Outline

This book is divided into eight chapters, a software list, a reference list, and an index. The first three chapters lay the ground in modeling, analysis, and numerical analysis. The following four chapters deal with algorithms for initial value problems, among them three with one-step methods and the fourth one with multistep methods. The final chapter is devoted to boundary value problems.

Chapter 1. Here we go into the scientific background of ordinary differential equations (ODEs) as examples of deterministic models. *Newton's celestial mechanics* still arises today in orbit calculation for satellites or asteroids. Classical *molecular dynamics*, which plays an increasing role in the design of drugs and in the understanding of viral diseases, is also based on the concept of Newtonian mechanics. At this point *Hamiltonian differential equations* already enter. Historically, stiff initial value problems (IVPs) arose for the first time in *chemical reaction kinetics*, which is an important part of industrial chemical engineering nowadays. As the last field of application we present the *electric circuit* models that arise in the design of rather diverse appliances, from mobile phones to automatic braking systems in cars. They lead naturally to IVPs for differential-algebraic equations (DAEs).

Chapter 2. In this chapter we lay the basis of analytical *existence and uniqueness theory* with a particular view toward application in *mathematical modeling*. At points where the right sides of ODEs are not Lipschitz continuous an interesting structure of nonunique solutions arises, which in this fine degree of representation can be found nearly nowhere else. *Singu-*

lar perturbation problems are a beautiful and useful tool for the analytical investigation of multiscale dynamical systems, and they also play a role in their numerical treatment. For their extension to general *quasilinear DAE* problems we introduce explicit expressions for orthogonal projectors that permit a characterization of an index-1 case that typically needs index-2 treatment in the literature. This characterization is of help later in the implementation of one-step and multistep methods for DAEs. The restriction to index 1 is made throughout the book.

Chapter 3. Here we turn to the practically important question of numerical analysis concerning the *sensitivity* of problems with respect to their typical *input data*. In the precise sense of our introductory textbook [58], Chapter 2, we define *condition numbers* for initial value problems. *Asymptotic stability* is studied first for linear autonomous ODEs, in which case a characterization purely via the real parts of the eigenvalues is possible. The extension to the nonlinear case is done for a neighborhood of fixed points decomposing the invariant tangent subspaces of the associated manifolds. Following the same pattern discrete dynamical systems are presented, which arise by discretization of ODEs: First linear autonomous recursions are treated where a characterization via the moduli of the eigenvalues is possible, then the extension by decomposition of the tangent space at fixed points. The connection of the eigenvalue real parts in the continuous case and the eigenvalue moduli in the discrete case is used to discuss the *inheritance* of properties from the matrix exponential to the approximating rational matrix functions.

After these three basic chapters we are prepared for the treatment of *numerical methods* for the actual solution of ODE problems.

Chapter 4. In this chapter we present explicit *one-step methods* for *nonstiff* initial value problems. From the beginning the notation includes the adaptive case of nonuniform grids. One-step methods transform the evolution of the ODE into a *discrete evolution* and correspondingly the ODE IVP condition number into associated *discrete condition numbers*. The comparison of continuous and discrete condition numbers easily defines the concept of *stiffness* of IVPs, even for a single scalar ODE. In Taylor expansions, which come up in the order conditions of any *Runge-Kutta method*, the occurring higher derivatives and coefficient products are written consistently as multilinear mappings. Thus we are able to interpret Butcher's rooted trees in an index-free form just as representations of an insertion structure within multilinear mappings. Especially in this slightly technical part, we have put considerable effort into a transparent presentation and suggestive notation and therefore hope to have made this not easily accessible material nevertheless quite readable. *Explicit extrapolation methods* with an asymptotic τ^2-expansion of the discretization error are characterized via the reversibility of discrete evolutions (Stetter trick). The asymptotic energy conservation of the Störmer/Verlet discretization is discussed by an example of the chaotic behavior of *Hamiltonian systems*; a deeper understanding of the associated numerical findings is obtained only via the condition of the IVPs.

Chapter 5. The *adaptive control* of step size and order in numerical integrators is, for strongly varying dynamics, of crucial importance in view of computational complexity. This chapter focuses on one-step methods. For a deeper understanding we make a methodical excursion into control theory and interpret the step-size control as a discrete controller. From this point of view we obtain an extremely useful stability condition that explains the empirically known robustness of step-size controls in higher-order methods in the presence of order reduction. This builds the bridge to stiff integrators.

