Numerical Analysis 2000, Volume 6

Ordinary Differential Equations and Integral Equations

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Preface

Numerical Analysis 2000
Vol. VI: Ordinary Differential Equations and Integral Equations

This volume contains contributions in the area of differential equations and integral equations. The editors wish to thank the numerous authors, referees, and fellow editors Claude Brezinski and Luc Wuytack, who have made this volume a possibility; it has been a major but personally rewarding effort to compile it. Due to the limited number of pages we were obliged to make a selection when composing this volume. At an early stage it was agreed that, despite the connections between the subject areas, it would be beneficial to allocate the area of partial differential equations to a volume for that area alone.

Many numerical methods have arisen in response to the need to solve "real-life" problems in applied mathematics, in particular problems that do not have a closed-form solution. It is particularly relevant to this comment that our Journal title involves the expression "Computational and Applied Mathematics". Applied mathematicians from differing academic cultures display differing approaches to computational techniques, but one might hazard the prophecy, based on current observations, that future generations of applied mathematicians will (without necessarily sacrificing mathematical rigour) *almost universally* regard the use of, and possibly the analysis and design of, robust numerical algorithms as an essential part of their research activity.

The differences seen in applied mathematics are reflected in differing approaches to the promotion of numerical analysis by those who today think of themselves as "numerical analysts": some, feeling that it is the mathematical modelling that supports the development of the subject, work closely in the area of mathematical modelling. Others, aware of the effect of advances in computers, are more concerned with accurate and efficient computational algorithms. Yet others prefer to construct more abstract mathematical theories that offer insight into, and justification (at least under well-formulated conditions) of, the numerical mathematics. Major contributions to topics represented here have been published in the past; many of the diverse approaches are represented in this volume. At the same time, there is a mixture of original and survey material represented here, often in the same paper.

Contributions on both initial-value problems and boundary-value problems in *ordinary differential equations* appear in this volume. Numerical methods for *initial-value problems* in ordinary differential equations fall naturally into two classes: those which use *one* starting value at each step (one-step methods) and those which are based on *several* values of the solution (multistep methods). Both methods were developed at the end of the 19th century.

- John Butcher has supplied an expert's perspective of the development of numerical methods for ordinary differential equations in the 20th century.

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For the one-step methods we can refer to the original work of Runge of 1895 (an extract is reproduced in John Butcher's paper), while for the multistep methods a first paper was published by Adams in 1883 (a copy of the title page appears in John's contribution). Advances in analysis and the advent of electronic computers has of course altered the scene drastically.

- Rob Corless and Lawrence Shampine talk about established technology, namely software for initial-value problems using Runge–Kutta and Rosenbrock methods, with interpolants to fill in the solution between mesh-points, but the 'slant' is new — based on the question, "How should such software integrate into the current generation of *Problem Solving Environments*?" They discuss specifically a new code they have written for the Maple environment and the similarities and differences with corresponding solvers for MATLAB and for traditional numerical libraries. The interplay between interface, environment and algorithm raises many subtle issues and provides an excellent example of mathematical software engineering.
- Natalia Borovykh and Marc Spijker study the problem of establishing upper bounds for the norm of the nth power of square matrices. This problem is of central importance in the stability analysis of numerical methods for solving (linear) initial-value problems for ordinary, partial or delay differential equations. In particular, they apply the new bounds in a stability analysis of the trapezoidal rule for delay differential equations (*vide infra*).

The dynamical system viewpoint has been of great benefit to ODE theory and numerical methods. The characterization and computation of *bifurcations* of parametrized ODEs is an active subfield created some 20 years ago. Related is the study of *chaotic behaviour*. To reproduce long-term behaviour realistically, special numerical methods are needed which *preserve invariants* of the exact system: symplectic methods are an example.

- In the first of three articles in the general area of *dynamical systems*, Willy Govaerts discusses the numerical methods for the computation and continuation of equilibria and bifurcation points of equilibria of dynamical systems. The computation of cycles as a boundary value problem, their continuation and bifurcations are considered. The basic numerical methods and the connections between various computational objects are discussed. References to the literature and software implementations are provided.
- In the second of this trio, Arieh Iserles and Antonella Zanna survey the construction of Runge–Kutta methods which preserve algebraic invariant functions. There is a well-known identity on the RK coefficients that is necessary and sufficient for the retention of a quadratic invariant. They extend this result and present a brief introduction to the Lie-group approach to methods that preserve more general invariants, referring to survey articles for fuller discussion.
- Symplectic methods for Hamiltonian systems are an important example of invariant-preserving methods. Valeria Antohe and Ian Gladwell present numerical experiments on solving a Hamiltonian system of Hénon and Heiles with a symplectic and a nonsymplectic method with a variety of precisions and initial conditions. The long-term behaviour of the Hamiltonian error, and the features of Poincaré sections, show interesting and unexpected phenomena.

