

# Appendix

# Appendix A

## List of Symbols

In this appendix, we collect a list of all the symbols that have been used in this book. If necessary, cross-references are also given.

### Functions

- $\|\cdot\|_\infty$  Chebyshev norm;  $\|f\|_\infty = \sup_{a \leq x \leq b} |f(x)|$
- $\|\cdot\|_p$   $L_p$  norm ( $1 \leq p < \infty$ );  $\|f\|_p = (\int_a^b |f(x)|^p dx)^{1/p}$
- $\lfloor \cdot \rfloor$  Floor function,  $\lfloor x \rfloor = \max\{z \in \mathbb{Z} : z \leq x\}$
- $\lceil \cdot \rceil$  Ceiling function,  $\lceil x \rceil = \min\{z \in \mathbb{Z} : z \geq x\}$
- $\binom{n}{k}$  Binomial coefficient,  $\binom{n}{k} = n(n-1)(n-2) \cdots (n-k+1)/k!$   
for  $n \in \mathbb{R}$  and  $k \in \mathbb{N}_0$
- $B_N[f]$   $N$ th Bernstein polynomial for the function  $f$ ,  
 $B_N[f](t) = \sum_{k=0}^N \binom{N}{k} t^k (1-t)^{N-k} f(k/N)$  (see Appendix D.5)
- $B$  Euler's Beta function,  $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$   
(cf. Appendix D.1)
- $\Gamma$  Euler's Gamma function,  $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$   
(cf. Definition 1.2)
- $\psi$  Digamma function,  $\psi(x) = \Gamma'(x)/\Gamma(x)$
- $E_n$  Mittag-Leffler function of order  $n$ ,  
 $E_n(x) = \sum_{j=0}^\infty x^j / \Gamma(jn+1)$  (cf. Definition 4.1)
- $E_{n_1, n_2}$  two-parameter Mittag-Leffler function,  
 $E_{n_1, n_2}(x) = \sum_{j=0}^\infty x^j / \Gamma(jn_1 + n_2)$  (cf. Definition 4.2)
- ${}_1F_1$  Kummer's confluent hypergeometric function [2, Chapter 13],  
 ${}_1F_1(a; b; z) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{k=0}^\infty \frac{\Gamma(a+k)}{\Gamma(b+k)k!} z^k \quad (a \in \mathbb{R}, -b \notin \mathbb{N}_0)$

- ${}_2F_1$  Gauss' hypergeometric function [2, Chapter 15],  

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{k=0}^{\infty} \frac{\Gamma(a+k)\Gamma(b+k)}{\Gamma(c+k)k!} z^k \quad (a, b \in \mathbb{R}, -c \notin \mathbb{N}_0)$$
- $o, O$  Landau symbols
- $T_j[f; a]$  Taylor polynomial of degree  $j$  for the function  $f$   
 centered at the point  $a$

## Sets

- $A^n, A^n[a, b]$  Set of functions with absolutely continuous derivative of  
 order  $n - 1$  (cf. Definition 1.5)
- $C, C[a, b]$  Set of continuous functions (cf. Definition 1.3)
- $C^k, C^k[a, b]$  Set of functions with continuous  $k$ th derivative  
 (cf. Definition 1.3)
- $H^*, H^*[a, b]$  Cf. Definition 1.4
- $H_\mu, H_\mu[a, b]$  Hölder space (cf. Definition 1.3)
- $L_p, L_p[a, b]$  Lebesgue space (cf. Definition 1.3)
- $\mathbb{N}$   $= \{1, 2, 3, \dots\}$ , the set of natural numbers
- $\mathbb{N}_0$   $= \mathbb{N} \cup \{0\}$
- $\mathbb{R}$  The set of real numbers
- $\mathbb{R}_+$   $= \{x \in \mathbb{R} : x > 0\}$ , the set of strictly positive real numbers
- $\mathbb{Z}$   $= \{0, \pm 1, \pm 2, \pm 3, \dots\}$ , the set of integer numbers

## Operators

- $\Delta_h^n$  Finite difference of order  $n$ ; cf. (2.11)
- $D$  Differential operator,  $Df(x) = f'(x)$  (cf. Definition 1.1)
- $D^n$   $n \in \mathbb{N}$ :  $n$ -fold iterate of the differential operator  $D$  (cf. Definition 1.1)
- $D_a^n$   $n \in \mathbb{R}_+$ : Riemann–Liouville fractional differential operator (cf. Definition 2.2)
- $\hat{D}_a^n$   $n \in \mathbb{R}_+$ : Grünwald–Letnikov fractional differential operator (cf. Definition 2.3)
- $\hat{D}_a^n$  Cf. Definition 3.1
- $D_{*a}^n$   $n \in \mathbb{R}_+$ : Caputo fractional differential operator (cf. Definition 3.2)
- $\mathcal{D}^n$   $n \in \mathbb{R}_+$ : Gel'fond–Leont'ev operator (cf. Definition 3.3)
- $I$  Identity operator
- $J_a$  Integral operator,  $J_a f(x) = \int_a^x f(t) dt$  (cf. Definition 1.1)

- $J_a^n$   $n \in \mathbb{N}$ :  $n$ -fold iterate of the integral operator  $J_a$  (cf. Definition 1.1)  
 $n \in \mathbb{R}_+ \setminus \mathbb{N}$ : Riemann–Liouville fractional integral operator (cf. Definition 2.1)  
 $n = 0$ : identity operator (cf. Definition 2.1)  
 $\tilde{J}_a^n$   $n \in \mathbb{R}_+$ : Grünwald–Letnikov fractional integral operator  
 (cf. Definition 2.4)  
 $\mathcal{L}$  Laplace transform operator (cf. Appendix D.3)  
 $\omega$  Modulus of continuity of the function  $g : [a, b] \rightarrow \mathbb{R}$ ,  
 $\omega(g; h) := \sup\{|g(y_1) - g(y_2)| : y_1, y_2 \in [a, b], |y_1 - y_2| \leq h\}$

## Other Symbols

$$\sim \quad a_j \sim b_j \Leftrightarrow \exists A, B > 0 \exists j_0 \in \mathbb{N} \forall j \geq j_0 : A \leq |a_j/b_j| \leq B$$

## Remarks

1. The power series for both types of Mittag-Leffler functions converge in the entire complex plane (cf. Theorem 4.1).
2. The power series for Kummer's confluent hypergeometric function converges in the entire complex plane.
3. For the Gauss hypergeometric function, the power series converges for all complex  $z$  with  $|z| < 1$  and may be extended analytically into the entire complex plane with a branch cut along the positive real axis from  $+1$  to  $+\infty$ . (In the formulas in Appendix B, we need to evaluate this function for  $z < 0$ , so the branch cut for  $z \geq 1$  gives no problems.)

## Appendix B

### A Table of Caputo Derivatives

For the convenience of the reader, we provide this appendix where we give some Caputo-type derivatives of certain important functions. We do not strive for completeness in any sense, but we do want to give at least the derivatives of the classical examples.

Throughout this appendix,  $n$  will always denote the order of the Caputo-type differential operator under consideration. We shall only consider the case  $n > 0$  and  $n \notin \mathbb{N}$ , and we use the notation  $m := \lceil n \rceil$  to denote the smallest integer greater than (or equal to)  $n$ . Recall that for  $n \in \mathbb{N}$ , the Caputo differential operator coincides with the usual differential operator of integer order, and for  $n < 0$ , the Caputo differential operator of negative order can be interpreted as the Riemann–Liouville differential operator of the same order. Tables of the latter are given in various places in the literature (cf., e.g., Podlubny [153] or Samko et al. [167]); we are not going to repeat those results here.

Various special functions will arise in this connection; for the precise definitions we refer to Appendix A. By  $i = \sqrt{-1}$  we denote the imaginary unit.

1. Let  $f(x) = x^j$ . Here we have to distinguish some cases:

$$(D_{*0}^n f)(x) = \begin{cases} 0 & \text{if } j \in \mathbb{N}_0 \text{ and } j < m, \\ \frac{\Gamma(j+1)}{\Gamma(j+1-n)} x^{j-n} & \text{if } j \in \mathbb{N}_0 \text{ and } j \geq m \\ \text{or } j \notin \mathbb{N} \text{ and } j > m-1. \end{cases}$$

2. Let  $f(x) = (x+c)^j$  for arbitrary  $c > 0$  and  $j \in \mathbb{R}$ . Then

$$(D_{*0}^n f)(x) = \frac{\Gamma(j+1)}{\Gamma(j+1-m)} \frac{c^{j-m-1} x^{m-n}}{\Gamma(m-n+1)} {}_2F_1(1, m-j; m-n+1; -x/c).$$

3. Let  $f(x) = \exp(jx)$  for some  $j \in \mathbb{R}$ . Then

$$(D_{*0}^n f)(x) = j^m x^{m-n} E_{1, m-n+1}(jx).$$

4. Let  $f(x) = x^j \ln x$  for some  $j > m - 1$ . Then

$$(D_{*0}^n f)(x) = x^{j-n} \sum_{k=0}^{m-1} (-1)^{m-k+1} \binom{j}{k} \frac{m!}{m-k} \frac{\Gamma(j-m+1)}{\Gamma(j-n+1)} \\ + \frac{\Gamma(j+1)}{\Gamma(j-n+1)} x^{j-n} (\psi(j-m+1) - \psi(j-n+1) + \ln x).$$

5. Let  $f(x) = \sin jx$  for some  $j \in \mathbb{R}$ . Here again we have two cases:

$$(D_{*0}^n f)(x) = \begin{cases} \frac{j^m i (-1)^{m/2} x^{m-n}}{2\Gamma(m-n+1)} [-{}_1F_1(1; m-n+1; i jx) \\ \quad + {}_1F_1(1; m-n+1; -i jx)] & (m \text{ even}), \\ \frac{j^m (-1)^{(m-1)/2} x^{m-n}}{2\Gamma(m-n+1)} [{}_1F_1(1; m-n+1; i jx) \\ \quad + {}_1F_1(1; m-n+1; -i jx)] & (m \text{ odd}). \end{cases}$$

6. Finally we consider  $f(x) = \cos jx$  with some  $j \in \mathbb{R}$ . As in the previous example, we obtain two cases:

$$(D_{*0}^n f)(x) = \begin{cases} \frac{j^m (-1)^{m/2} x^{m-n}}{2\Gamma(m-n+1)} [{}_1F_1(1; m-n+1; i jx) \\ \quad + {}_1F_1(1; m-n+1; -i jx)] & (m \text{ even}), \\ \frac{j^m i (-1)^{(m-1)/2} x^{m-n}}{2\Gamma(m-n+1)} [{}_1F_1(1; m-n+1; i jx) \\ \quad - {}_1F_1(1; m-n+1; -i jx)] & (m \text{ odd}). \end{cases}$$

# Appendix C

## Numerical Solution of Fractional Differential Equations

For most fractional differential equations we cannot provide methods to compute the exact solutions analytically. Therefore it is necessary to revert to numerical methods. In order to give the reader a tool that can be applied to a very wide class of equations, we now present a method that is well understood and that has proven to be efficient in many practical applications [50, 51, 65, 182, 183]. We begin by discussing this problem for single-term equations and later extend our idea to multi-term problems.

### C.1 An Algorithm for Single-Term Equations

The method can be called *indirect* because, rather than discretizing the differential equation

$$D_{*0}^n y(x) = f(x, y(x))$$

with appropriate initial conditions

$$D^k y(0) = y_0^{(k)}, \quad k = 0, 1, \dots, [n] - 1,$$

directly, it requires some preliminary analytical manipulation, namely an application of Lemma 6.2 in order to convert the initial value problem for the differential equation into an equivalent Volterra integral equation,

$$y(x) = \sum_{k=0}^{m-1} \frac{x^k}{k!} D^k y(0) + \frac{1}{\Gamma(n)} \int_0^x (x-t)^{n-1} f(t, y(t)) dt \quad (\text{C.1})$$

where  $m = [n]$ . We shall therefore now look at a method for the numerical solution of (C.1).

The algorithm that we shall consider can be interpreted as a fractional variant of the classical second-order Adams–Bashforth–Moulton method. It has been introduced and briefly discussed in [50]; more information is given in [51]. Some additional results for a specific initial value problem are contained in [44], a detailed mathematical analysis is provided in [49], and additional practical remarks can be

found in [48]. Numerical experiments and comparisons with other methods are reported in [52, 65, 182, 183]. Here we shall give an even more detailed analysis under quite general assumptions.

*Remark C.1.* Before starting the investigations, we need to give a note of caution. It is common to construct methods for fractional differential equations by taking methods for classical (typically first-order) equations and then generalizing the concepts in an appropriate way. The resulting formulas are then usually given the same name as the underlying classical algorithm, possibly extended by the adjective “fractional”. However, many classical numerical schemes can be extended in more than one way. This may lead to the problem that, in two different items of literature, two different algorithms are denoted in identical ways. Of course, this is a potential source for confusion, and the reader must be very careful in this respect. For example, the fractional Adams–Moulton rules of Galeone and Garrappa [70] do not coincide with the methods of the same name that we shall develop below.

### *Classical Formulation*

In order to motivate the construction of the method, we shall first briefly recall the idea behind the classical Adams–Bashforth–Moulton algorithm for first-order equations. So, for a start, we focus our attention on the well-known initial-value problem for the first-order differential equation

$$Dy(x) = f(x, y(x)), \quad (\text{C.2a})$$

$$y(0) = y_0. \quad (\text{C.2b})$$

We assume the function  $f$  to be such that a unique solution exists on some interval  $[0, T]$ , say. Following [88, §III.1], we suggest to use the predictor-corrector technique of Adams where, for the sake of simplicity, we assume that we are working on a uniform grid  $\{t_j = jh : j = 0, 1, \dots, N\}$  with some integer  $N$  and  $h = T/N$ . In some applications it may be more efficient to use a non-uniform grid, and we will develop the numerical approximation formulas in this generalized sense. However, for the subsequent analysis of the properties of the scheme we will then restrict ourselves to the equispaced case.

