Chapter 4
Summary and Outlook

4.1 Comparison of Numerical Methods

Remark 4.1. Motivation. Given an initial value problem in practice, one has to choose a method for its numerical solution. It is desirable to use a method that is appropriate for the given problem, since there is no method that is the best in all aspects and for all situations. This section discusses some criteria for making the choice. □

Remark 4.2. Criteria for comparing numerical methods for solving initial value problems.

- *Computing time.* Computing time is important in many applications. If the evaluation of the right-hand side of the initial value problem is time-consuming, the number of evaluations is important. For implicit methods, the number of calculations of the Jacobian and the number of LU factorizations is of importance.
- *Accuracy.* Computing an accurate numerical solution is of course desirable. However, aiming for high accuracy is often in conflict with having short computing times. An easy step length control should be possible.
- *Memory.* On modern computers, the amount of memory is usually not a big issue. However, if the given initial value problem has special structures, like a sparse Jacobian, such structures should be supported by the numerical method. It should be kept into consideration that on modern computers the access to the memory determines essentially the computing time (and not the number of floating point operations).
- *Reliability.* The step length control (or order control) should be sensitive with respect to local changes of the right-hand side and act in a correct way.
- *Robustness.* The method should work also for complicated examples. It should be flexible with the step length control, e.g., reduce the step length appropriately if the right-hand side has steep gradients.

- *Simplicity.* In complex applications, often the simplicity of the method is of importance.

□

Remark 4.3. Some experience. There are much more numerical methods for solving initial value problems than presented in this course. Here, only some remarks to the presented methods are given.

- *Non-stiff problems.* For such problems, explicit one-step and linear multi-step methods were presented. Often, one-step methods need less steps than multi-step methods. In addition, they are easier to implement and allow an efficient step length control. A few popular explicit one-step methods are given in Remark 1.45.
- *Complex problems.* For complex problems, e.g., from fluid dynamics, where one has an initial value problem with respect to time, very often only the simplest methods are used, like the explicit or implicit Euler method, the trapezoidal rule (Crank–Nicolson scheme), or BDF(2). An efficient and theoretically supported step length control is not possible with these methods. Other methods, like Rosenbrock schemes, have been used only for academic problems so far, e.g., in John & Rang (2010).

□

4.2 Boundary Value Problems

Remark 4.4. A one-dimensional boundary value problem. Boundary value problems prescribe, in contrast to initial value problems, values at (some part of) the boundary of the domain. A typical example in one dimension is

$$-u'' = f \quad \text{in } (0,1), \quad u(0) = a,\ u(1) = b, \tag{4.1}$$

with given values $a, b \in \mathbb{R}$. Solving (4.1) can be performed in principal by integrating the right-hand side of the differential equation twice. Whether or not this analytic calculation can be performed depends on f. Each integration gives a constant, such that the general solution of the differential equation has two constants. The values of these constants can be determined with the given boundary conditions. □

Remark 4.5. Boundary value problems in higher dimensions. Let $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, be a bounded domain. Then, a typical boundary value problem is

$$-\Delta u = -\sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2} = f \quad \text{in } \Omega, \quad u = g \quad \text{on } \partial\Omega, \tag{4.2}$$

where Δ is the Laplacian and $\partial\Omega$ is the boundary of Ω. Solutions of problems of type (4.2) can be hardly found analytically.

The topic of Numerical Mathematics III will be the introduction of numerical methods for solving problems of type (4.2). Such methods include Finite Difference Methods, Finite Element Methods, and Finite Volume Methods. □

4.3 Differential-Algebraic Equations

Remark 4.6. Differential-Algebraic Equations (DAEs). In many applications, the modeling of processes leads to a coupled system of equations of different type. A typical example are systems of the form

$$\begin{aligned} y'(t) &= f(t, y(t), z(t)), \\ 0 &= g(t, y(t), z(t)), \end{aligned} \tag{4.3}$$

with given functions f and g. In (4.3), the derivative of y with respect to t occurs, but not the derivative of z with respect to t. Problem (4.3) is called semi-explicit differential-algebraic equation (DAE), the variable y is the differential variable, and z is the algebraic variable. In this context, the notion 'algebraic' means that there are no derivatives. □

Example 4.7. Equations for incompressible fluids. Equations for the behavior of incompressible fluids are derived on the basis of two conservation laws. The first one is Newton's second law of motion (net force equals mass times acceleration, conservation of linear momentum) and the second one is the conservation of mass. The unknown variables in these equations are the velocity $\boldsymbol{u}(t, x, y, z)$ and the pressure $p(t, x, y, z)$, where t is the time, (x, y, z) the spatial variable, and

$$\boldsymbol{u}(t, x, y, z) = \begin{pmatrix} u_1(t, x, y, z) \\ u_2(t, x, y, z) \\ u_3(t, x, y, z) \end{pmatrix}.$$

Whereas the conservation of linear momentum contains the temporal derivative $\partial_t \boldsymbol{u}$ of the velocity, i.e., it is a differential equation with respect to time, the conservation of mass reads as follows

$$\nabla \cdot \boldsymbol{u} = \partial_x u_1 + \partial_y u_2 + \partial_z u_3 = 0. \tag{4.4}$$

Thus, one obtains a coupled model, the Stokes or Navier–Stokes equations, of the differential equation (with respect to time) and the algebraic equation (4.4). □

Remark 4.8. Theory of DAEs. There is not sufficient time for presenting the theory of DAEs. One can find it, e.g., in (Strehmel *et al.*, 2012, Chapter 13) or (Kunkel & Mehrmann, 2006, Part I). □

Remark 4.9. Direct approach for the discretization of DAEs. In the so-called direct approach, the DAE (4.3) is embedded in the so-called singularly perturbed problem

$$\begin{aligned} y'(t) &= f(t, y(t), z(t)), \\ \varepsilon z'(t) &= g(t, y(t), z(t)), \end{aligned} \tag{4.5}$$

with $0 < \varepsilon \ll 1$. Problem (4.5) is an ODE, for which the methods presented in this course can be applied. Formulating these methods for problem (4.5), then the so-called singular perturbation parameter ε appears. Setting then $\varepsilon = 0$ in these formulations leads formally to methods for the DAE (4.3). Now, one has to study the properties of these methods. □