Stiff differential equations first became recognized as special during the 1950s. In 1963 two seminal publications laid to the foundations for later development: Dahlquist's paper on A-stable multistep methods and Butcher's first paper on implicit Runge–Kutta methods. Later, order stars became a fundamental tool for the theoretical understanding of order and stability properties of stiff differential equations. Variable-order variable-step methods were the next for study.

- Ernst Hairer and Gerhard Wanner deliver a survey which retraces the discovery of the order stars as well as the principal achievements obtained by that theory, which has become a fundamental role for the understanding of order and stability properties of numerical methods for stiff differential equations. Some later extensions as well as recent developments and open questions are discussed.
- Guido Vanden Berghe, Hans De Meyer, Marnix Van Daele and Tanja Van Hecke construct exponentially fitted Runge–Kutta methods with s stages, which exactly integrate differential initial-value problems whose solutions are linear combinations of functions of the form $\{x^j \exp(\omega x), x^j \exp(-\omega x)\}$, ($\omega \in \mathbb{R}$ or $i\mathbb{R}$, $j = 0, 1, \ldots, j\max$), where $0 \leqslant j\max \leqslant \lfloor s/2 - 1 \rfloor$, the lower bound being related to explicit methods, the upper bound applicable for collocation methods. Explicit methods with $s \in \{2, 3, 4\}$ belonging to that class are constructed. For these methods a study of the local truncation error is made, out of which follows a simple heuristic to estimate the ω-value. Error and step length control is introduced based on Richardson extrapolation ideas.

Differential-algebraic equations arise in control, in modelling of mechanical systems and in many other fields. They differ fundamentally from ODEs, and an *index* can be defined that measures (in some sense) how far a given DAE is from being an ODE. DAEs can in some cases be regarded as infinitely stiff ODEs, and methods for stiff problems work well for problems of index 1 or 2 at least. Examples are the classical backward differentiation formulas (BDF). Recent modifications of BDF due to Cash, using the so-called super-future points, have also proved very effective on DAEs as well as on highly oscillatory problems. Other variants on the classical Runge–Kutta and multistep approaches have been studied in recent decades, such as special-purpose "exponentially fitted" methods when the solution of the problem exhibits a pronounced oscillatory or exponential character. A good theoretical foundation of this technique was given by Gautschi in 1961 and Lyche in 1972. Automatic error control when solving DAEs is harder than for ODEs because changing dominance of different solution components may make both index and order of accuracy seem to vary over the range, especially for boundary-value problems. New meshing algorithms have been developed to cope with this.

- Jeff Cash describes a fairly recent class of formulae for the numerical solution of initial-value problems for *stiff and differential-algebraic systems*. These are the modified extended backward differentiation formulae (MEBDF), which offer some important advantages over the classical BDF methods, for general stiff nonoscillatory problems, for damped highly oscillatory problems and for linearly implicit DAEs of index up to 3. Numerical results are given for a simple DAE example with references to other performance tests. Pointers to down-loadable software are given.
- In the same area, Shengtai Li and Linda Petzold describe methods and software for *sensitivity analysis* of solutions of DAE initial-value problems: that is, for computing derivatives of a solution of $F(t, y, y', p) = 0$ with respect to one or more parameters p. As with similar methods for ODEs, they integrate auxiliary systems, incorporating local Jacobians which may be computed by *automatic differentiation* using a package such as ADIFOR. Consistent initialization is shown to need special care and suitable algorithms described. Several numerical experiments illustrate the performance; pointers to down-loadable software are given.
- Again in the area of differential-algebraic systems, Neil Biehn, John Betts, Stephen Campbell and William Huffman present current work on mesh adaptation for DAE two-point boundary-value problems. The context is an optimal control problem, which discretizes to a nonlinear

programming problem, but the problem of "order variation" is more general. Not only are different components of a DAE computed to different order of accuracy as a function of step-size, but the "real order" can vary at different points of the interval and from iteration to iteration. They discuss the principles and details of a new meshing algorithm and show its effectiveness on a computational example.

