italy, the Netherlands, Poland, Spain, Switzerland, and the USA. The hospitality and generosity of the CIME foundation are gratefully acknowledged.

This volume addresses some current research directions in the general area of stability studies for differential equations. ODEs (Ordinary Differential Equations), PDEs (Partial Differential Equations) and SDEs (Stochastic Differential Equations) are all treated in this monograph.

Although the emphasis of the volume is on issues of concern for numerical studies of differential equations, the arguments treated here will be of interest also to people working on qualitative theory of differential equations.

Above, the word *stability* has to be understood in a broad sense, to indicate some of the many issues which arise in numerical studies of differential equations. These issues range from the need to develop stable and reliable algorithms preserving some qualitative properties of the computed solutions, to the development of tools which are helpful to assess the onset of potential instabilities, to tools which assess the asymptotic properties of the solution or its discretization.

The topics considered in this volume involve the computation of dynamic patterns in evolution PDEs, the long-time integration of conservative ODEs and highly oscillatory systems, the Markov chain Monte Carlo method establishing a connection between SDEs and geometric integration, the continuous decomposition of matrices depending on parameters and the localization of singularities, and the uniform stability analysis of time-dependent linear initial value ODE problems.

In the end, the motivation of the authors remains the one of robust algorithmic development for use in approximation of differential equations. And, in all of the issues considered by the authors, the concerns for reliable approximations

lead to considerations of stability and to the development of new analytical tools. In turn, these tools will be useful to analyze discretization schemes both for differential equations and for different applications, as the authors will clarify in their contributions.

1. The first chapter is authored by Paola Console and Ernst Hairer and is entitled "Long-Term Stability of Symmetric Partitioned Linear Multistep Methods".

The importance of good numerical properties in the time integration of Hamiltonian systems is a well-known and deeply studied subject. Here, the authors analyze the properties of (possibly partitioned) multistep methods, which present parasitic solutions. The results presented in this chapter exploit the combination of two powerful techniques: backward error analysis of numerical integrators and modulated Fourier expansions theory. In the first part of the chapter, the authors treat stability of the parasitic solution components over long time intervals. The results, which are obtained exploiting backward error analysis, are not covered by classical convergence estimates, when a multistep method is applied to a Hamiltonian system (not highly oscillatory), and they clarify the conditions under which such integrators are of interest. In the second part, the authors analyze the near-conservation of oscillatory energies (adiabatic invariants) by numerical discretization. These two seemingly unrelated topics are in fact closely connected by the use of the same technique of proof: *modulated Fourier expansions*. The inverse of the high frequency in the second topic plays the role of the step size of multistep methods in the first topic. Near-preservation of oscillatory energies in the second topic corresponds to the boundedness of parasitic solution components for multistep methods in the first topic.

2. The second chapter is authored by Sanz-Serna and is entitled "Markov Chain Monte Carlo and Numerical Differential Equations".

Markov Chain Monte Carlo algorithms are among the most widely used algorithms in just about any of the applied sciences: e.g. physics, chemistry and statistics. In many implementations of these techniques, at each step of the chain it is required to produce a numerical approximation of an initial value problem, where the initial condition or the differential equation or both are subject to random perturbations (stochastic differential equations). The author emphasizes how ideas from *geometric integration* play an important role in these numerical simulations. The initial part of the chapter is devoted to background in stochastic processes and Hamiltonian dynamics. In the second part, first the author presents in detail the basic Random Walk Metropolis algorithm for discrete or continuous distributions. Then, MALA (Metropolis Adjusted Langevin Algorithm) is presented; this is an algorithm based on a stochastic differential equations proposal. Finally, the Hybrid Monte Carlo method, which is based on ideas from Hamiltonian mechanics, is presented.

3. The third chapter is authored by Wolf-Jürgen Beyn, Denny Otten and Jens Rottmann-Matthes and is entitled "Stability and Computation of Dynamic Patterns in PDEs".