The basic idea is, assuming that we have already calculated approximations  $y_j \approx y(t_j)$  ( $j = 1, 2, \dots, k$ ), that we try to obtain the approximation  $y_{k+1}$  by means of the equation

$$y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(z, y(z)) dz. \quad (\text{C.3})$$

This equation follows upon integration of (C.2a) on the interval  $[t_k, t_{k+1}]$ . Of course, we know neither of the expressions on the right-hand side of (C.3) exactly, but we do have an approximation for  $y(t_k)$ , namely  $y_k$ , that we can use instead. The integral is then replaced by the two-point trapezoidal quadrature formula



$$\int_a^b g(z) dz \approx \frac{b-a}{2} (g(a) + g(b)), \quad (\text{C.4})$$

thus giving an equation for the unknown approximation  $y_{k+1}$ , it being

$$y_{k+1} = y_k + \frac{t_{k+1} - t_k}{2} (f(t_k, y(t_k)) + f(t_{k+1}, y(t_{k+1}))), \quad (\text{C.5})$$

where again we have to replace  $y(t_k)$  and  $y(t_{k+1})$  by their approximations  $y_k$  and  $y_{k+1}$ , respectively. This yields the equation for the implicit one-step *Adams–Moulton method*, which is

$$y_{k+1} = y_k + \frac{t_{k+1} - t_k}{2} (f(t_k, y_k) + f(t_{k+1}, y_{k+1})). \quad (\text{C.6})$$

The problem with this equation is that the unknown quantity  $y_{k+1}$  appears on both sides, and due to the nonlinear nature of the function  $f$ , we cannot solve for  $y_{k+1}$  directly in general. Therefore, we may use (C.6) in an iterative process, inserting a preliminary approximation for  $y_{k+1}$  in the right-hand side in order to determine a better approximation that we can then use.

The preliminary approximation  $y_{k+1}^P$ , the so-called predictor, is obtained in a very similar way, only replacing the trapezoidal quadrature formula by the rectangle rule

$$\int_a^b g(z) dz \approx (b-a)g(a), \quad (\text{C.7})$$

giving the explicit (forward Euler or one-step *Adams–Bashforth*) method

$$y_{k+1}^P = y_k + hf(t_k, y_k). \quad (\text{C.8})$$

It is well known [88, p. 372] that the process defined by (C.8) and

$$y_{k+1} = y_k + \frac{h}{2} (f(t_k, y_k) + f(t_{k+1}, y_{k+1}^P)), \quad (\text{C.9})$$

known as the one-step *Adams–Bashforth–Moulton* technique, is convergent of order 2, i.e.

$$\max_{j=1,2,\dots,N} |y(t_j) - y_j| = O(h^2). \quad (\text{C.10})$$

Moreover, this method behaves satisfactorily from the point of view of its numerical stability [89, Chap. IV]. It is said to be of the PECE (Predict, Evaluate, Correct, Evaluate) type because, in a concrete implementation, we would start by calculating the predictor in (C.8), then we evaluate  $f(t_{k+1}, y_{k+1}^P)$ , use this to calculate the corrector in (C.9), and finally evaluate  $f(t_{k+1}, y_{k+1})$ . This result is stored for future use in the next integration step.

## Fractional Formulation

Having introduced this concept, we now try to carry over the essential ideas to the fractional-order problem with some unavoidable modifications. The key is to derive an equation similar to (C.3). Fortunately, such an equation is available, namely (C.1). This equation looks somewhat different from (C.3), because the range of integration now starts at 0 instead of  $t_k$ . This is a consequence of the non-local structure of the fractional-order differential operators. This however does not cause major problems in our attempts to generalize the Adams method. What we do is simply use the product trapezoidal quadrature formula to replace the integral, i.e. we use the nodes  $t_j$  ( $j = 0, 1, \dots, k+1$ ) and interpret the function  $(t_{k+1} - \cdot)^{n-1}$  as a weight function for the integral. In other words, we apply the approximation

$$\int_0^{t_{k+1}} (t_{k+1} - z)^{n-1} g(z) dz \approx \int_0^{t_{k+1}} (t_{k+1} - z)^{n-1} \tilde{g}_{k+1}(z) dz, \quad (\text{C.11})$$

where  $\tilde{g}_{k+1}$  is the piecewise linear interpolant for  $g$  with nodes and knots chosen at the  $t_j$ ,  $j = 0, 1, 2, \dots, k+1$ .

It is clear by construction that the required weighted trapezoidal quadrature formula can be represented as a weighted sum of function values of the integrand  $g$ , taken at the points  $t_j$ . Specifically, we find that we can write the integral on the right-hand side of (C.11) as

$$\int_0^{t_{k+1}} (t_{k+1} - z)^{n-1} \tilde{g}_{k+1}(z) dz = \sum_{j=0}^{k+1} a_{j,k+1} g(t_j) \quad (\text{C.12a})$$

where

$$a_{j,k+1} = \int_0^{t_{k+1}} (t_{k+1} - z)^{n-1} \phi_{j,k+1}(z) dz \quad (\text{C.12b})$$

and

$$\phi_{j,k+1}(z) = \begin{cases} (z - t_{j-1})/(t_j - t_{j-1}) & \text{if } t_{j-1} < z \leq t_j, \\ (t_{j+1} - z)/(t_{j+1} - t_j) & \text{if } t_j < z < t_{j+1}, \\ 0 & \text{else.} \end{cases} \quad (\text{C.12c})$$

This is clear because the functions  $\phi_{j,k+1}$  satisfy

$$\phi_{j,k+1}(t_\mu) = \begin{cases} 0 & \text{if } j \neq \mu, \\ 1 & \text{if } j = \mu, \end{cases}$$

and that they are continuous and piecewise linear with breakpoints at the nodes  $t_\mu$ , so that they must be integrated exactly by our formula.

An easy explicit calculation yields that, for an arbitrary choice of the  $t_j$ , (C.12b) and (C.12c) produce

$$a_{0,k+1} = \frac{(t_{k+1} - t_1)^{n+1} + t_{k+1}^n [nt_1 + t_1 - t_{k+1}]}{t_1 n(n+1)}, \quad (\text{C.13a})$$

$$a_{j,k+1} = \frac{(t_{k+1} - t_{j-1})^{n+1} + (t_{k+1} - t_j)^n [n(t_{j-1} - t_j) + t_{j-1} - t_{k+1}]}{(t_j - t_{j-1})n(n+1)} + \frac{(t_{k+1} - t_{j+1})^{n+1} - (t_{k+1} - t_j)^n [n(t_j - t_{j+1}) - t_{j+1} + t_{k+1}]}{(t_{j+1} - t_j)n(n+1)}, \quad (\text{C.13b})$$

if  $1 \leq j \leq k$ , and

$$a_{k+1,k+1} = \frac{(t_{k+1} - t_k)^n}{n(n+1)}. \quad (\text{C.13c})$$

In the case of equispaced nodes ( $t_j = jh$  with some fixed  $h$ ), these relations reduce to

$$a_{j,k+1} = \begin{cases} \frac{h^n}{n(n+1)} (k^{n+1} - (k-n)(k+1)^n) & \text{if } j = 0, \\ \frac{h^n}{n(n+1)} ((k-j+2)^{n+1} + (k-j)^{n+1} - 2(k-j+1)^{n+1}) & \text{if } 1 \leq j \leq k, \\ \frac{h^n}{n(n+1)} & \text{if } j = k+1. \end{cases} \quad (\text{C.14})$$

This then gives us our corrector formula (i.e. the fractional variant of the one-step *Adams–Moulton method*), which is

$$y_{k+1} = \sum_{j=0}^{m-1} \frac{t_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(n)} \left( \sum_{j=0}^k a_{j,k+1} f(t_j, y_j) + a_{k+1,k+1} f(t_{k+1}, y_{k+1}^p) \right). \quad (\text{C.15})$$

The remaining problem is the determination of the predictor formula that we require to calculate the value  $y_{k+1}^p$ . The idea we use to generalize the one-step Adams–Bashforth method is the same as the one described above for the Adams–Moulton technique: We replace the integral on the right-hand side of (C.1) by the product rectangle rule

$$\int_0^{t_{k+1}} (t_{k+1} - z)^{n-1} g(z) dz \approx \sum_{j=0}^k b_{j,k+1} g(t_j), \quad (\text{C.16})$$

where now

$$b_{j,k+1} = \int_{t_j}^{t_{j+1}} (t_{k+1} - z)^{n-1} dz = \frac{(t_{k+1} - t_j)^n - (t_{k+1} - t_{j+1})^n}{n}. \quad (\text{C.17})$$

This expression for weights can be derived in a way similar to the method used in the derivation of (C.13). However, here we are dealing with a piecewise constant approximation and not a piecewise linear one, and hence we have to replace the “hat-shaped” functions  $\phi_{kj}$  by functions being of constant value 1 on  $[t_j, t_{j+1}]$  and 0

on the remaining parts of the interval  $[0, t_{k+1}]$ . Again, in the equispaced case, we have the simpler expression

$$b_{j,k+1} = \frac{h^n}{n} ((k+1-j)^n - (k-j)^n). \quad (\text{C.18})$$

Thus, the predictor  $y_{k+1}^P$  is determined by the fractional *Adams–Bashforth method*

$$y_{k+1}^P = \sum_{j=0}^{m-1} \frac{t_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(n)} \sum_{j=0}^k b_{j,k+1} f(t_j, y_j). \quad (\text{C.19})$$

Our basic algorithm, the fractional *Adams–Bashforth–Moulton method*, is therefore completely described now by (C.19) and (C.15) with the weights  $a_{j,k+1}$  and  $b_{j,k+1}$  being defined according to (C.13) and (C.17), respectively.

## Error Analysis

For the error analysis of this algorithm, we restrict our attention to the case of an equispaced grid, i.e. from now on we assume that  $t_j = jh = jT/N$  with some  $N \in \mathbb{N}$ . Essentially we follow the structure of [49] and begin by stating some auxiliary results.

What we need for our purposes is some information on the errors of the quadrature formulas that we have used in the derivation of the predictor and the corrector, respectively. We first give a statement on the product rectangle rule that we have used for the predictor.

**Theorem C.1.** (a) Let  $z \in C^1[0, T]$ . Then,

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \leq \frac{1}{n} \|z'\|_{\infty} t_{k+1}^n h.$$

(b) Let  $z(t) = t^p$  for some  $p \in (0, 1)$ . Then,

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \leq C_{n,p}^{\text{Re}} t_{k+1}^{n+p-1} h$$

where  $C_{n,p}^{\text{Re}}$  is a constant that depends only on  $n$  and  $p$ .

*Proof.* By construction of the product rectangle formula, we find in both cases that the quadrature error has the representation

$$\begin{aligned}
& \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \\
&= \sum_{j=0}^k \int_{jh}^{(j+1)h} (t_{k+1} - t)^{n-1} (z(t) - z(t_j)) dt. \tag{C.20}
\end{aligned}$$

To prove statement (a), we apply the Mean Value Theorem of Differential Calculus to the second factor of the integrand on the right-hand side of (C.20) and derive

$$\begin{aligned}
& \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \\
& \leq \|z'\|_\infty \sum_{j=0}^k \int_{jh}^{(j+1)h} (t_{k+1} - t)^{n-1} (t - jh) dt \\
& = \|z'\|_\infty \frac{h^{1+n}}{n} \sum_{j=0}^k \left( \frac{1}{1+n} [(k+1-j)^{1+n} - (k-j)^{1+n}] - (k-j)^n \right) \\
& = \|z'\|_\infty \frac{h^{1+n}}{n} \left( \frac{(k+1)^{1+n}}{1+n} - \sum_{j=0}^k j^n \right) \\
& = \|z'\|_\infty \frac{h^{1+n}}{n} \left( \int_0^{k+1} t^n dt - \sum_{j=0}^k j^n \right).
\end{aligned}$$

Here the term in parentheses is simply the remainder of the standard rectangle quadrature formula, applied to the function  $t^n$ , and taken over the interval  $[0, k+1]$ . Since the integrand is monotonic, we may apply some standard results from quadrature theory [19, Thm. 97] to find that this term is bounded by the total variation of the integrand, viz. the quantity  $(k+1)^n$ . Thus,

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \leq \|z'\|_\infty \frac{h^{1+n}}{n} (k+1)^n.$$

Similarly, to prove (b), we use the monotonicity of  $z$  in (C.20) and derive

$$\begin{aligned}
& \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \\
& \leq \sum_{j=0}^k |z(t_{j+1}) - z(t_j)| \int_{jh}^{(j+1)h} (t_{k+1} - t)^{n-1} dt \\
& = \frac{h^{n+p}}{n} \sum_{j=0}^k ((j+1)^p - j^p)((k+1-j)^n - (k-j)^n)
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{h^{n+p}}{n} \left( (k+1)^n - k^n + (k+1)^p - k^p + pn \sum_{j=1}^{k-1} j^{p-1} (k-j+q)^{n-1} \right) \\
&\leq \frac{h^{n+p}}{n} \left( n(k+q)^{n-1} + pk^{p-1} + pn \sum_{j=1}^{k-1} j^{p-1} (k-j+q)^{n-1} \right)
\end{aligned}$$

by additional applications of the Mean Value Theorem. Here  $q = 0$  if  $n \leq 1$ , and  $q = 1$  otherwise. In either case a brief asymptotic analysis using the Euler–MacLaurin formula [188, Thm. 3.7] yields that the term in parentheses is bounded from above by  $C_{n,p}^{\text{Re}}(k+1)^{p+n-1}$  where  $C_{n,p}^{\text{Re}}$  is a constant depending on  $n$  and  $p$  but not on  $k$ .  $\square$

Next we come to a corresponding result for the product trapezoidal formula that we have used for the corrector. The proof of this theorem is very similar to the proof of Theorem C.1; we therefore omit the details.