Contrasting approaches to the question of how good an approximation is as a solution of a given equation involve (i) attempting to estimate the actual *error* (i.e., the difference between the true and the approximate solutions) and (ii) attempting to estimate the *defect* — the amount by which the approximation fails to satisfy the given equation and any side-conditions. (In collocation and Galerkin techniques, the defect is required to satisfy certain constraints. Generally speaking, the relationship between defect and error can be analyzed using results on the stability or conditioning of the solution of the original problem.)

- The paper by Wayne Enright on defect control relates to carefully analyzed techniques that have been proposed both for ordinary differential equations and for delay differential equations in which an attempt is made to control an estimate of the size of the defect.

Many phenomena incorporate noise, and the numerical solution of *stochastic differential equations* has developed as a relatively new item of study in the area.

- Kevin Burrage, Pamela Burrage and Taketomo Mitsui review the way numerical methods for solving stochastic differential equations (SDEs) are constructed. SDEs arise from physical systems where the parameters describing the system can only be estimated or are subject to noise. The authors focus on two important topics: the numerical stability and the implementation of the method. Different types of stability are discussed and illustrated by examples. The introduction of variable step-size implementation techniques is stressed under the proviso that different numerical simulations must follow the same Brownian path.

One of the more recent areas to attract scrutiny has been the area of *differential equations with after-effect* (retarded, delay, or neutral delay differential equations) and in this volume we include a number of papers on evolutionary problems in this area. The problems considered are in general initial-function problems rather than initial-value problems. The analytical study of this area was already well-advanced in the 1960s, and has continued to develop (some of the names that spring to mind are: in the fSU, Myskhis, Krasovskii, Kolmanovskii; in the USA, Bellman and Cooke, and later Driver, Hale, etc.; in Europe, Diekmann, Halanay, Verduyn Lunel and Stépán). There has been an increasing interest in the use of such equations in mathematical modelling. For numerical analysts, one significant issue is the problem of the possible lack of smoothness of the solution, for which various strategies have been advanced, whilst another is the richer dynamics encountered in problems with delay.

- The paper of Genna Bocharov and Fathalla Rihan conveys the importance in mathematical biology of models using retarded differential equations. Although mathematical analysis allows deductions about the qualitative behaviour of the solutions, the majority of models can only be solved approximately using robust numerical methods. There are now a number of papers on the use of delay and neutral delay equations in parameter fitting to biological data; the most recent work relates to a sensitivity analysis of this data-fitting process.

- Delay differential equations also arise in mechanical systems, and the paper by John Norbury and Eddie Wilson relates to a form of constrained problem that has application to the control of a motor.
- The contribution by Christopher Baker, whose group has for some years been working in this area, is intended to convey much of the background necessary for the application of numerical methods and includes some original results on stability and on the solution of approximating equations.
- Alfredo Bellen, Nicola Guglielmi and Marino Zennaro contribute to the analysis of stability of numerical solutions of nonlinear neutral differential equations; they look at problems that display a form of contractivity. This paper extends earlier work on nonlinear delay equations by Torelli, Bellen, and Zennaro. We note that Alfredo Bellen and Marino Zennaro are preparing a book on the numerical solution of delay equations.
- In the papers by Koen Engelborghs, Tatyana Luzyanina and Dirk Roose and by Neville Ford and Volker Wulf, the authors consider the numerics of bifurcation in delay differential equations. Oscillations in biological phenomena have been modelled using delay equations. For some time, it has been realized that the onset of periodicity in such equations can be associated with a Hopf bifurcation and that chaotic behaviour can arise in scalar delay differential equations.
- Christopher Paul, who is the author of a code for the numerical solution of retarded equations (named `Archi`) addresses various issues in the design of efficient software and proposes methods for determining automatically information about the delay equation.
- The preceding papers relate to deterministic problems. Evelyn Buckwar contributes a paper indicating the construction and analysis of a numerical strategy for stochastic delay differential equations (SDDEs). The theory of SDDEs has been developed in books written by Mohammed and by Mao, but the numerics have been neglected. Unlike the corresponding results for stochastic differential equations without time lag (represented herein by the paper of Burrage et al.) some of the basic elements required in the numerical analysis have previously been lacking.