Nonlinear waves are a common feature in many applications such as the spread of epidemics, electric signaling in nerve cells, excitable chemical reactions and models of combustion.

The mathematical models of such systems lead to time-dependent partial differential equations (PDEs) of parabolic or hyperbolic type. In one space dimension, typical examples of waves are fronts and pulses, in two space dimensions we have rotating and spiral waves, and in three space dimensions there appear the so-called scroll waves. When the PDE is posed on the whole space, these dynamic patterns can be viewed as relative equilibria of an equivariant evolution equation. Here equivariance means that the spatial differential operator commutes with the action of a Lie group. One of the major theoretical concerns is to prove nonlinear stability with asymptotic phase based on linearized stability. Typically the differential operators obtained by linearizing at a relative equilibrium have both essential and isolated spectrum with several eigenvalues lying on the imaginary axis, and one of the computational challenges is to develop robust methods which locate critical isolated parts of the spectrum. For the time-dependent PDEs the authors present the freezing method which makes use of equivariance and allows to compute moving coordinate frames in which solutions converging to dynamic patterns become stationary in the classical sense. The numerical analysis of this method is intimately connected to the stability issues considered before. The aim of this contribution is to give an overview of the field, while also providing analytical details for some core topics.

The last two chapters are concerned with spectral properties of families of matrices in connection to stability.

4. The fourth chapter is authored by Luca Dieci, Alessandra Papini, Alessandro Pugliese and Alessandro Spadoni and is entitled "Continuous Decompositions and Coalescing Eigenvalues for Matrices Depending on Parameters".

The eigendecomposition and singular value decomposition of a matrix are surely some of the most useful theoretical and numerical tools. They form the backbone of local stability analysis and subspace approximation, to name a few of their applications. Suppose to have a matrix valued function which depends on several parameters, and that it has some degree of smoothness with respect to these parameters. It is natural to inquire whether the factors of—say—a singular value decomposition of this function inherit some smoothness. In general, the answer is not positive, and one may experience a total loss of smoothness when the singular values coalesce. Some of this theory will be reviewed, and then the authors will address a revised question: is it possible to give localization results for where (in parameter space) the singular values will coalesce? Some old and some new results will be presented on this topic, as well as numerical methods that find the location of these coalescing points. Applications range from structural engineering to best approximation studies.

5. The fifth and final chapter of the volume is authored by Nicola Guglielmi and Marino Zennaro and is entitled “Stability of Linear Problems: Joint Spectral Radius of Sets of Matrices”.

It is known that the stability analysis of step-by-step numerical methods for differential equations often reduces to the analysis of linear difference equations with variable coefficients. This class of difference equations leads to a family $\mathscr{F}$ of matrices depending on some parameters, and the behaviour of the solutions depends on the convergence properties of the products of the matrices of $\mathscr{F}$. To date, the techniques mainly used in the literature are confined to the search for a suitable norm and for conditions on the parameters such that the matrices of $\mathscr{F}$ are contractive in that norm. In general, the resulting conditions are more restrictive than necessary. An alternative and more rigorous approach is based on the concept of “joint spectral radius” of the family $\mathscr{F}$. It is known that, in analogy with the case of a single matrix, all the products of matrices of $\mathscr{F}$ asymptotically vanish if and only if the joint spectral radius is less than 1. The aim of this chapter is to discuss the main theoretical and computational aspects involved in the analysis of the joint spectral radius and in applying this tool to the stability analysis of the discretizations of differential equations, as well as to other stability problems. It is worth stressing that both theory and numerical methods for the computation of the joint spectral radius still present many open problems.

It is the expectation of the editors that this volume will serve a twofold purpose. On the one hand, the volume will be a valuable entry point into the topics herein considered, with ample and exhaustive references on each subject, and a didactic style of presentation on cutting-edge techniques. On the other hand, this volume will hopefully stimulate researchers to pursue further the topics presented in this volume.

Atlanta, GA, USA — Luca Dieci
L’Aquila, Italy — Nicola Guglielmi

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