- $q \geq 3$. The derivation of higher order methods proceeds in the same way. One obtains, e.g., as BDF(3) method

$$\frac{11}{6} y_{k+1} - \frac{18}{6} y_k + \frac{9}{6} y_{k-1} - \frac{2}{6} y_{k-2} = hf\left(x_{k+1}, y_{k+1}\right). \tag{3.32}$$

It should be emphasized that in BDF methods the right-hand side of the initial value problem appears only in one term, namely $f\left(x_{k+1}, y_{k+1}\right)$. This situation is in contrast to the predictor-corrector methods from Section 3.2. This property of BDF methods is of advantage if the computation of the right-hand side is complicated or numerically expensive, like for special discretizations of partial differential equations. □

Lemma 3.33. Null stability of BDF(1), BDF(2), and BDF(3). *The methods BDF(1), BDF(2), and BDF(3) are null stable.*

Proof. The statement of the lemma is obtained by computing the roots of the first characteristic polynomial.

- $q = 1$. The characteristic polynomial is $\lambda - 1$ with the root $\lambda_1 = 1$.
- $q = 2$. The characteristic polynomial of BDF(2) (3.31) is

$$\lambda^2 - \frac{4}{3}\lambda + \frac{1}{3}.$$

  A straightforward calculation gives

$$\lambda_1 = \frac{2}{3} + \frac{1}{3} = 1, \quad \lambda_2 = \frac{2}{3} - \frac{1}{3} = \frac{1}{3}.$$

- $q = 3$. For BDF(3), see (3.32), one obtains the characteristic polynomial

$$\lambda^3 - \frac{18}{11}\lambda^2 + \frac{9}{11}\lambda - \frac{2}{11}.$$

  By inserting, one checks that $\lambda_1 = 1$ is a root of this polynomial. Extracting the linear factor with this root yields

$$\frac{\lambda^3 - \frac{18}{11}\lambda^2 + \frac{9}{11}\lambda - \frac{2}{11}}{\lambda - 1} = \lambda^2 - \frac{7}{11}\lambda + \frac{2}{11}.$$

  The remaining roots are given by the roots of the quadratic polynomial, which are

$$\lambda_2 = \frac{7 + i\sqrt{39}}{22}, \quad \lambda_3 = \frac{7 - i\sqrt{39}}{22},$$

  such that $|\lambda_2| = |\lambda_3| = \sqrt{22}/11 \approx 0.4264$.

■

Remark 3.34. Null stability of BDF(q) methods. It can be shown that BDF(q) methods are null stable only for $q \leq 6$, e.g., see Cryer (1972). Hence, BDF(q) methods for $q > 6$ are not of interest. □

Lemma 3.35. Consistency of BDF(q) methods. *BDF(q) methods with $q \leq 6$ are consistent of order q.*

Proof. The proof is obtained by a Taylor series expansion (*exercise*). ■

Theorem 3.36. Convergence of BDF(q) methods. *Let $f \in C^q([a,b] \times \mathbb{R})$ and Lipschitz continuous with respect to the second argument, then the BDF(q) methods with $q \le 6$ are convergent of order q.*

Proof. The incremental function of BDF(q) methods is

$$\Phi(x_{k+1}, \ldots, x_{k+1-q}, y_{k+1}, \ldots, y_{k+1-q}, h) = f\left(x_{k+1}, y_{k+1}\right),$$

such that the assumptions of Theorem 3.27 are satisfied. Because BDF(q) methods with $q \le 6$ are null stable and consistent of order q, the other assumptions of Theorem 3.29 are also satisfied and the statement of the theorem follows now from Theorem 3.29. ■

Remark 3.37. On the stability. Stability of multi-step methods is studied at the same initial value problem (2.7) as it was used for one-step methods. In the same way as in Example 3.17, one obtains a homogeneous difference equation

$$y_{k+1} - \sum_{j=0}^{q-1} a_j y_{k-j} = z \sum_{j=-1}^{q-1} b_j y_{k-j}$$

with $z = \lambda h$. With the ansatz $y_k = \xi^k$ and after division by ξ^{k+1-q}, one obtains a characteristic equation

$$\Psi(\xi) - z\sigma(\xi) = 0, \tag{3.33}$$

compare (3.16), where $\Psi(\xi)$ is the first characteristic polynomial (3.18). The polynomial σ has the coefficients b_j, compare (3.19).

Note that for $z = 0$, only the roots of the first characteristic polynomial are considered, which are important for the null stability of the method. This relation might be the reason for the notion 'null' stable. □

Definition 3.38. Stability domain. The set

$$S = \big\{ z \in \mathbb{C} \ : \ \text{for all roots } \xi_l \text{ of (3.33) it holds } |\xi_l| \le 1; \\ \text{if } \xi_l \text{ is a multiple root, then it holds } |\xi_l| < 1 \ \big\}$$

is called stability domain of a linear multi-step method. □

Definition 3.39. A-stability, $A(\alpha)$-stability. A linear multi-step method is called A-stable if $\mathbb{C}^- \subset S$. It is called $A(\alpha)$-stable with $\alpha \in (0, \pi/2)$ if

$$\big\{ z \in \mathbb{C}^- \text{ with } |\arg(z) - \pi| \le \alpha \big\} \subset S,$$

with $\arg(z) \in [0, 2\pi)$. □

Theorem 3.40 (Second Dahlquist barrier). *An A-stable linear multi-step method is at most of second order.*

Table 3.1 Values of α (in degree) for the A(α)-stability of BDF(q) methods.

q	1	2	3	4	5	6
α	90	90	86.03	73.35	51.84	17.84

Proof. See literature, e.g., (Strehmel *et al.*, 2012, Section 9.1). ■

Remark 3.41. A(α)-stability of BDF(q) methods. BDF(q) methods are $A(\alpha)$-stable for $q \le 6$ and even A-stable for $q \le 2$. The values of α for BDF(q) methods are given in Table 3.1. Because of the small value of α for $q = 6$, the method BDF(6) is not used in practice. □

Remark 3.42. Variable step size for BDF(q) methods. BDF(q) methods can be used on non-equidistant grids, e.g., a formula for BDF(2) with variable step size can be derived on the basis of the quadratic interpolation polynomial (3.30). For $q > 1$ there is some restriction on the admissible change of the mesh size from one mesh cell to its neighbor, e.g., for BDF(2) stability is guaranteed as long as $h_{k+1}/h_k \le 2.41421$, see (Strehmel *et al.*, 2012, p. 328) for more details. □

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. 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, 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.
- *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 and they require fewer evaluations of the right-hand side. 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 sometimes BDF2. An efficient and theoretically supported step length control is not possible with these methods. Other methods, like Rosenbrock schemes, are 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 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 the singularly perturbed problem (4.5), the parameter ε appears. Setting then $\varepsilon = 0$ in these formulations leads to methods for the DAE (4.3). Now, one has to study the properties of these methods. □