Chapter 6. This chapter is concerned with *one-step methods* for *stiff* and *differential-algebraic* initial value problems. We analyze the inheritance of properties of a continuous phase flow to discrete flows. The solution of the scalar linear ODE is the complex exponential function, known to have an *essential singularity* at the point $z = \infty$. Among the corresponding rational approximations we select those that in the approach to $z = \infty$ for $\Re(z) < 0$ vanish, thus arriving at the fundamental concept of *L-stability*. The approach for $\Re(z) = 0$ cannot realize the zero at infinity, and is therefore treated in connection with the *isometric* structure of phase flows. Following this analysis our presentation naturally bifurcates into implicit and linearly implicit one-step methods. In the Runge-Kutta frame of Butcher this leads to *implicit Runge-Kutta methods* where *nonlinear* systems of equations must be solved. Among these methods we focus on *collocation methods*, which stand out due to their transparent methods of proof and their beautiful inheritance properties. Apart from that they represent an important class of methods for the treatment of boundary value problems (see below). The direct realization of the concept of perturbations of linear phase flows leads to *linearly implicit one-step methods* where only *linear* systems of equations must be solved. Among these methods we emphasize the extrapolated linearly implicit Euler method, which at present is the only usable W-method of higher and even variable order; it is applicable to DAE problems only up to index 1, a restriction made throughout the book. The latter class of methods is especially well suited for use within a *method of lines* approach to *partial differential equations* (PDEs). Moreover, they are a convenient basis for a realization of *numerical singular perturbation computations*, which recently have played an important role in the elimination of fast modes, in particular in the context of *model reduction* for time dependent PDEs of diffusion reaction type.

This completes the presentation of one-step methods.

Chapter 7. The chapter on *multistep methods* deals with *nonstiff* and *stiff* initial value problems in parallel. At the beginning the classical convergence theory over *uniform* grids is presented. The traditional derivation formulates k-step methods as one-step methods of k-times the ODE dimension, an approach that leads, however, to an unwieldy norm defined via the Jordan canonical form. In contrast to that standard derivation we apply some quite simple *sequence calculus* that permits estimates in the maximum norm. Our sequence calculus takes up an old idea of P. Henrici, where we, however, have avoided the use of complex analysis, which was typical for this grand classic of ODE methods. The point of view of inheritance of stability of the phase flow supplies the essential structures of multistep methods for both nonstiff and stiff IVPs out of one hand: Via the stability at $z = 0$ we arrive at Adams methods; via the stability at $z = \infty$ we are led to BDF methods. On the one hand, the family of Adams methods can be interpreted as numerical integration based on interpolation of the direction field. On the other hand, the family of BDF methods can be interpreted as numerical differentiation based on interpolation of the approximate solution. Both classes are presented in a unified framework over a *variable* grid and also in Nordsieck form, down to important details of *adaptive* control of step sizes and order. By the construction selected here the extension of BDF methods to DAE problems follows immediately.

The four chapters on *initial value problems* are strictly oriented toward only a small number of efficient numerical integrators:

- for *nonstiff* problems to
  1. the explicit Runge-Kutta methods of Dormand and Prince,
  2. the explicit extrapolation methods based on the midpoint rule and on the Störmer/Verlet discretization,
  3. the Adams methods in various implementations;
- for *stiff* and *differential-algebraic* problems to
  1. the Radau collocation method due to Hairer and Wanner,
  2. the extrapolation method based on the linearly implicit Euler discretization due to Deuflhard and Nowak,
  3. the BDF or Gear method in various implementations.

Chapter 8. In the treatment of *boundary value problems* we again start from (local) uniqueness results. They form the basis for the definition of *condition numbers* for BVPs that are invariant under affine transformation of the boundary conditions. The comparison with IVPs suggests a distinction between timelike and spacelike BVPs. For *timelike* BVPs there exists a clearly preferable direction in which the associated IVP is well-conditioned; typically, the independent variable is a time variable. For *spacelike* BVPs no such preferable direction exists; typically, the independent variable is a spatial variable; in fact, these BVPs often stem from a reduction of BVPs for PDEs to one spatial dimension. Accordingly, this chapter is oriented toward two classes of efficient BVP solvers:

- for *timelike* problems to multiple shooting methods,
- for *spacelike* problems to adaptive collocation methods.

Both classes give rise to corresponding definitions of *discrete condition numbers*. These terms also emerge from the analysis of elimination methods for the *cyclic* systems of linear equations that arise. Beyond the classical two-point BVPs we give some insight into underdetermined BVPs, exemplified by *periodic orbit computation*, and into overdetermined BVPs, exemplified by *parameter identification* in ODEs. Finally, we mention, of necessity briefly to remain within the scope of the book, problems of *variational calculus* and of *optimal control*, which as a rule lead to multipoint BVPs.