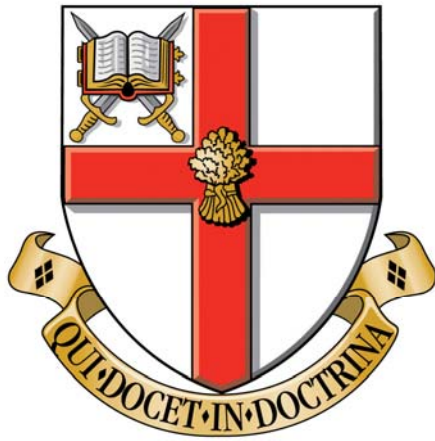


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# DETAILED ERROR ANALYSIS FOR A FRACTIONAL ADAMS METHOD\*

KAI DIETHELM<sup>†</sup>, NEVILLE J. FORD<sup>‡</sup>, AND ALAN D. FREED<sup>§</sup>

**Abstract.** We investigate a method for the numerical solution of the nonlinear fractional differential equation  $D_*^\alpha y(t) = f(t, y(t))$ , equipped with initial conditions  $y^{(k)}(0) = y_0^{(k)}$ ,  $k = 0, 1, \dots, [\alpha] - 1$ . Here  $\alpha$  may be an arbitrary positive real number, and the differential operator is the Caputo derivative. The numerical method can be seen as a generalization of the classical one-step Adams-Bashforth-Moulton scheme for first-order equations. We give a detailed error analysis for this algorithm. This includes, in particular, error bounds under various types of assumptions on the equation. Asymptotic expansions for the error are also mentioned briefly. The latter may be used in connection with Richardson's extrapolation principle to obtain modified versions of the algorithm that exhibit faster convergence behaviour.

**Key words.** Fractional differential equation, Caputo derivative, Adams-Bashforth-Moulton method.

**AMS subject classifications.** Primary 65L06; secondary 26A33, 65B05, 65L05, 65L20, 65R20.

**1. Introduction.** We discuss a numerical method for the fractional initial value problem

$$(1.1) \quad D_*^\alpha y(t) = f(t, y(t)), \quad y^{(k)}(0) = y_0^{(k)}, \quad k = 0, 1, \dots, [\alpha] - 1,$$

where the  $y_0^{(k)}$  may be arbitrary real numbers and where  $\alpha > 0$ . In (1.1),  $D_*^\alpha$  denotes the differential operator in the sense of Caputo [19], defined by

$$D_*^\alpha z(t) = J^{\beta-\alpha} D^\beta z(t)$$

where  $\beta := [\alpha]$  is the smallest integer  $\geq \alpha$ . Here  $D^\beta$  is the usual differential operator of (integer) order  $\beta$ , and for  $\mu > 0$ ,  $J^\mu$  is the Riemann-Liouville integral operator of order  $\mu$ , defined by

$$J^\mu z(t) = \frac{1}{\Gamma(\mu)} \int_0^t (t-u)^{\mu-1} z(u) du.$$

Equations of this type arise in a number of applications where models based on fractional calculus are used. Some early examples for such models are given in the book of Oldham and Spanier [33] (diffusion processes) and the classical papers of Caputo [5], Caputo and Mainardi [6, 7] and Torvik and Bagley [41] (these papers dealing with the modeling of materials) as well as in the publications of Marks and Hall [28] (signal processing) and Olmstead and Handelsman [34] (also dealing with diffusion problems); more recent results are described, e.g., in the work of Benson [2] (advection and dispersion of solutes in natural porous or fractured media), Chern [8] and Diethelm and