**Theorem C.2.** (a) If  $z \in C^2[0, T]$  then there is a constant  $C_n^{\text{Tr}}$  depending only on  $n$  such that

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} z(t_j) \right| \leq C_n^{\text{Tr}} \|z''\|_{\infty} t_{k+1}^n h^2.$$

(b) Let  $z \in C^1[0, T]$  and assume that  $z'$  fulfils a Lipschitz condition of order  $\mu$  for some  $\mu \in (0, 1)$ . Then, there exist positive constants  $B_{n,\mu}^{\text{Tr}}$  (depending only on  $n$  and  $\mu$ ) and  $M(z, \mu)$  (depending only on  $z$  and  $\mu$ ) such that

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} z(t_j) \right| \leq B_{n,\mu}^{\text{Tr}} M(z, \mu) t_{k+1}^n h^{1+\mu}.$$

(c) Let  $z(t) = t^p$  for some  $p \in (0, 2)$  and  $\rho := \min(2, p+1)$ . Then,

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} z(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} z(t_j) \right| \leq C_{n,p}^{\text{Tr}} t_{k+1}^{n+p-\rho} h^\rho$$

where  $C_{n,p}^{\text{Tr}}$  is a constant that depends only on  $n$  and  $p$ .

**Remark C.2.** Notice that in part (c) of Theorem C.2 it may happen that  $n < 1$  and  $p < 1$ . This implies  $\rho = p+1$ . Thus, the exponent of  $t_{k+1}$  on the right-hand side of the inequality is equal to  $n-1$  which is negative. At first sight this may seem counter-intuitive because it means that the overall integration error becomes larger if the size of the interval of integration becomes smaller. The explanation for this phenomenon is that by making  $t_{k+1}$  smaller we do not only shorten the length of the integration interval (which should lead to a smaller error) but we also change the weight function in a way that makes the integral more difficult, and this second feature leads to an increase in the error.

A similar observation can be made in Theorem C.1 (b).

We now present the main results concerning the error of our Adams scheme. It is useful to distinguish a number of cases. Specifically, we shall see that the precise behaviour of the error differs depending on whether  $n < 1$  or  $n > 1$ . Moreover, the smoothness properties of the given function  $f$  and the unknown solution  $y$  play an important role. In view of the results of Sect. 6.4, we find that smoothness of one of these functions will imply non-smoothness of the other unless some special conditions are fulfilled. Therefore we shall also investigate the error under those two different smoothness assumptions.

Based on the error estimates above we shall first present a general convergence result for the Adams–Bashforth–Moulton method. In the theorems below we shall specialize this result to particularly important special cases.

**Lemma C.3.** *Assume that the solution  $y$  of the initial value problem is such that*

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} D_{*0}^n y(t) dt - \sum_{j=0}^k b_{j,k+1} D_{*0}^n y(t_j) \right| \leq C_1 t_{k+1}^{\gamma_1} h^{\delta_1}$$

and

$$\left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} D_{*0}^n y(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} D_{*0}^n y(t_j) \right| \leq C_2 t_{k+1}^{\gamma_2} h^{\delta_2}$$

with some  $\gamma_1, \gamma_2 \geq 0$  and  $\delta_1, \delta_2 > 0$ . Then, for some suitably chosen  $T > 0$ , we have

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^q)$$

where  $q = \min\{\delta_1 + n, \delta_2\}$  and  $N = \lfloor T/h \rfloor$ .

*Proof.* We will show that, for sufficiently small  $h$ ,

$$|y(t_j) - y_j| \leq Ch^q \tag{C.21}$$

for all  $j \in \{0, 1, \dots, N\}$ , where  $C$  is a suitable constant. The proof will be based on mathematical induction. In view of the given initial condition, the induction basis ( $j = 0$ ) is presupposed. Now assume that (C.21) is true for  $j = 0, 1, \dots, k$  for some  $k \leq N - 1$ . We must then prove that the inequality also holds for  $j = k + 1$ . To do this, we first look at the error of the predictor  $y_{k+1}^P$ . By construction of the predictor we find that

$$\begin{aligned} |y(t_{k+1}) - y_{k+1}^P| &= \frac{1}{\Gamma(n)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} f(t, y(t)) dt - \sum_{j=0}^k b_{j,k+1} f(t_j, y_j) \right| \\ &\leq \frac{1}{\Gamma(n)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} D_{*0}^n y(t) dt - \sum_{j=0}^k b_{j,k+1} D_{*0}^n y(t_j) \right| \\ &\quad + \frac{1}{\Gamma(n)} \sum_{j=0}^k b_{j,k+1} |f(t_j, y(t_j)) - f(t_j, y_j)| \end{aligned}$$

$$\begin{aligned}
&\leq \frac{C_1 t_{k+1}^{\gamma_1}}{\Gamma(n)} h^{\delta_1} + \frac{1}{\Gamma(n)} \sum_{j=0}^k b_{j,k+1} L C h^q \\
&\leq \frac{C_1 T^{\gamma_1}}{\Gamma(n)} h^{\delta_1} + \frac{CLT^n}{\Gamma(n+1)} h^q.
\end{aligned} \tag{C.22}$$

Here we have used the Lipschitz property of  $f$ , the assumption on the error of the rectangle formula, and the facts that, by construction of the quadrature formula underlying the predictor,  $b_{j,k+1} > 0$  for all  $j$  and  $k$  and

$$\sum_{j=0}^k b_{j,k+1} = \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} dt = \frac{1}{n} t_{k+1}^n \leq \frac{1}{n} T^n.$$

On the basis of the bound (C.22) for the predictor error we begin the analysis of the corrector error. We recall the relation (C.14) which we shall use in particular for  $j = k + 1$  and find, arguing in a similar way to above, that

$$\begin{aligned}
&|y(t_{k+1}) - y_{k+1}| \\
&= \frac{1}{\Gamma(n)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} f(t, y(t)) dt \right. \\
&\quad \left. - \sum_{j=0}^k a_{j,k+1} f(t_j, y_j) - a_{k+1,k+1} f(t_{k+1}, y_{k+1}^p) \right| \\
&\leq \frac{1}{\Gamma(n)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{n-1} D_{*0}^n y(t) dt - \sum_{j=0}^{k+1} a_{j,k+1} D_{*0}^n y(t_j) \right| \\
&\quad + \frac{1}{\Gamma(n)} \sum_{j=0}^k a_{j,k+1} |f(t_j, y(t_j)) - f(t_j, y_j)| \\
&\quad + \frac{1}{\Gamma(n)} a_{k+1,k+1} |f(t_{k+1}, y(t_{k+1})) - f(t_{k+1}, y_{k+1}^p)| \\
&\leq \frac{C_2 t_{k+1}^{\gamma_2}}{\Gamma(n)} h^{\delta_2} + \frac{CL}{\Gamma(n)} h^q \sum_{j=0}^k a_{j,k+1} + a_{k+1,k+1} \frac{L}{\Gamma(n)} \left( \frac{C_1 T^{\gamma_1}}{\Gamma(n)} h^{\delta_1} + \frac{CLT^n}{\Gamma(n+1)} h^q \right) \\
&\leq \left( \frac{C_2 T^{\gamma_2}}{\Gamma(n)} + \frac{CLT^n}{\Gamma(n+1)} + \frac{C_1 LT^{\gamma_1}}{\Gamma(n)\Gamma(n+2)} + \frac{CL^2 T^n}{\Gamma(n+1)\Gamma(n+2)} h^n \right) h^q
\end{aligned}$$

in view of the nonnegativity of  $\gamma_1$  and  $\gamma_2$  and the relations  $\delta_2 \leq q$  and  $\delta_1 + n \leq q$ . By choosing  $T$  sufficiently small, we can make sure that the second summand in the parentheses is bounded by  $C/2$ . Having fixed this value for  $T$ , we can then make the sum of the remaining expressions in the parentheses smaller than  $C/2$  too (for sufficiently small  $h$ ) simply by choosing  $C$  sufficiently large. It is then obvious that the entire upper bound does not exceed  $Ch^q$ .  $\square$

As a first application of this Lemma we assume that the given data is such that the solution  $y$  itself is sufficiently differentiable. As mentioned above, the result depends on whether  $n > 1$  or  $n < 1$ .



**Theorem C.4.** Let  $0 < n$  and assume  $D_{*0}^n y \in C^2[0, T]$  for some suitable  $T$ . Then,

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = \begin{cases} O(h^2) & \text{if } n \geq 1, \\ O(h^{1+n}) & \text{if } n < 1. \end{cases}$$

Before we come to the proof, we note one particular point: The order of convergence depends on  $n$ , and it is a non-decreasing function of  $n$ . This is due to the fact that we discretize the integral operator in (C.1) which behaves more smoothly (and hence can be approximated with a higher accuracy) as  $n$  increases. In contrast, so-called *direct methods* like the backward differentiation method of [34] use a different approach; as the name suggests they directly discretize the differential operator in the given initial value problem. The smoothness properties of such operators (and thus the ease with which they may be approximated) deteriorate as  $n$  increases, and so we find that the convergence order of the method from [34] is a non-increasing function of  $n$ ; in particular no convergence is achieved there for  $n \geq 2$ . It is a distinctive advantage of the Adams scheme presented here that it converges for all  $n > 0$ .

*Remark C.3.* We formally recover the error bound (C.10) if we set  $n = 1$ .

*Proof (of Theorem C.4).* In view of Theorems C.1 and C.2, we may apply Lemma C.3 with  $\gamma_1 = \gamma_2 = n > 0$ ,  $\delta_1 = 1$  and  $\delta_2 = 2$ . Thus, defining

$$q = \min\{1 + n, 2\} = \begin{cases} 2 & \text{if } n \geq 1, \\ 1 + n & \text{if } n < 1, \end{cases}$$

we find an  $O(h^q)$  error bound. □

Note that in a certain sense the theorem above deals with the “optimal” situation: The function that we approximate in our process is  $f(\cdot, y(\cdot)) = D_{*0}^n y$ . In order to obtain very good error bounds, we need to make sure that the quadrature errors for this function are (asymptotically) as small as possible. A sufficient condition for this to hold is, as is well known from quadrature theory [19], that this function is in  $C^2$  on the interval of integration. This is precisely the setting discussed in Theorem C.4. So this theorem shows us what kind of performance the Adams method can give under optimal circumstances, and it also states sufficient conditions for such results to hold.

An objection against the use of this Adams–Bashforth–Moulton scheme may be the very slow rate of convergence if  $n$  is close to 0. However, a careful inspection of the proof of the error bound reveals a fact that is well known in the error analysis for methods of this structure for first-order equations (cf., e.g., [179]): The application of the corrector formula improves the accuracy of its input (the predictor) by a factor of  $h^n$  until an order of  $O(h^2)$  (i.e. a saturation) is reached. Thus we may replace the plain PECE structure by a P(EC) $^\mu$ E method, i.e. by introducing additional corrector iterations.

*Remark C.4.* An interesting observation here is that by choosing a larger number of corrector iterations, we essentially leave the computational complexity unchanged: A corrector iteration is of the form

$$y_{j+1}^{[\ell]} = \sum_{r=0}^{[n]-1} \frac{t_{j+1}^r}{r!} y_0^{(r)} + \frac{h^n}{\Gamma(n+2)} f(t_{j+1}, y_{j+1}^{[\ell-1]}) \\ + \frac{h^n}{\Gamma(n+2)} \sum_{r=0}^j a_{r,j+1} f(t_r, y_r),$$

cf. (C.15). Here  $y_{j+1}^{[\ell]}$  denotes the approximation after  $\ell$  corrector steps,  $y_{j+1}^{[0]} = y_{j+1}^P$  is the predictor, and  $y_{j+1} := y_{j+1}^{[\mu]}$  is the final approximation after  $\mu$  corrector steps that we actually use. We can rewrite this as

$$y_{j+1}^{[\ell]} = \beta_{j+1} + \frac{h^n}{\Gamma(n+2)} f(t_{j+1}, y_{j+1}^{[\ell-1]})$$

where

$$\beta_{j+1} = \sum_{r=0}^{[n]-1} \frac{t_{j+1}^r}{r!} y_0^{(r)} + \frac{h^n}{\Gamma(n+2)} \sum_{r=0}^j a_{r,j+1} f(t_r, y_r)$$

is independent of  $\ell$ . Thus the total arithmetic complexity of the corrector part of the  $(j+1)$ st step (taking us from  $t_j$  to  $t_{j+1}$ ) is  $O(j)$  for the calculation of  $\beta_{j+1}$  plus  $O(\mu)$  for the  $\mu$  corrector steps, which (since  $\mu$  is constant) is asymptotically the same as the complexity in the case  $\mu = 1$ .

For the error of the scheme outlined in Remark C.4 we find, as indicated above, by a repeated application of the considerations of the proof of Theorem C.4 (see [36] for details):

**Theorem C.5.** *Under the assumptions of Theorem C.4, the approximation obtained by the  $P(EC)^\mu E$  method described above satisfies*

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^q)$$

where  $q = \min\{2, 1 + \mu n\}$ .

For the moment we leave the topic of general  $P(EC)^\mu E$  methods in favour of a more detailed investigation of its special case  $\mu = 1$ , i.e. the original Adams–Bashforth–Moulton method introduced in (C.19) and (C.15). In this context we note an apparent disadvantage in the formulation of the hypotheses of the theorems above: They are stated in terms of the solution  $y$  (or, more precisely, its Caputo derivative of order  $n$ ), which is unknown in general. Even though it is sometimes possible to determine the smoothness properties of  $D_{*0}^n y$  from the given data, there still is some need for a corresponding error theory for the Adams method under assumptions formulated directly in terms of the given data, i.e. in terms of the function  $f$ . Such results will be derived later in this section.

Before we come to those results however, we want to give some more information under assumptions similar to those of Theorem C.4. Specifically we want to state the conjecture that the error of our scheme, taken at a fixed abscissa, possesses an asymptotic expansion in powers of the step size  $h$  under additional smoothness conditions on  $D_{*0}^n y$ . If this were true (as, e.g., numerical results in Example C.1 below indicate), we could construct a Richardson extrapolation algorithm based on the Adams method in a way similar to the construction in [53] which is based on the scheme of [34]. The use of this extrapolation procedure then would permit us to obtain more accurate numerical approximations for the desired solution.