One could perhaps argue that stochastic differential equations (since they are really Itô or Stratonovitch integral equations) should be classified under the heading of integral equations. In any event, this volume contains contributions on both *Volterra and Fredholm-type integral equations.*

- Christopher Baker responded to a late challenge to craft a review of the theory of the basic numerics of Volterra integral and integro-differential equations; it is intended to serve as an introduction to the research literature. The very comprehensive book by Hermann Brunner and Pieter van der Houwen on the numerical treatment of Volterra integral equations remains a standard reference work.
- Simon Shaw and John Whiteman discuss Galerkin methods for a type of Volterra integral equation that arises in modelling viscoelasticity, an area in which they have already made a number of useful contributions.

Volterra integral and integro-differential equations are examples of causal or nonanticipative problems, as are retarded differential equations. It seems likely that such causal (abstract Volterra) problems will, increasingly, be treated together, since mathematical models frequently involve both discretely distributed and continuously distributed delays. The basic discretization theory is concerned with replacing the continuous problem with another causal problem (if one considers a vectorized formulation, this statement is true of block-by-block methods as well as step-by-step methods), and the study of *discrete Volterra equations* is a feature of increasing importance in the analysis.

We turn now to a subclass of *boundary-value problems* for ordinary differential equation, that comprises *eigenvalue problems* such as Sturm–Liouville problems (SLP) and Schrödinger equations. They are important for their role in physics and engineering and in spurring the development of spectral theory. For the classical (second-order) SLP there is reliable software for eigenvalues (less reliable for eigenfunctions) for commonly occurring types of singular behaviour. The underlying self-adjointness is important for these methods. Among current developments are new methods for *higher-order problems*, both self-adjoint and nonself-adjoint. Also of interest are the Constant Potential (CP) methods, which have recently been embodied in good software for the classical regular SLP, and whose efficiency makes them likely to supplant existing methods.

- In the first of a number of articles on *ODE eigenvalue problems*, Liviu Ixaru describes the advances made over the last three decades in the field of piecewise perturbation methods for the numerical solution of Sturm–Liouville problems in general and systems of Schrödinger equations in particular. He shows that the most powerful feature of the introduced constant potential (CP) methods is the uniformity of accuracy with respect to the eigen-parameter. He presents basic formulae and characteristics of a class of CP methods, based on piecewise approximation by a constant and a polynomial perturbation term. He illustrates by means of the Coffey–Evans equation — a standard example with pathologically clustered eigenvalues — the superiority of his code over some other standard codes, such as SLEDGE, SLEIGN and SL02F.
- Alan Andrew surveys the asymptotic correction method for regular Sturm–Liouville problems. Simple but unexpectedly powerful, it applies to finite difference and finite element methods which reduce the problem to a matrix eigenproblem. It greatly improves the accuracy of higher eigenvalues and generally improves lower ones as well, which makes it especially useful where long runs of eigenvalues need to be computed economically. The Coffey–Evans equation is used to show the good performance of the method even on tightly clustered eigenvalues.
- Leon Greenberg and Marco Marletta survey methods for higher-order Sturm–Liouville problems. For the self-adjoint case, the elegant basic theory generalizes the Prüfer phase-angle, used in theory and numerical methods for the classical SLP, to a complex unitary matrix. This was introduced by Atkinson in the 1960s, but the obstacles to using it numerically are considerable. The authors' considerable achievement over the last few years has been to identify suitable subclasses of the problem, and a general strategy (coefficient approximation) that leads to a usably efficient numerical method with error control. They also discuss theory and methods for the very different nonself-adjoint case. Numerical examples of both types are given.
- R. Moore in the 1960s first showed the feasibility of *validated solution* of differential equations, that is, of computing guaranteed enclosures of solutions. Validated methods use outward-rounded interval floating point arithmetic as the computing tool, and fixed-point theorems as the mathematical foundation. An important development in this area was the appearance in 1988 of Lohner's code, AWA, for ODE initial-value problems, which he also applied to the validated solution of boundary-value problems. Recently, these techniques have been extended to eigenvalue problems, e.g. to prove the existence of, and enclose, certain kinds of eigenvalue of a singular Sturm–Liouville problem, and the paper of Malcolm (B.M.) Brown, Daniel McCormack and Anton Zettl describes validated SLP eigenvalue calculation using Lohner's code.