**Conjecture C.1.** *Let  $n > 0$  and assume that  $D_{*0}^n y \in C^k[0, T]$  for some  $k \geq 3$  and some suitable  $T$ . Then,*

$$y(T) - y_{T/h} = \sum_{j=1}^{k_1} c_j h^{2j} + \sum_{j=1}^{k_2} d_j h^{j+n} + O(h^{k_3})$$

where  $k_1, k_2$  and  $k_3$  are certain constants depending only on  $k$  and satisfying  $k_3 > \max(2k_1, k_2 + n)$ .

Notice that the asymptotic expansion begins with an  $h^2$  term and continues with  $h^{1+n}$  for  $1 < n < 3$ , whereas it begins with  $h^{1+n}$ , followed by  $h^2$ , for  $0 < n < 1$ .

*Example C.1.* Consider the equation

$$\begin{aligned} D_{*0}^n y(x) = & \frac{40320}{\Gamma(9-n)} x^{8-n} - 3 \frac{\Gamma(5+n/2)}{\Gamma(5-n/2)} x^{4-n/2} + \frac{9}{4} \Gamma(n+1) \\ & + \left( \frac{3}{2} x^{n/2} - x^4 \right)^3 - [y(x)]^{3/2} \end{aligned}$$

for  $x \in [0, 1]$  with homogeneous initial conditions ( $y(0) = 0$ ,  $y'(0) = 0$ ; the latter only in the case  $n > 1$ ).

The exact solution of this initial value problem is

$$y(x) = x^8 - 3x^{4+n/2} + \frac{9}{4}x^n,$$

and hence

$$D_{*0}^n y(x) = \frac{40320}{\Gamma(9-n)} x^{8-n} - 3 \frac{\Gamma(5+n/2)}{\Gamma(5-n/2)} x^{4-n/2} + \frac{9}{4} \Gamma(n+1),$$

i.e.  $D_{*0}^n y \in C^2[0, 1]$  if  $n \leq 4$ , and thus the conditions of Theorem C.4 are fulfilled. Moreover, assuming that Conjecture C.1 holds, the application of Richardson extrapolation is also justified. We display some of the results in Tables C.1 and C.2 where, e.g., the notation  $-5.53(-3)$  stands for  $-5.53 \cdot 10^{-3}$ . In each case, the left-most column shows the step size used, the following column gives the error of our

**Table C.1** Errors for Example C.1 with  $n = 1.25$ , taken at  $x = 1$

Step size	Error of				
	Adams scheme	Extrapolated values			
1/10	-5.53(-3)				
1/20	-1.59(-3)	-2.80(-4)			
1/40	-4.33(-4)	-4.60(-5)	1.63(-5)		
1/80	-1.14(-4)	-8.17(-6)	1.90(-6)	2.13(-7)	
1/160	-2.97(-5)	-1.54(-6)	2.24(-7)	2.71(-8)	1.47(-8)
1/320	-7.66(-6)	-3.04(-7)	2.56(-8)	2.28(-9)	6.24(-10)
1/640	-1.96(-6)	-6.16(-8)	2.85(-9)	1.73(-10)	3.25(-11)
EOC	1.97	2.30	3.17	3.72	4.26

**Table C.2** Errors for Example C.1 with  $n = 0.25$ , taken at  $x = 1$

Step size	Error of				
	Adams scheme	Extrapolated values			
1/10	2.50(-1)				
1/20	1.81(-2)	-1.50(-1)			
1/40	3.61(-3)	-6.91(-3)	4.09(-2)		
1/80	1.45(-3)	-1.10(-4)	2.16(-3)	-8.15(-3)	
1/160	6.58(-4)	8.19(-5)	1.46(-4)	-3.89(-4)	1.28(-4)
1/320	2.97(-4)	3.49(-5)	1.92(-5)	-1.45(-5)	1.05(-5)
1/640	1.31(-4)	1.12(-5)	3.37(-6)	-8.50(-7)	6.01(-8)
EOC	1.18	1.63	2.51	4.09	7.44

scheme at  $x = 1$ , and the columns after that give the extrapolated values. The bottom line (marked “EOC”) states the experimentally determined order of convergence for each of the columns on the right of the table. According to our theoretical considerations, these values should be  $1 + n, 2, 2 + n, 3 + n, 4, 4 + n, \dots$  in the case  $0 < n < 1$  and  $2, 1 + n, 2 + n, 4, 3 + n, 4 + n, \dots$  for  $1 < n < 2$ . The numerical data in the following tables show that these values are reproduced approximately at least for  $n > 1$  (see Table C.1). In the case  $0 < n < 1$ , displayed in Table C.2, the situation seems to be less obvious. Apparently, we need to use much smaller values for  $h$  than in the case  $n > 1$  before we can see that the asymptotic behaviour really sets in. This would normally correspond to the situation that the coefficients of the leading terms are small in magnitude compared to the coefficients of the higher-order terms.

Our belief in the truth of Conjecture C.1 is not only supported by the numerical results but also by the results of de Hoog and Weiss [32, §5] who show that asymptotic expansions of this form hold if we use the fractional Adams–Moulton method (i.e. if we solve the corrector equation exactly) and that a similar expansion can be derived for the fractional Adams–Bashforth method (using the predictor as the final approximation rather than correcting once with the Adams–Moulton formula). For the moment however, we leave the question of the influence of the corrector step (that combines the two approaches) on this expansion open.

Rather, we turn our attention to another related problem. In the previous theorems we had formulated our hypotheses in the form of smoothness assumptions on  $D_{*0}^n y$ . Now we want to replace this by similar assumptions on  $y$  itself. In view of Theorem 3.15 we must be aware of the fact that smoothness of  $y$  in general implies non-smoothness of  $D_{*0}^n y$  (the function that we have to approximate), so some difficulties are likely. Fortunately Theorem 3.15 also informs us about the precise nature of the singularities in the derivatives of  $D_{*0}^n y$ . We can exploit this information to obtain the following results.

**Theorem C.6.** *Let  $n > 1$  and assume that  $y \in C^{1+\lceil n \rceil}[0, T]$  for some suitable  $T$ . Then,*

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^{1+\lceil n \rceil - n}).$$

*Proof.* By Theorem 3.15 we find that  $D_{*0}^n y(x) = cx^{\lceil n \rceil - n} + g(x)$  where  $g \in C^1[0, T]$  and  $g'$  fulfils a Lipschitz condition of order  $\lceil n \rceil - n$ . Thus, according to Theorems C.1 and C.2 we can apply Lemma C.3 with  $\gamma_1 = 0$ ,  $\gamma_2 = n - 1 > 0$ ,  $\delta_1 = 1$  and  $\delta_2 = 1 + \lceil n \rceil - n$ . Because of  $n > 1$  we then find that  $\delta_1 + n = 1 + n > 2 > \delta_2$ , and hence  $\min\{\delta_1 + n, \delta_2\} = \delta_2$ . So the overall error bound is  $O(h^{\delta_2})$ .  $\square$

Notice that a reformulation of Theorem C.6 yields that, if  $1 < n = k_1 + k_2$  with  $k_1 \in \mathbb{N}$  and  $0 < k_2 < 1$ , then the error is  $O(h^{2-k_2})$ . Thus the fractional part of  $n$  plays the decisive role for the order of the error. In particular, we find slow convergence if the fractional part of  $n$  is large. Consequently, under these assumptions we cannot expect the convergence order to be a monotone function of  $n$  any more. Nevertheless we can prove that the method converges for all  $n > 0$ :

**Theorem C.7.** *Let  $0 < n < 1$  and assume that  $y \in C^2[0, T]$  for some suitable  $T$ . Then, for  $1 \leq j \leq N$  we have*

$$|y(t_j) - y_j| \leq Ct_j^{n-1} \times \begin{cases} h^{1+n} & \text{if } 0 < n < 1/2, \\ h^{2-n} & \text{if } 1/2 \leq n < 1, \end{cases} \quad (\text{C.23})$$

where  $C$  is a constant independent of  $j$  and  $h$ .

We obtain two immediate consequences.

**Corollary C.8.** *Under the assumptions of Theorem C.7, we have*

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = \begin{cases} O(h^{2n}) & \text{if } 0 < n < 1/2, \\ O(h) & \text{if } 1/2 \leq n < 1. \end{cases}$$

Moreover, for every  $\varepsilon \in (0, T)$  we have

$$\max_{t_j \in [\varepsilon, T]} |y(t_j) - y_j| = \begin{cases} O(h^{1+n}) & \text{if } 0 < n < 1/2, \\ O(h^{2-n}) & \text{if } 1/2 \leq n < 1. \end{cases}$$

*Proof (of Theorem C.7).* The first steps of the proof are as in the proof of Theorem C.6. The key difference is that now  $\gamma_2 < 0$  (note that we still have  $\gamma_2 = n - 1$ , but now  $n < 1$ ). Thus we cannot apply Lemma C.3. Instead we modify its proof so that it fits to our requirements: We keep the inductive structure and remember that our claim is now (C.23) rather than (C.21). With this change in the induction hypothesis we proceed much as in the proof of Lemma C.3. However, because of this new hypothesis, we now have to estimate terms of the form  $\sum_{j=1}^{k-1} b_{j,k+1} t_j^{\gamma_2}$  and  $\sum_{j=1}^{k-1} a_{j,k+1} t_j^{\gamma_2}$ . By the Mean Value Theorem we have  $0 \leq b_{j,k+1} \leq h^n (k-j)^{n-1}$  and  $0 \leq a_{j,k+1} \leq c h^n (k-j)^{n-1}$  for  $1 \leq j \leq k-1$  (where the constant  $c$  is independent of  $j$  and  $k$ ), respectively, so that the problem reduces to finding a bound for  $S_k := \sum_{j=1}^{k-1} j^{\gamma_2} (k-j)^{n-1}$ . Under our assumptions, both the exponents  $\gamma_2$  and  $n-1$  are in the interval  $(-1, 0)$ , and then it is easily seen that  $S_k = O(k^{\gamma_2+n})$ . Using this relation we can complete the proof of Theorem C.7 by following along the lines of the rest of the proof of Lemma C.3.  $\square$

We conclude the discussion of error bounds with a result where we formulate the hypotheses in terms of the given data and not in terms of the unknown solution. We give a result in the case  $n > 1$  and later discuss properties of the numerical scheme when  $n < 1$ .

**Theorem C.9.** *Let  $n > 1$ . Then, if  $f \in C^2(G)$ ,*

$$\max_{0 \leq j \leq N} |y(t_j) - y_j| = O(h^2).$$

*Proof (of Theorem C.9).* We begin by discussing the case  $n \geq 2$ . Then, according to Theorem 6.25, we find that  $y \in C^2[0, T]$ . Thus, in view of the smoothness assumption on  $f$  and the chain rule,  $D_{*0}^n y := f(\cdot, y(\cdot)) \in C^2[0, T]$  too, and the claim follows by virtue of Theorem C.4.

For the case  $1 < n < 2$ , we want to apply Lemma C.3 and hence we have to determine the constants  $\gamma_1, \gamma_2, \delta_1$  and  $\delta_2$  in its hypotheses. In order to do so we need more precise information about the behaviour of  $y$ . This information can be found in Theorem 6.38 which asserts that  $y(x) = cx^n + \psi(x)$  with some  $c \in \mathbb{R}$  and some  $\psi \in C^2[0, T]$ . This implies, in particular, that  $y \in C^1[0, T]$ . As in the case  $n > 2$  above we can then deduce  $D_{*0}^n y \in C^1[0, T]$  too, and by Theorem C.1(a), we find that we may choose  $\gamma_1 = n$  and  $\delta_1 = 1$ . Moreover, using again the fact that  $y(x) = cx^n + \psi(x)$  with some  $c \in \mathbb{R}$  and some  $\psi \in C^2[0, T]$  and applying Theorem C.2(a) and (c), we determine the correct values for the remaining quantities as  $\gamma_2 = \min\{n, 2n-2\} = 2n-2 \geq 0$  and  $\delta_2 = 2$ . The claim then follows from Lemma C.3.  $\square$

In the case  $n < 1$  the situation seems to be less clear. According to the theorems presented at the end of Sect. 6.4, smoothness conditions on  $f$  imply that the exact solution is of the form

$$y(t) = \psi(t) + \sum_{v=1}^{\hat{v}} c_v t^{vn} + \sum_{v=1}^{\tilde{v}} d_v t^{1+vn}$$

where  $\psi$  is twice differentiable. The first sum consists of terms which are not differentiable, and the second sum is of terms that are differentiable once but not twice. As remarked by Lubich [120] it seems unlikely that numerical schemes will be rapidly convergent over any interval that contains the origin. Indeed we can prove that the error  $y(t_1) - y_1$  of the approximation after just one step behaves as  $O(h^{2n})$  if  $f \in C^2(G)$ . Simple numerical experiments indicate that this result cannot be improved. However this error introduced in the initial phase is transient and from numerical results reported in [49, Table 4.5] we believe the following conjecture to be true.

**Conjecture C.2.** *Let  $0 < n < 1$ . Then, if  $f \in C^3(G)$ , for every  $\varepsilon > 0$  we have*

$$\max_{t_j \in [\varepsilon, T]} |y(t_j) - y_j| = O(h^{1+n}).$$

## C.2 Numerical Schemes for Multi-Term Equations

We now come to the extension of the numerical methods discussed in the previous section to multi-term equations. The most important theoretical properties of these multi-term equations have been discussed in Chap. 8. As in that chapter we restrict our attention to equations of the form

$$D_{*0}^{n_k} y(x) = f(x, y(x), D_{*0}^{n_1} y(x), D_{*0}^{n_2} y(x), \dots, D_{*0}^{n_{k-1}} y(x)) \quad (\text{C.24a})$$

(where  $0 < n_1 < n_2 < \dots < n_k$ ) with a suitable function  $f$  and initial conditions

$$y^{(j)}(0) = y_0^{(j)}, \quad j = 0, 1, \dots, \lceil n_k \rceil - 1. \quad (\text{C.24b})$$

For initial value problems of this type we shall discuss the various approaches introduced in Chap. 8 and find out their respective advantages and disadvantages.

### *Conversion to Single-Order Systems*

Our first attempt consists in a direct application of the result of Theorem 8.1 or 8.2 (depending on whether  $n_k > 1$  or not) to the given initial value problem. In this way we transform the given initial value problem into a system of equations of the form

$$\begin{aligned}
D_{*0}^{\gamma} y_0(x) &= y_1(x), \\
D_{*0}^{\gamma} y_1(x) &= y_2(x), \\
&\vdots \\
D_{*0}^{\gamma} y_{N-2}(x) &= y_{N-1}(x), \\
D_{*0}^{\gamma} y_{N-1}(x) &= f(x, y_0(x), y_{n_1/\gamma}(x), \dots, y_{n_{k-1}/\gamma}(x)),
\end{aligned} \tag{C.25a}$$

together with the initial conditions

$$y_j(0) = \begin{cases} y_0^{(j\gamma)} & \text{if } j\gamma \in \mathbb{N}_0, \\ 0 & \text{else,} \end{cases} \tag{C.25b}$$

with the precise choice of the new parameters  $\gamma$  and  $N$  being according to Theorems 8.1 or 8.2, as appropriate. We have thus formally obtained an equation of the type

$$D_{*0}^{\gamma} Y(x) = F(x, Y(x)), \quad Y(0) = Y_0, \tag{C.26}$$

with certain vector-valued functions  $F$  (known) and  $Y$  (unknown) and an initial condition vector  $Y_0$ , i.e. a single-term equation of order  $\gamma$  with vector-valued data. Thus we may apply any numerical method for such single-term equations and calculate an approximate solution for this system; for the sake of simplicity we shall restrict ourselves to the Adams–Bashforth–Moulton scheme developed above. The first component of the (numerical) solution vector (with index 0) is then the required approximate solution for the original equation. We illustrate the procedure by a simple example taken from [44].

*Example C.2.* Solve the Bagley–Torvik equation

$$Ay''(x) + BD_{*0}^{3/2}y(x) + Cy(x) = C(x+1)$$

(where  $A \neq 0$  and  $B, C \in \mathbb{R}$ ) with initial conditions

$$y(0) = y'(0) = 1$$

with the approach described above.

It is easily verified that the exact solution of this problem is

$$y(x) = x + 1$$

independent of the choice of the coefficients  $A$ ,  $B$ , and  $C$ . Thus, the resulting system is

$$D_{*0}^{1/2} \begin{pmatrix} y_0(x) \\ y_1(x) \\ y_2(x) \\ y_3(x) \end{pmatrix} = \frac{1}{A} \begin{pmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \\ -By_3(x) - Cy_0(x) + C(x+1) \end{pmatrix},$$



$$\begin{pmatrix} y_0(0) \\ y_1(0) \\ y_2(0) \\ y_3(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

We have solved this problem on the interval  $[0, 5]$  with the Adams–Bashforth–Moulton scheme. The numerical results at  $x = 5$  were as shown in Table C.3.

These data indicate that the convergence behaviour is  $O(h^{3/2})$ . To understand how this relates to the error estimates of Sect. C.1, we must recall that we now construct an approximate solution for the entire system and not just for its first component. Thus we see that, as a by-product of the method, we do not only obtain information on  $y$  but also on its fractional derivatives of order  $\gamma, 2\gamma, \dots, (N-1)\gamma$ . Depending on the task at hand this information can be anything between highly useful and absolutely unnecessary. In any case the error estimate is dominated by the worst error estimate of the four components. Since the exact solution for the system is  $(x+1, x^{1/2}/\Gamma(3/2), 1, 0)^T$  we see that the second, third and fourth components of the exact solution have smooth derivatives of order  $1/2$ ; thus they may be approximated with order  $O(h^{3/2})$  according to Theorem C.4. The first component is smooth itself; it allows an application of Corollary C.8 that gives an  $O(h)$  error estimate on the full interval  $[0, T]$  and an  $O(h^{3/2})$  estimate on each interval of the form  $[\varepsilon, T]$  with  $\varepsilon > 0$ . Since the latter case covers the problem considered in Table C.3, we have agreement between theoretical and numerical results.

In order to explain the weaknesses of this concept, we look at a second example, already considered in [45] and [35].

*Example C.3.* Solve the nonlinear three-term equation

$$D_{*0}^{1.455}y(x) = -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} e^x y(x) D_{*0}^{0.555}y(x) + e^{-2x} - [D_{*0}^1 y(x)]^2 \quad (\text{C.27})$$

for  $0 \leq x \leq 1$ , equipped with the initial conditions  $y(0) = 1$  and  $y'(0) = -1$ , with the same algorithm.

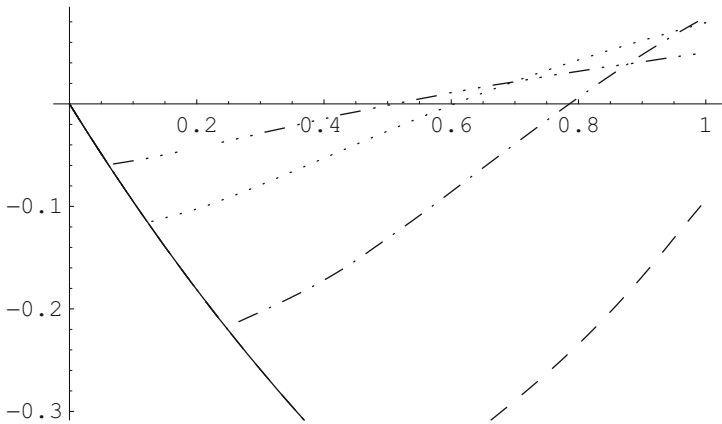
The exact solution of this problem is  $y(x) = \exp(-x)$ . When applying our idea to this equation, we first need to calculate the order  $\gamma$  of the new system as described in Theorem 8.1. In our case the result is  $\gamma = 1/200$ , and hence the dimension of the resulting system is  $N = 1.455/\gamma = 291$  – a rather large number. In a first attempt we have tried to solve the system with the Adams–Bashforth–Moulton scheme as

**Table C.3** Bagley–Torvik equation solved with Adams method

Step size	Numerical solution	Error	Estimated order of convergence
0.5	6.15131473519232	−0.15131473519232	
0.25	6.04684102179946	−0.04684102179946	1.69
0.125	6.01602947553912	−0.01602947553912	1.55
0.0625	6.00562770408881	−0.00562770408881	1.51

**Table C.4** Numerical results for Example C.3 (system with  $N = 291$ ,  $\gamma = 0.005$ ) using the standard PECE-type Adams algorithm

Step size	Maximal error	Run time
1/200	0.3904	101.2 s
1/400	0.2193	368.4 s
1/800	0.1164	1358.0 s
1/1,600	0.0600	5017.4 s



**Fig. C.1** Approximation errors for Example C.3 with  $h = 1/100$  (solid line),  $h = 1/200$  (dashed line),  $h = 1/400$  (dot-dashed line),  $h = 1/800$  (dotted line),  $h = 1/1,600$  (dashed and triple-dotted line)

above. The resulting errors are reported in Table C.4 and Fig. C.1. For the purpose of comparison with later methods we have also included information about the run time of the algorithm on a standard 500 MHz Pentium PC in double precision arithmetic.

It is clearly seen that the results for  $h = 1/100$  and  $h = 1/200$  are totally unacceptable. There is a simple explanation for this phenomenon which becomes evident when one takes a look at the numerical solution of the initial value problem and not at the approximation error: In each case the first 99 steps of the algorithm do not change the first component of the approximate solution. In other words we get stuck at the initial value instead of following the exact solution. The reason for this behaviour can be found in the structure of the function  $F$  on the right-hand side of the system (C.26) and of its initial condition: The first component (index 0) is  $y_0$ , the component with index 200 ( $= 1/\gamma$ ) is  $y'_0 (\neq 0)$ , and all the components in between vanish. The interaction of the Adams–Bashforth–Moulton method with the function  $F$  now implies that the non-zero component is propagated by one row in each predictor step and another row in each corrector step, so in the first 99 steps only a total of 198 zeros are added to the initial value of the leading component of the numerical solution. The last (199th) zero is then used in the predictor of the 100th step, and the corrector of step 100 is actually the first operation where a non-zero entry reaches the first component of the solution. Thus we always have an initial

interval of  $2/\gamma - 1$  steps where the numerical solution is constant before it can start to make progress towards the exact solution. Notice that in our Bagley–Torvik example above we had  $\gamma = 1/2$ , and so (since here  $2/\gamma - 1 = 3$ ) the effect is negligible. This means that, if one wants to keep the structure of the algorithm and the uniform step size, then the only way to reduce this effect is a drastic reduction of the step size  $h$ , essentially by the rule  $h = O(\gamma)$ . A look at Fig. C.1 confirms this observation.

Let us briefly summarize what we have achieved so far: The approach described above has the advantage of producing a system of equations with a very simple structure. As a consequence of this structure, numerical schemes for this system can be implemented on a parallel computer architecture in a rather efficient way. However we have also seen some disadvantages:

- (a) The method only works in the case of commensurate multi-term equations (if  $n_k \leq 1$ ) or under the even more restrictive assumption that all the  $n_j$  are rational (if  $n_k > 1$ )
- (b) The dimension of the system can be very large (depending on the precise values of the parameters of the original equation); this can lead to very long run times on sequential machines
- (c) The structure of the initial conditions of the new system can be problematic for some types of numerical algorithms; in particular we may be forced to use excessively small step sizes

In order to overcome these problems (at least partially), we propose two possible strategies. The first one, taken from [45], is a slight refinement of the idea used so far that works in two stages. We recall that the problem is mainly due to the large dimension of the system, and this in turn is a consequence of the size of the greatest common divisor of the orders of the differential operators in the given system. Therefore we introduce a stage of preliminary manipulations before actually starting the numerical algorithm.

This first stage consists of replacing the given initial value problem (C.24) by a new differential equation

$$D_{*0}^{\tilde{n}_k} \tilde{y}(x) = f(x, \tilde{y}(x), D_{*0}^{\tilde{n}_1} \tilde{y}(x), D_{*0}^{\tilde{n}_2} \tilde{y}(x), \dots, D_{*0}^{\tilde{n}_{k-1}} \tilde{y}(x)) \quad (\text{C.28})$$

with identical initial conditions (C.24b). We thus perturb the orders of the differential operators, but all other parameters of the given problem (the function  $f$  on the right-hand side and the initial conditions) remain unchanged.

The essence of this idea is that, according to Theorem 8.8, the exact solution  $\tilde{y}$  of this new initial value problem and the exact solution  $y$  of the original problem differ only by

$$\|y - \tilde{y}\|_\infty = O\left(\max_{j=1,2,\dots,k} |n_j - \tilde{n}_j|\right). \quad (\text{C.29})$$

Here by  $\|\cdot\|_\infty$  we denote the Chebyshev norm taken over a suitable finite interval  $[0, T]$ , say, where both problems have a solution.

In order to exploit the capabilities of this approach, we need to choose the new parameters  $\tilde{n}_1, \dots, \tilde{n}_k$  in such a way that they have the following three properties:

- (a)  $\tilde{n}_1, \dots, \tilde{n}_k \in \mathbb{Q}$
- (b) The least common multiple of the denominators of  $\tilde{n}_1, \dots, \tilde{n}_k$  is small
- (c)  $\max_j |n_j - \tilde{n}_j|$  is small

Here condition (a) asserts that a conversion of (C.28) to a single-term system (as described in Chap. 8) is possible. Specifically, since only the new values  $\tilde{n}_j$  enter the later stages of the scheme, such a conversion is always possible, without any restrictions on the original values  $n_j$ . The purpose of condition (b) is to keep the dimension  $N$  of this system small (remember that in Theorem 8.1 we had seen that essentially  $N = Mn_k$  where  $M$  is the least common multiple mentioned in condition (b)), which – according to our initial idea – was the main point of the concept. Condition (c) finally makes sure that the error introduced by this perturbation remains small, cf. (C.29).

It must be noted of course that there is a conflict between conditions (b) and (c): In many cases it will be possible to improve the approximation required in (c) at the price of increasing the least common multiple mentioned in (b). A proper compromise must be found in this case. It seems to be impossible however to state a generally valid strategy for the solution of this conflict; a good compromise will likely depend on the specific parameters of the equation under consideration.

This completes the first stage of the algorithm. At the end of this stage we have found a new initial value problem that consists of the perturbed differential equation (C.28) together with the original (unperturbed) initial conditions (C.24b).

The second stage of the algorithm is then the stage where the initial value problem that was constructed in stage 1 will be solved numerically. In practice we will first use the approach described at the beginning of this section: We convert the new initial value problem into a single-term system, and then we will solve this system numerically (for example by means of the Adams method).

*Example C.4.* Construct an approximate solution for the problem from Example C.3 by the two-stage strategy outlined above.

As a first attempt to solve the problem with our refined method, we approximate (C.27) by

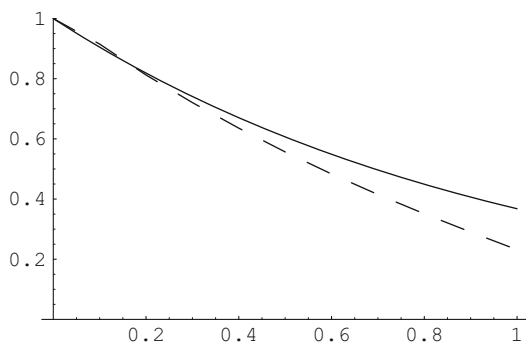
$$D_{*0}^{1.5} \tilde{y}(x) = -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} e^x \tilde{y}(x) D_{*0}^{0.5} \tilde{y}(x) + e^{-2x} - [D_{*0}^1 \tilde{y}(x)]^2, \quad (\text{C.30})$$

convert (C.30) to a three-dimensional system of order  $\gamma = 0.5$ , and solve this system numerically with the Adams method in its standard form using various step sizes. The results are described in Table C.5.