We turn to papers on *boundary integral equations*. In the last 20 years, the numerical solution of integral equations associated with boundary-value problems has experienced continuing interest. This is because of the many intriguing theoretical questions that still needed to be answered, and the many complications that arise in applications, particularly in the engineering fields. Coming from the reformulation of PDE boundary value problems in terms of boundary integral equations, such problems often have complex geometries, bad aspect ratios, corners and other difficulties, all of which challenge existing numerical techniques. In particular, much effort has been concentrated on the following research themes:

— equations with singular and hyper-singular kernels,
— equations of Mellin type and equations defined on nonsmooth regions,
— fast solution numerical methods, especially for three-dimensional problems,
— domain decomposition, and
— the coupling of finite element and boundary element methods.

Many numerical analysts have made major contributions to the above themes, and to other important topics. With a limited number of pages at our disposal, we have included the seven papers below:

- Peter Junghanns and Bernd Silbermann present a selection of modern results concerning the numerical analysis of one-dimensional Cauchy singular integral equations, in particular the stability of operator sequences associated with different projection methods. They describe the main ideas and approaches. Computational aspects, in particular the construction of fast algorithms, are also discussed.
- Johannes Elschner and Ivan Graham summarize the most important results achieved in the last years about the numerical solution of one-dimensional integral equations of Mellin type by means of projection methods and, in particular, by collocation methods. They also consider some examples arising in boundary integral methods for the two-dimensional Laplace equation on bounded polygonal domains.
- A survey of results on quadrature methods for solving boundary integral equations is presented by Andreas Rathsfeld. The author gives, in particular, an overview on well-known stability and convergence results for simple quadrature methods based on low-order composite quadrature rules and applied to the numerical solution of integral equations over smooth manifolds. Useful "negative results" are also presented.
- Qualocation was introduced in the late 1980s as a compromise between Galerkin and collocation methods. It aimed, in the context of spline approximation methods for boundary integral equations on smooth curves, to achieve the benefits of the Galerkin method at a cost comparable to the collocation method. Ian Sloan reviews this method with an emphasis on recent developments.
- Wolfgang Hackbusch and Boris Khoromski present a novel approach for a very efficient treatment of integral operators. They propose and analyze a quite general formulation of the well-known panel clustering method for boundary integral equations, introduced by Hackbusch and Z.P. Nowak in the late 1980s. Their approach may be applied for the fast solution of the linear integral equations which arise in the boundary element methods for elliptic problems.
- Ernst Stephan examines multilevel methods for the *h*-, *p*- and *hp*- versions of the boundary element method, including pre-conditioning techniques. In his paper he reviews the additive Schwarz methods for the above versions of the Galerkin boundary element method applied to first kind (weakly singular and hyper-singular) integral equations on surfaces.

- Domain decomposition methods are well suited for the coupling of different discretization schemes such as finite and boundary element methods. George Hsiao, Olaf Steinbach and Wolfgang Wendland analyze various boundary element methods employed in local discretization schemes. They also describe appropriate iterative strategies, using both local and global pre-conditioning techniques, for the solution of the resulting linear systems.

The latter papers not only present overviews of some of the authors' recent research activities, but, in some cases, also contain original results and new remarks. We think that they will constitute fundamental references for any further research work on the numerical resolution of boundary integral equations.

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Numerical methods for ordinary differential equations in the 20th century

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Abstract

Numerical methods for the solution of initial value problems in ordinary differential equations made enormous progress during the 20th century for several reasons. The first reasons lie in the impetus that was given to the subject in the concluding years of the previous century by the seminal papers of Bashforth and Adams for linear multistep methods and Runge for Runge–Kutta methods. Other reasons, which of course apply to numerical analysis in general, are in the invention of electronic computers half way through the century and the needs in mathematical modelling of efficient numerical algorithms as an alternative to classical methods of applied mathematics. This survey paper follows many of the main strands in the developments of these methods, both for general problems, stiff systems, and for many of the special problem types that have been gaining in significance as the century draws to an end.

Keywords: Initial value problems; Adams–Bashforth method; Adams–Moulton method; Runge–Kutta method; Consistency; Stability and convergence; Order of methods; Stiff problems; Differential equation software

1. Introduction

It is not possible to assess the history of this subject in the 20th century without first recognizing the legacy of the previous century on which it has been built. Notable are the 1883 paper of Bashforth and Adams [5] and the 1895 paper of Runge [57]. Not only did the former present the famous Adams–Bashforth method, which plays an essential part in much modern software, but it also looked ahead to the Adams–Moulton method and to the practical use of Taylor series methods. The paper by Runge is now recognized as the starting point for modern one-step methods. These early contributions, together with a brief introduction to the fundamental work of Euler, will form the subject matter of Section 2.

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