**Table C.5** Numerical results of first approximation ( $N = 3$ ,  $\gamma = 0.5$ )

Step size	Maximal error	Run time
1/10	0.136	0.07 s
1/20	0.124	0.18 s
1/40	0.118	0.56 s

**Fig. C.2** Exact solution and first approximation ( $N = 3$ ,  $\gamma = 0.5$ , step size  $h = 0.1$ )



We can see that there is almost no improvement when we change the step size from  $1/20$  to  $1/40$ . This indicates that the error of the Adams scheme (i.e. the error introduced in the second stage) is already very small compared to the error of the first stage (i.e. the error introduced by perturbing the differential equation). Therefore there is no need to look for an improved scheme for the solution of this simple system. Note in particular (see Fig. C.2) that even the crudest of these three approximations (the dashed line) gives a *qualitatively* correct picture of the exact solution (the solid line). Certainly this cannot be said to be true for our plain and simple first approach discussed above.

In order to obtain a better approximation with our method we must now reduce the error of stage 1, i.e. we need to introduce smaller perturbations in the orders of the differential operators. We thus try to approximate the given equation (C.27) not by (C.30) but by

$$D_{*0}^{1.45} \tilde{y}(x) = -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} e^x \tilde{y}(x) D_{*0}^{0.55} \tilde{y}(x) + e^{-2x} - [D_{*0}^1 \tilde{y}(x)]^2 \quad (\text{C.31})$$

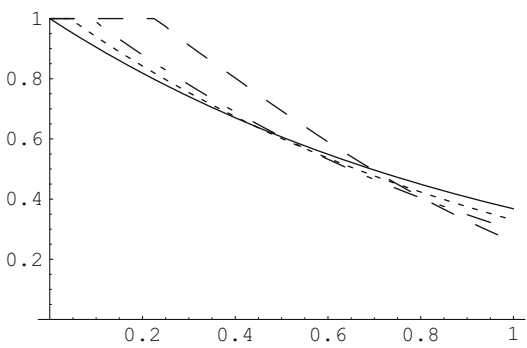
and proceed as above. Consequently we find that we have to solve a 29-dimensional system of order 0.05 numerically. This task is (in particular due to the nature of the initial conditions) much more difficult than the previous one, and therefore we need to put more effort into the numerical scheme. For the moment we interpret this requirement as a demand for a smaller step size; an alternative will be considered later. The results are given in Table C.6.

For the purpose of comparison with the previous example we have included the case of a step size of  $1/40$ . As can be seen by comparing Tables C.5 and C.6, the error is much larger now than it was before. The reason is the problem that we mentioned above: Since the dimension of the system has been increased, the numerical solution needs more time to get away from the initial value. An even more obvious picture of the situation appears when we look at the graphical data provided in Fig. C.3. Here again the solid line is the exact solution, the other lines correspond to the numerical solutions (dashed line:  $h = 1/40$ ; dash-dotted line:  $h = 1/100$ ;

**Table C.6** Numerical results of second approximation ( $N = 29$ ,  $\gamma = 0.05$ )

Step size	Maximal error	Run time
1/40	0.2015	0.9 s
1/100	0.0861	5.5 s
1/200	0.0440	21.5 s
1/400	0.0222	82.4 s

**Fig. C.3** Exact solution and second approximation ( $N = 29$ ,  $\gamma = 0.05$ , various step sizes)



dotted line:  $h = 1/200$ ). We thus have to say that the graph for  $h = 1/40$  does *not* give a qualitatively correct picture of the true solution.

As pointed out above, we will sometimes be forced to choose the parameters in such a way that the dimension of the system is larger than desirable. In this context the present 29-dimensional system may be considered to be such a case. That means that also the number of zeros in the initial condition of the resulting system is larger than one would like it to be, which forces us to use a very small step size.

This is where our second strategy mentioned above comes into play as a possible alternative. Specifically, it may be useful to replace the plain PECE structure by a  $P(EC)^\mu E$  method (i.e. by introducing additional corrector iterations) as described in Theorem C.5. This allows for a quicker propagation of the non-zero elements, and it may be possible to avoid the use of excessively small step sizes. We shall provide a numerical example now. This flexibility in the number of corrector steps is actually one of the main reasons why we suggest the Adams scheme and not, e.g., the method of [34]. Recall that, as derived in Remark C.4, by (for example) doubling the number of corrector iterations, we essentially leave the computational complexity unchanged.

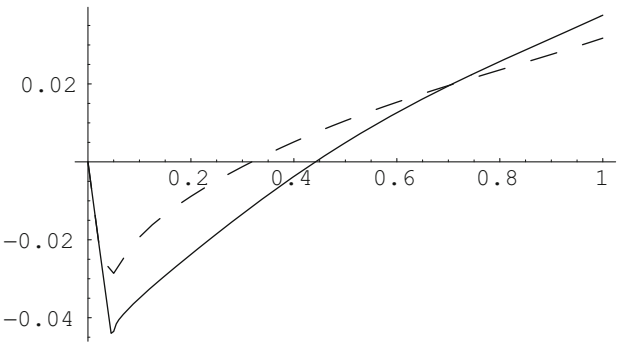
If we would use the other option and reduce the step size by a factor of two, then the run time would increase by a factor of four because the complexity of the algorithm is  $O(h^{-2})$ . Both approaches would reduce the size of the initial interval where the numerical solution gets stuck at the initial value by a factor of 1/2.

The data obtained by our  $P(EC)^\mu E$  approach are given in Table C.7. Note that the data of Table C.6 correspond to this method with  $\mu = 1$ .

It is clearly seen that there is a significant advantage in this approach: By choosing  $\mu = 10$  and  $h = 1/40$  for example, we obtain an absolute error that is about 25% smaller than in the case  $\mu = 1$  and  $h = 1/200$ , and at the same time the run time is

**Table C.7** Numerical results of second approximation ( $N = 29, \gamma = 0.05$ ) as in (C.31) with  $P(EC)^\mu E$  algorithm

Number $\mu$ of corrector iterations	Step size	Maximal error	Run time
10	1/40	0.03175	4.9 s
10	1/100	0.01174	28.6 s
20	1/40	0.00989	9.3 s
20	1/100	0.00379	55.0 s



**Fig. C.4** Errors for second approximation ( $N = 29, \gamma = 0.05$ ) as in (C.31) with various combinations of step size and number of corrector steps

75% shorter. The reason is the following. In the case  $\mu = 1$  the numerical solution gets stuck at the initial value for a rather long interval. At the end of this interval the true solution has moved away significantly from the initial value, and here the error attains its maximum. Over the remainder of the interval  $[0, 1]$  the numerical solution then has to creep towards the exact solution, and the error gets smaller. If we choose a larger value for  $\mu$ , we make the problematic initial interval smaller, and therefore we also diminish the error attained over this interval. This is apparent from Fig. C.4 where we have compared the absolute errors for  $\mu = 1, h = 1/200$  (solid line) and  $\mu = 10, h = 1/40$  (dashed line).

In this example one can of course now apply the idea of using many corrector steps also to the given equation (C.27) itself. This is equivalent to skipping stage 1 of our two-stage process. It is clear that the run times of the plain PECE scheme (see Table C.4) are not competitive. Therefore we once again revert to the  $P(EC)^\mu E$  structure with larger values for  $\mu$  and larger step sizes as before. Some results are stated in Table C.8.

Comparing Tables C.4 and C.8 we once again find a significant run time advantage in the  $P(EC)^\mu E$  method as compared to the PECE method without losing accuracy, but even the approximations obtained by the faster  $P(EC)^\mu E$  approach are less accurate and more time consuming than the results presented in Table C.7 where we had used a simpler differential equation system.

**Table C.8** Numerical results for unperturbed equation ( $N = 291$ ,  $\gamma = 0.005$ ), with  $P(EC)^\mu E$  algorithm

Number $\mu$ of corrector iterations	Step size	Maximal error	Run time
10	1/100	0.16473	117.3 s
10	1/200	0.08607	446.8 s
20	1/100	0.08607	222.8 s
20	1/200	0.04400	811.0 s

Based on our theoretical considerations here and in Sect. C.1 and on heuristical arguments coming from the numerical results, we now give a complete description of a possible algorithm for the approximate solution of the initial value problem (C.24). The algorithm will follow the basic ideas outlined above. The fundamental concept is that we assume a bound on the complexity to be given (expressed in terms of the least common multiple of the denominators of the orders  $\tilde{n}_j$ ) and that we try to achieve a high accuracy in the solution without exceeding the complexity limit.

Specifically, we assume that the user specifies a parameter  $M \in \mathbb{N}$  which we interpret as an upper bound for the least common multiple of the denominators of  $\tilde{n}_1, \dots, \tilde{n}_k$ . Since the dimension  $N$  of the system that we shall construct in stage 2 of the algorithm is given by  $N = M\tilde{n}_k \approx Mn_k$ , this data gives us an upper bound on the dimension and hence an upper bound on the arithmetic complexity.

We begin by constructing the perturbations required for the first stage. This is very simple; for  $j = 1, 2, \dots, k$  we only have to set  $\tilde{n}_j := \alpha_j/M$  where  $\alpha_j \in \mathbb{N}$  is chosen to be the natural number closest to  $Mn_j$  (i.e.  $\alpha_j = \lfloor Mn_j + 0.5 \rfloor$ ). In this way we make sure that, for every single  $j$ , the quantity  $|\tilde{n}_j - n_j|$  is minimized under the condition that the least common multiple of the denominators of  $\tilde{n}_1, \dots, \tilde{n}_k$  is bounded by  $M$ . This essentially completes the first stage.

The second stage begins by rewriting the perturbed equations as a system of order  $\gamma = 1/M$  and dimension  $N$  as described in Theorem 8.1. This system is solved by the  $P(EC)^\mu E$  scheme indicated above. To avoid the problems caused by the large number of zeros in the new initial condition, we choose the parameter  $\mu$  in a way that depends on the number of zeros (i.e. on  $M$ ); specifically we set  $\mu := M$  as suggested in [36]. Note that it follows from our considerations that it is neither necessary nor helpful to introduce additional flexibility by choosing different values for the parameter  $\mu$  in each step. The choice that we propose here is sufficient to avoid the problems caused by the (possibly) large number of zeros in the initial condition. Choosing  $\mu$  larger than this would not give a better order of accuracy, so there is no point in doing that (cf. the considerations on (C.32) below). Choosing  $\mu$  smaller (permanently or temporarily) would mean that the problem cannot be avoided totally, so one would have to assume a deterioration of the approximation quality, but on the other hand it would not lead to a significantly faster algorithm because the arithmetic complexity of the entire scheme is (asymptotically) independent of  $\mu$ .



Another advantage of the  $P(EC)^\mu E$  scheme with the choice of  $\mu$  indicated above can be explained by a look at Theorem C.5: The algorithm converges to the true solution of the perturbed equation with an error of

$$\max_{j=0,1,\dots,N} |y(t_j) - y_h(t_j)| = O(h^p) \quad \text{where} \quad p = \min(2, 1 + \gamma\mu). \quad (C.32)$$

Since here we have  $\mu = M = 1/\gamma$  by construction, this means that in the proposed scheme we actually have  $p = 2$  in every case, so we find slightly better convergence behaviour than in the simple PECE approach; indeed this is the maximum order than one can possibly obtain by an algorithm that uses the approximation method underlying our scheme.

This approach is particularly useful when one is looking for a computationally inexpensive but still reasonably accurate approximation. In many applications this will be what is desired because often one needs to solve a great number of such initial value problems whose solutions are then required as input data for other problems. Additionally, high accuracy is frequently impossible to obtain anyway because the given data (in particular the orders  $n_j$  of the differential operators) are something like material constants known only up to a certain (usually moderate) precision.

### Conversion to Multi-Order Systems

An alternative approach has been suggested in [59]. Two variants are possible; we begin with the one that is simpler to describe and discuss the other one later.

The basic idea is to use a completely different transformation of the given initial value problem into the form of a system of fractional differential equations. Essentially this amounts to replacing the path that uses Theorem 8.1 or 8.2 that we had used above by the transformation to a multi-order system according to Theorem 8.9 or Theorem 8.10. We begin with the former and, as above, assume that the original initial value problem is given in the form

$$D_{*0}^{n_k} y(x) = f(x, y(x), D_{*0}^{n_1} y(x), D_{*0}^{n_2} y(x), \dots, D_{*0}^{n_{k-1}} y(x)) \quad (C.33a)$$

(where  $0 < n_1 < n_2 < \dots < n_k$ ) with a suitable function  $f$  and initial conditions

$$y^{(j)}(0) = y_0^{(j)}, \quad j = 0, 1, \dots, \lceil n_k \rceil - 1. \quad (C.33b)$$

However we now assume (without loss of generality) that additionally we have

$$\{1, 2, \dots, \lceil n_k \rceil - 1\} \subset \{n_1, n_2, \dots, n_k\}. \quad (C.34)$$

This implies  $n_j - n_{j-1} \leq 1$  for all  $j$ . Consider now the differences  $d_j := n_j - n_{j-1}$  for  $j = 1, 2, 3, \dots, k$ , where we have defined  $n_0 := 0$ . We then introduce the new functions

$$y_0 := y, \quad y_j := D_{*0}^{d_j} y_{j-1} \quad (j = 1, 2, \dots, k),$$

such that

$$\begin{aligned}
 y_1 &= D_{*0}^{d_1} y_0 = D_{*0}^{n_1 - n_0} y_0 = D_{*0}^{n_1} y, \\
 y_2 &= D_{*0}^{d_2} y_1 = D_{*0}^{n_2 - n_1} D_{*0}^{n_1} y = D_{*0}^{n_2} y, \\
 &\vdots \\
 y_k &= D_{*0}^{d_k} y_{k-1} = D_{*0}^{n_k - n_{k-1}} D_{*0}^{n_{k-1}} y = D_{*0}^{n_k} y.
 \end{aligned}$$

For the derivation of these identities one can proceed as in the proof of Lemma 3.13; the key point is that – due to our assumption (C.34) – we never jump across an integer when moving from  $n_{j-1}$  to  $n_j$ . Thus we may rewrite (C.33a) in the form

$$\begin{aligned}
 D_{*0}^{d_1} y_0 &= y_1, \\
 D_{*0}^{d_2} y_1 &= y_2, \\
 &\vdots \\
 D_{*0}^{d_{k-1}} y_{k-2} &= y_{k-1}, \\
 D_{*0}^{d_k} y_{k-1} &= f(x, y_0(x), y_1(x), y_2(x), \dots, y_{k-1}(x)). \tag{C.35a}
 \end{aligned}$$

We have found the required system of differential equations; the corresponding initial values obviously have to be

$$y_j(0) = \begin{cases} y_0^{(n_j)} & \text{if } n_j \in \mathbb{N}_0, \\ 0 & \text{else} \end{cases} \tag{C.35b}$$

in view of the fact that  $y_j = D_{*0}^{n_j} y$ , Lemma 3.11 and the given initial values (C.33b). A comparison of this multidimensional initial value problem with its counterpart (C.25) constructed above reveals a number of substantial differences even though formally they are equivalent in the sense that the first components of the solutions of the two problems coincide:

- (a) The dimension of the new system is  $k$  (a small number in typical applications), independent of the values of the  $n_j$ ; we had seen above (see, e.g., Example C.3) that the other approach could give rise to systems of very large dimension even if  $k$  was small.
- (b) The number of zeros in the initial condition (C.33b) relates to the number of zeros in its counterpart (C.25b) in the same way as the dimensions.
- (c) The structure of the left-hand side of the new system (C.35a) is much more complicated than it was in the old system (C.25a).
- (d) The formal structures of the right-hand sides of the two system do not differ from each other at all.

It turns out that, in view of the considerations with respect to the approach using single-order systems, the first two points mentioned above indicate the capability of the new approach to avoid the potentially serious problems encountered in the first approach. On the other hand, the third item reveals that we have to pay a certain price for this improvement: Instead of requiring an approximation for only one differential operator we now need to work with operators of order  $d_1, d_2, \dots, d_k$ . These orders may or may not coincide with each other.

*Example C.5.* We rewrite the equations from Examples C.2 and C.3 as systems of equations according to the ideas outlined above.

For the Bagley–Torvik equation

$$Ay''(x) = -BD_{*0}^{3/2}y(x) - Cy(x) + C(x+1), \quad y(0) = y'(0) = 1,$$

from Example C.2, we have

$$n_1 = 1, \quad n_2 = \frac{3}{2} \quad \text{and} \quad n_3 = 2,$$

such that

$$d_1 = 1, \quad d_2 = \frac{1}{2} \quad \text{and} \quad d_3 = \frac{1}{2}.$$

The resulting system thus is three-dimensional and reads

$$\begin{aligned} D_{*0}^1 y_0(x) &= y_1(x), \\ D_{*0}^{1/2} y_1(x) &= y_2(x), \\ D_{*0}^{1/2} y_2(x) &= -\frac{B}{A} y_2(x) - \frac{C}{A} y_0(x) + \frac{C}{A} (x+1) \end{aligned}$$

with initial conditions

$$y_0(0) = y_1(0) = 1 \quad \text{and} \quad y_2(0) = 0.$$

A comparison with Example C.2 shows that the differences for this simple example are small: The dimension is reduced by one, and two different fractional derivatives appear on the left-hand side of the system.

In the other example, the equation was

$$\begin{aligned} D_{*0}^{1.455} y(x) &= -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} \exp(x) y(x) D_{*0}^{0.555} y(x) \\ &\quad + \exp(-2x) - [D_{*0}^1 y(x)]^2, \end{aligned}$$

with initial conditions  $y(0) = 1$  and  $y'(0) = -1$ . Here the new approach uses the parameters

$$n_1 = 0.555, \quad n_2 = 1 \quad \text{and} \quad n_3 = 1.455,$$

such that

$$d_1 = 0.555, \quad d_2 = 0.445 \quad \text{and} \quad d_3 = 0.455.$$

Once again we obtain a three-dimensional system; this time it has the form

$$\begin{aligned} D_{*0}^{0.555} y_0(x) &= y_1(x), \\ D_{*0}^{0.445} y_1(x) &= y_2(x), \\ D_{*0}^{0.455} y_2(x) &= -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} \exp(x) y_0(x) y_1(x) + \exp(-2x) - [y_2(x)]^2 \end{aligned}$$

with initial conditions

$$y_0(0) = 1, \quad y_1(0) = 0 \quad \text{and} \quad y_2(0) = -1.$$

Now the difference to the single-order system approach is enormous: The dimension of the system is reduced from 291 to 3, but of course we now have to work with three different differential operators.

Before we come to the question for a suitable numerical scheme for systems of this structure, let us briefly introduce a small modification of the idea presented so far that may lead to a slightly more efficient scheme. This is motivated by the observation from the two examples above that integer order differential operators that are local by nature are decomposed into two (or more) non-local fractional differential operators: In the Bagley–Torvik example we have  $y'' = D_{*0}^{1/2} y_2 = D_{*0}^{1/2} D_{*0}^{1/2} y_1 = D_{*0}^{1/2} D_{*0}^{1/2} D_{*0}^1 y_0$ , and so in any approximation method the possibility to save time by making use of the locality is lost. A similar decomposition  $y_2 = y' = D_{*0}^{0.445} y_1 = D_{*0}^{0.445} D_{*0}^{0.555} y_0$  is used in the other example. It would thus be preferable to use the alternative systems

$$\begin{aligned} D_{*0}^1 y_0(x) &= y_1(x), \\ D_{*0}^{1/2} y_1(x) &= y_2(x), \\ D_{*0}^1 y_1(x) &= -\frac{B}{A} y_2(x) - \frac{C}{A} y_0(x) + \frac{C}{A} (x+1) \end{aligned}$$

with initial conditions

$$y_0(0) = y_1(0) = 1 \quad \text{and} \quad y_2(0) = 0$$

for the Bagley–Torvik problem and

$$\begin{aligned} D_{*0}^{0.555} y_0(x) &= y_1(x), \\ D_{*0}^1 y_0(x) &= y_2(x), \\ D_{*0}^{0.455} y_2(x) &= -x^{0.1} \frac{E_{1.545}(-x)}{E_{1.445}(-x)} \exp(x) y_0(x) y_1(x) + \exp(-2x) - [y_2(x)]^2 \end{aligned}$$

with initial conditions

$$y_0(0) = 1, \quad y_1(0) = 0 \quad \text{and} \quad y_2(0) = -1$$

for the other example. In this way we simplify the structure somewhat because some of the fractional differential operators on the left-hand side can be replaced by integer-order operators. This modification is equivalent to using Theorem 8.10 instead of Theorem 8.9 in our multi-order system approach.

For the numerical solution of these systems of equations one can then use a numerical scheme for scalar fractional differential equations for each component separately. Of course one needs to take into account that the individual equations now will typically not be of the same order, so numerical methods for different orders must be used. In general, there do not seem to be any advantages in using differently constructed methods for the individual equations; rather one would usually prefer to use just one class of numerical schemes and merely change the orders of the algorithms as prescribed by the orders of the differential operators on the left-hand side of the system.

In either of the two multi-order system approaches, Edwards et al. [59] have investigated the use of the formula of [34] for the numerical solution of the resulting system of equations; later results [65] indicate that our Adams–Bashforth–Moulton method is likely to be more efficient. As far as the error is concerned, it turns out that the behaviour of the entire scheme is dominated by the component with the worst behaviour.

A comparison with the single-order system approach shows that the multi-order system approach is always applicable (there are no number-theoretic restrictions on the orders  $n_1, \dots, n_k$ ), and it will in many cases lead to a system with a considerably smaller dimension. However the structure of the left-hand side becomes more complicated.

The numerical experiments of Ford and Connolly [66] indicate that the conversion to a multi-order system via Theorem 8.10 tends to be the computationally least efficient of the approaches presented here. They found the conversion to a multi-order system via Theorem 8.9 and the approach using the transformation to single-order systems by means of Theorem 8.1 or 8.2 to be usually preferable. Which of these ideas works best seems to depend on the particular problem under consideration, so a generally valid advice cannot be given.

## Exercise

**Exercise C.1.** Give an explicit proof of Theorem C.2.

## Appendix D

### Useful Results from Analysis

In this chapter we collect some information on some concepts from Analysis that is useful in the remainder of the text.

#### D.1 Euler's Gamma Function

We begin with the Gamma function.

We recall the definition

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt$$

for  $x > 0$ . Elementary considerations from the theory of improper integrals reveal that the integral exists. Moreover, upon setting  $x = 1$  we easily see

$$\Gamma(1) = \int_0^{\infty} e^{-t} dt = \lim_{z \rightarrow \infty} \int_0^z e^{-t} dt = \lim_{z \rightarrow \infty} [-e^{-t}]_0^z = \lim_{z \rightarrow \infty} (1 - e^{-z}) = 1. \quad (\text{D.1})$$

Additionally we may, for arbitrary  $x > 0$ , manipulate the integral in the definition of the Gamma function by means of a partial integration. This yields

$$\begin{aligned} \Gamma(x+1) &= \int_0^{\infty} t^x e^{-t} dt = \lim_{z \rightarrow \infty, y \rightarrow 0+} \int_y^z t^x e^{-t} dt \\ &= \lim_{z \rightarrow \infty, y \rightarrow 0+} \left( [-e^{-t} t^x]_{t=y}^{t=z} + x \int_y^z t^{x-1} e^{-t} dt \right) \\ &= x \int_0^{\infty} t^{x-1} e^{-t} dt = x\Gamma(x). \end{aligned}$$

We have thus shown

**Theorem D.1 (Functional Equation for  $\Gamma$ ).** *If  $x > 0$  then  $x\Gamma(x) = \Gamma(x+1)$ .*

Now we may prove the all important relation between the Gamma function and the factorial:

*Proof (of Theorem 1.3).* The proof uses mathematical induction. The induction basis ( $n = 1$ ) reads  $\Gamma(1) = 0! = 1$  which is true in view of (D.1). For the induction step, we use the functional equation and the induction hypothesis:

$$\Gamma(n+1) = n\Gamma(n) = n(n-1)! = n!$$

as desired.  $\square$

There is one other important application of the functional equation of the Gamma function. We solve it for  $\Gamma(x)$ ; it then reads

$$\Gamma(x) = \frac{\Gamma(x+1)}{x} \quad (\text{D.2})$$

if  $x > 0$ . Now the expression on the right-hand side is meaningful not only if  $x > 0$  but also in the case  $-1 < x < 0$ . Therefore we may use it as a definition for the left-hand side, i.e. for  $\Gamma(x)$ , in that case (which is not covered by the original definition because the defining integral is divergent for  $x < 0$ ). Having done this extension, the Gamma function is also defined for  $-1 < x < 0$ , and we may return to (D.2) with  $x$  in that range. This allows us to extend the definition to  $-2 < x < -1$ . Proceeding in this manner, we find a definition for the Gamma function that can be applied for all  $x \in \mathbb{R}$  with the exception of those for which  $-x \in \mathbb{N}_0$ .

As a consequence of these considerations, we find another important identity involving the Gamma function:

**Theorem D.2.** *Let  $n \notin \mathbb{Z}$  and  $k \in \mathbb{N}_0$ . Then,*

$$(-1)^{k+1} \Gamma(n-k) \Gamma(k+1-n) = \Gamma(-n) \Gamma(n+1).$$

Another useful identity in this context is

**Theorem D.3 (Reflection Formula for  $\Gamma$ ).** *Let  $0 < x < 1$ . Then,*

$$\Gamma(x) \Gamma(1-x) = \frac{\pi}{\sin \pi x}.$$

It is also possible to find an alternative representation, due to Gauss, for the Gamma function. This representation actually holds for the extension indicated above. However, in practical calculations one frequently observes that the integral representation is easier to handle.

**Theorem D.4 (Gauss' Product Formula for  $\Gamma$ ).** *Let  $x \in \mathbb{R}$ ,  $-x \notin \mathbb{N}_0$ . Then,*

$$\Gamma(x) = \lim_{n \rightarrow \infty} \frac{n! n^x}{x(x+1)(x+2) \cdots (x+n)}.$$

The asymptotic behaviour of  $\Gamma(x)$  as  $x \rightarrow \infty$  is sometimes important; it can be described by the following result [2, Chapter 6].

**Theorem D.5 (Stirling's Formula).** *For  $x \rightarrow \infty$  we have*

$$\Gamma(x+1) = \left(\frac{x}{e}\right)^x \sqrt{2\pi x} (1 + o(1)).$$

One last result that we shall mention explicitly is the following integral identity. We leave the proof as an exercise.

**Theorem D.6.** *Let  $\alpha, \beta \in \mathbb{R}_+$ . Then*

$$\int_0^1 t^{\alpha-1} (1-t)^{\beta-1} dt = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)},$$

and hence

$$\int_0^x t^{\alpha-1} (x-t)^{\beta-1} dt = x^{\alpha+\beta-1} \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}.$$

The integral in the first equation of Theorem D.6 is known as *Euler's integral of the first kind* or *Euler's Beta function*  $B(\alpha, \beta)$ .

More information on the Gamma function may be found, e.g., in the classical work of Artin [6] or in the usual reference works on special functions like [2, Chapter 6] or [62, Chapter I].

## D.2 Fixed Point Theorems

The proofs of various existence and uniqueness theorems throughout this text have been based on classical theorems asserting existence or uniqueness of fixed points of certain operators.

The first of these theorems is the following generalization of Banach's fixed point theorem that we take from [189].

**Theorem D.7 (Weissinger's Fixed Point Theorem).** *Assume  $(U, d)$  to be a non-empty complete metric space, and let  $\alpha_j \geq 0$  for every  $j \in \mathbb{N}_0$  and such that  $\sum_{j=0}^{\infty} \alpha_j$  converges. Furthermore, let the mapping  $A : U \rightarrow U$  satisfy the inequality*

$$d(A^j u, A^j v) \leq \alpha_j d(u, v) \tag{D.3}$$

*for every  $j \in \mathbb{N}$  and every  $u, v \in U$ . Then,  $A$  has a uniquely determined fixed point  $u^*$ . Moreover, for any  $u_0 \in U$ , the sequence  $(A^j u_0)_{j=1}^{\infty}$  converges to this fixed point  $u^*$ .*

An immediate consequence is

**Corollary D.8 (Banach's Fixed Point Theorem).** *Assume  $(U, d)$  to be a non-empty complete metric space, let  $0 \leq \alpha < 1$ , and let the mapping  $A : U \rightarrow U$  satisfy the inequality*



$$d(Au, Av) \leq \alpha d(u, v) \quad (\text{D.4})$$

for every  $u, v \in U$ . Then,  $A$  has a uniquely determined fixed point  $u^*$ . Furthermore, for any  $u_0 \in U$ , the sequence  $(A^j u_0)_{j=1}^\infty$  converges to this fixed point  $u^*$ .

Moreover we also used a slightly different result that asserts only the existence but not the uniqueness of a fixed point. Here we may work with weaker assumptions on the operator in question. A proof may be found, e.g., in [29].

**Theorem D.9 (Schauder's Fixed Point Theorem).** *Let  $(E, d)$  be a complete metric space, let  $U$  be a closed convex subset of  $E$ , and let  $A : U \rightarrow U$  be a mapping such that the set  $\{Au : u \in U\}$  is relatively compact in  $E$ . Then  $A$  has at least one fixed point.*

In this context we recall a definition:

**Definition D.1.** Let  $(E, d)$  be a metric space and  $F \subseteq E$ . The set  $F$  is called *relatively compact in  $E$*  if the closure of  $F$  is a compact subset of  $E$ .

A helpful classical result from Analysis in connection with such sets is as follows. The proof can be found in many standard textbooks, e.g. in [30, p. 30].

**Theorem D.10 (Arzelà–Ascoli).** *Let  $F \subseteq C[a, b]$  for some  $a < b$ , and assume the sets to be equipped with the Chebyshev norm. Then,  $F$  is relatively compact in  $C[a, b]$  if  $F$  is equicontinuous (i.e. for every  $\varepsilon > 0$  there exists some  $\delta > 0$  such that for all  $f \in F$  and all  $x, x^* \in [a, b]$  with  $|x - x^*| < \delta$  we have  $|f(x) - f(x^*)| < \varepsilon$ ) and uniformly bounded (i.e. there exists a constant  $C > 0$  such that  $\|f\|_\infty \leq C$  for every  $f \in F$ ).*

### D.3 The Laplace Transform

The Laplace transform method is an extremely useful tool for the analysis of linear (fractional or classical) initial value problems. In particular, it allows us to replace a differential equation by an algebraic equation. We take the fundamental definition from the classical book of Doetsch [56] where the interested reader may find a comprehensive treatment of the Laplace transform.

**Definition D.2.** Let  $f : [0, \infty) \rightarrow \mathbb{R}$  be given. The function  $F$  defined by

$$F(s) := \mathcal{L}f(s) := \int_0^\infty f(x)e^{-sx} dx$$

is called the *Laplace transform* of  $f$  whenever the integral exists.

It is rather simple to calculate the Laplace transform of some elementary functions.

- Example D.1.* (a) For  $f(x) = \exp(ax)$  with  $a \in \mathbb{R}$  we have  $\mathcal{L}f(s) = 1/(s-a)$  whenever  $s > a$ .  
 (b) For  $f(x) = x^k$  with  $k > -1$  we find  $\mathcal{L}f(s) = \Gamma(k+1)/s^{k+1}$  whenever  $s > 0$ .  
 (c) For  $f(x) = \sin \omega x$  with  $\omega > 0$  we have  $\mathcal{L}f(s) = \omega/(s^2 + \omega^2)$ , again for  $s > 0$ .

We cite the most important rules for Laplace transforms.

**Theorem D.11.** Assume the functions  $f_1$ ,  $f_2$  and  $f_3$  to be given on  $[0, \infty)$  and to be such that their Laplace transforms exist for all  $s \geq s_0$  with some suitable  $s_0 \in \mathbb{R}$ . Then we have the following rules.

- (a) If  $f_3 = a_1 f_1 + a_2 f_2$  with arbitrary real constants  $a_1$  and  $a_2$  then

$$\mathcal{L}f_3(s) = a_1 \mathcal{L}f_1(s) + a_2 \mathcal{L}f_2(s)$$

(linearity of the Laplace transform).

- (b) If  $f_3$  is the convolution of  $f_1$  and  $f_2$ , i.e. if

$$f_3(x) = \int_0^x f_1(x-t)f_2(t) dt,$$

then

$$\mathcal{L}f_3(s) = \mathcal{L}f_1(s) \cdot \mathcal{L}f_2(s)$$

(the convolution theorem). In other words: The convolution in the original domain corresponds to the usual product in the Laplace domain.

- (c) If  $f_3(x) = \int_0^x f_1(t) dt$  then we have for  $s > \max\{0, s_0\}$

$$\mathcal{L}f_3(s) = \frac{1}{s} \mathcal{L}f_1(s)$$

(the integration theorem).

- (d) Let  $m \in \mathbb{N}$ . If  $f_3 = D^m f_1$  is the  $m$ th derivative of  $f_1$  then

$$\mathcal{L}f_3(s) = s^m \mathcal{L}f_1(s) - \sum_{k=1}^m s^{m-k} f_1^{(k-1)}(0)$$

(the differentiation theorem).

- (e) Let  $a > 0$  and  $f_3(x) = f_1(ax)$ . Then

$$\mathcal{L}f_3(s) = \frac{1}{a} \mathcal{L}f_1(s/a).$$

- (f) Let  $a \in \mathbb{R}$  and  $f_3(x) = e^{-ax} f_1(x)$ . Then

$$\mathcal{L}f_3(s) = \mathcal{L}f_1(s+a).$$

(g) Let  $m \in \mathbb{N}$  and  $f_3(x) = x^m f_1(x)$ . Then

$$\mathcal{L}f_3(s) = (-1)^m \frac{d^m}{ds^m} \mathcal{L}f_1(s).$$

(h) Let  $f_3(x) = f_1(x)/x$ . Then

$$\mathcal{L}f_3(s) = \int_s^\infty \mathcal{L}f_1(\sigma) d\sigma.$$

(i) Let  $a \in \mathbb{R}$  and

$$f_3(x) = \begin{cases} 0 & \text{for } x < a, \\ f_1(x-a) & \text{for } x \geq a. \end{cases}$$

Then

$$\mathcal{L}f_3(s) = e^{-as} \mathcal{L}f_1(s).$$

Part (d), the differentiation theorem, is of particular interest to us. Specifically this result needed to be generalized to  $m \notin \mathbb{N}$  with a suitable definition of the differential operator. We have dealt with this question in Theorem 7.1.

Of course it is not sufficient to have the Laplace transform; for practical work the inverse transform is required too. There are various ways to express this inverse; one possibility is contained in the following result. We refer to the standard books on Laplace transforms for details on the “suitable assumptions”.

**Theorem D.12.** *Under suitable assumptions on  $f$  we have*

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \exp(sx) \mathcal{L}f(s) ds.$$

Under certain conditions, the long-term behaviour of functions may also be expressed with the help of Laplace transforms, see [27, 76, 158] and the references cited therein:

**Theorem D.13 (Final Value Theorem).** *Assume that  $\mathcal{L}f$  does not have any singularities in the closed right half-plane  $\{s \in \mathbb{C} : \operatorname{Re} s \geq 0\}$ , except for possibly a simple pole at the origin. Then,*

$$\lim_{x \rightarrow \infty} f(x) = \lim_{s \rightarrow 0+} s \mathcal{L}f(s).$$

*Remark D.1.* The condition on the singularities of  $\mathcal{L}f$  is essential here: If  $\mathcal{L}f$  has a pole with positive real part, then  $f(x)$  is unbounded as  $x \rightarrow \infty$ , and if  $\mathcal{L}f$  has a pole on the imaginary axis (but not at the origin) then  $f$  has persistent oscillations, so  $\lim_{x \rightarrow \infty} f(x)$  does not exist either.

## D.4 Hadamard's Finite-Part Integral

The integral  $\int_a^b (x-a)^{-\mu} f(x) dx$  is divergent for  $\mu \geq 1$  whenever  $f(a) \neq 0$ . Nevertheless it is sometimes useful to assign a finite value to such integrals. This has been observed by Hadamard [86] in connection with solution methods for certain partial differential equations, and he introduced the following idea for the solution of this problem, known as the *finite-part integral*. We shall mainly require this concept for  $\mu \notin \mathbb{N}$ , and therefore we will restrict our attention to these values of  $\mu$ . The consideration of integer values requires some small modifications.

The Hadamard finite-part of the integral (that we will, for the sake of simplicity, denote by the same symbol as the standard integral) is, roughly speaking, defined by a Taylor expansion of  $f$  at  $x = a$  where the resulting singular integrals are defined by

$$\int_a^b (x-a)^{-\mu} dx = \frac{1}{1-\mu} (b-a)^{1-\mu} \quad (\mu > 1). \quad (\text{D.5})$$

Essentially this means that we first replace the integral  $\int_a^b (x-a)^{-\mu} dx$  by the expression  $\int_{a+\varepsilon}^b (x-a)^{-\mu} dx$  for  $\varepsilon > 0$ . This is a convergent integral; its value is simply  $(1-\mu)^{-1} [(b-a)^{1-\mu} - \varepsilon^{1-\mu}]$ . Then we let  $\varepsilon \rightarrow 0$ . Of course the limit does not exist for  $\mu \geq 1$ , and so Hadamard suggested simply to ignore the unbounded contribution  $\lim_{\varepsilon \rightarrow 0} \varepsilon^{1-\mu} / (1-\mu)$  and to assign the value of the remaining (finite) expression  $(1-\mu)^{-1} (b-a)^{1-\mu}$  – hence the name “finite-part integral”.

A precise way to define the finite-part integral is (for  $\mu \notin \mathbb{N}$ )

$$\begin{aligned} \int_a^b (x-a)^{-\mu} f(x) dx &:= \sum_{k=0}^{[\mu]-1} \frac{f^{(k)}(a)(b-a)^{k+1-\mu}}{(k+1-\mu)k!} \\ &\quad + \int_a^b (x-a)^{-\mu} R_{[\mu]-1}(x, a) dx. \end{aligned} \quad (\text{D.6a})$$

Here,

$$R_p(x, a) := \frac{1}{p!} \int_a^x (x-y)^p f^{(p+1)}(y) dy \quad (\text{D.6b})$$

is the remainder of the  $p$ th degree Taylor polynomial of  $f$  with expansion point  $a$ . It is well known that a sufficient condition for the existence of the integral (D.6a) is that  $f \in C^s[a, b]$  with  $\mu - 1 < s \in \mathbb{N}$ . This is due to the fact that then the remainder term of the Taylor expansion has a zero at  $a$  whose order is so high that the singularity in the other factor in the last integral in (D.6a) is almost being cancelled; the remaining singularity is weak and integrable in the improper sense.

An alternative representation that is helpful for us can be taken from [61, eq. (A17)]:

**Theorem D.14.** *Let  $\mu > 1$  but  $\mu \notin \mathbb{N}$  and  $m := \lceil \mu - 1 \rceil$ . For  $f \in C^m[a, b]$  we have*

$$\frac{1}{\Gamma(1-\mu)} \int_a^b (b-x)^{-\mu} f(x) dx = \sum_{k=0}^{m-1} \frac{(b-a)^{k-\mu+1}}{\Gamma(k-\mu+2)} f^{(k)}(a) + J_a^{m-\mu+1} f^{(m)}(b).$$

We mention here the most important properties of the finite-part integral:

- In contrast to the classical Riemann or Lebesgue integral, the finite-part integral is not a positive functional, i.e. the inequality

$$\left| \int_a^b (x-a)^{-\mu} f(x) dx \right| \leq \int_a^b (x-a)^{-\mu} |f(x)| dx$$

is not true in general.

- The finite-part integral is a consistent extension of the concept of regular integrals, i.e. whenever the integral  $\int_a^b (x-a)^{-\mu} f(x) dx$  exists in the classical sense, then it also exists in the finite-part sense, and the two integrals have the same value.
- The finite-part integral is additive with respect to the union of integration intervals and invariant with respect to translation.
- The finite-part integral is linear.
- The usual change-of-variables rule remains valid if  $\mu \notin \mathbb{N}$ .

A very useful result on these integrals is as follows.

**Theorem D.15.** *Let  $f \in C^k[a, b]$  for some  $k \in \mathbb{N}_0$ , and let  $p < k$ . Then, for  $a < x < b$ ,*

$$\frac{d}{dx} \int_a^x f(t)(x-t)^{-p} dt = -p \int_a^x f(t)(x-t)^{-p-1} dt.$$

We leave the proof as an exercise to the reader.

## D.5 Approximation Theory

A well-known concept from approximation theory that we had to use in the proof of Theorem 2.25 was the *Bernstein polynomial*. A classical reference is the book of Lorentz [117]. The definition is

$$B_N[f](t) := \sum_{k=0}^N \binom{N}{k} t^k (1-t)^{N-k} f\left(\frac{k}{N}\right)$$

where  $f : [0, 1] \rightarrow \mathbb{R}$ . The fundamental result that we require is a convergence theorem:

**Theorem D.16.** *Let  $f \in C^\ell[0, 1]$  for some  $\ell \in \mathbb{N}_0$ . Then, for all  $\mu \in \{0, 1, 2, \dots, \ell\}$ , the sequence  $(D^\mu B_N[f])_{N=1}^\infty$  converges uniformly towards  $D^\mu f$ .*

A proof may be found in [117, §1.8].

## Exercises

**Exercise D.1.** Give a proof for Theorem D.6.

**Exercise D.2.** Give a proof for Theorem D.2.

**Exercise D.3.** Prove the relations stated in Example D.1.

**Exercise D.4.** Evaluate the finite-part integral  $\int_0^1 x^{-\mu} dx$  for  $\mu > 1$ .

**Exercise D.5.** Give a proof for Theorem D.15.

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