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Freed [13, 14, 15] (modeling of the behaviour of viscoelastic and viscoplastic materials under external influences), Gaul, Klein, and Kempfle [16] (description of mechanical systems subject to damping), Glöckle and Nonnenmacher [17] (relaxation and reaction kinetics of polymers), Gorenflo and Rutman [21] (so-called ultraslow processes), Gorenflo, Mainardi et al. [18, 20, 27, 39] (connections to the theory of random walks, the latter two papers especially with respect to applications to mathematical models in finance), Metzler et al. [30] (relaxation in filled polymer networks), Podlubny [35] (control theory), Podlubny et al. [37] (heat propagation), and Shaw, Warby and Whiteman [40] (modeling of viscoelastic materials). Surveys or collections of applications can also be found in Gorenflo and Mainardi [19], Mainardi [26], Matignon and Montseny [29], Nonnenmacher and Metzler [32] and Podlubny [36]. Finally we refer to the work of Woon [43] that essentially mentions mathematical applications that, in turn, have important implications in other sciences like physics. Note that many of those papers formally use Riemann-Liouville fractional derivatives instead of Caputo derivatives. Typically those authors then require homogeneous initial conditions. It is known [36] that under those homogeneous conditions the equations with Riemann-Liouville operators are equivalent to those with Caputo operators. We chose the Caputo version because it allows us to specify inhomogeneous initial conditions too if this is desired. For the Riemann-Liouville approach, this generalization is connected with major practical difficulties; cf., e.g., [12, 15].

It is well known that the initial value problem (1.1) is equivalent to the Volterra integral equation

$$(1.2) \quad y(t) = \sum_{\nu=0}^{[\alpha]-1} y_0^{(\nu)} \frac{t^\nu}{\nu!} + \frac{1}{\Gamma(\alpha)} \int_0^t (t-u)^{\alpha-1} f(u, y(u)) du$$

in the sense that a continuous function is a solution of (1.1) if and only if it is a solution of (1.2). For a brief derivation we refer to [11, Lemma 2.3].

In order to indicate the approach that we will use for the fractional equation and to help highlight the distinctive features of our method, we shall first briefly recall the idea behind the classical one-step 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

$$(1.3a) \quad Dy(t) = f(t, y(t)),$$

$$(1.3b) \quad y(0) = y_0.$$

We assume the function  $f$  to be such that a unique solution exists on some interval  $[0, T]$ , say. Following [22, §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  $h = T/N$ . 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

$$(1.4) \quad y(t_{k+1}) = y(t_k) + \int_{t_k}^{t_{k+1}} f(z, y(z)) dz.$$

This equation follows upon integration of (1.3a) on the interval  $[t_k, t_{k+1}]$ . Of course, we know neither of the expressions on the right-hand side of eq. (1.4) 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

$$(1.5) \quad \int_a^b g(z) dz \approx \frac{b-a}{2} (g(a) + g(b)),$$

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

$$(1.6) \quad y_{k+1} = y_k + \frac{h}{2} [f(t_k, y(t_k)) + f(t_{k+1}, y(t_{k+1}))],$$

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

$$(1.7) \quad y_{k+1} = y_k + \frac{h}{2} [f(t_k, y_k) + f(t_{k+1}, y_{k+1})].$$

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 eq. (1.7) 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

$$(1.8) \quad \int_a^b g(z) dz \approx (b-a)g(a),$$

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

$$(1.9) \quad y_{k+1}^P = y_k + hf(t_k, y_k).$$

It is well known [22, p. 372] that the process defined by eq. (1.9) and

$$(1.10) \quad y_{k+1} = y_k + \frac{h}{2} (f(t_k, y_k) + f(t_{k+1}, y_{k+1}^P)),$$

called the one-step Adams-Bashforth-Moulton method, is convergent of order 2, i.e.

$$(1.11) \quad \max_{j=0,1,\dots,N} |y(t_j) - y_j| = O(h^2).$$

Moreover, this method behaves satisfactorily from the point of view of its numerical stability [23, 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 eq. (1.9), then we evaluate  $f(t_{k+1}, y_{k+1}^P)$ , use this to calculate the corrector in eq. (1.10), and finally evaluate  $f(t_{k+1}, y_{k+1})$ . This result is stored for future use in the next integration step.

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 (1.4). Fortunately, such an equation is available, namely eq. (1.2). This equation looks somewhat different from eq. (1.4), 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. It is straightforward in principle to construct a formula that generalizes the Adams method to fractional equations. However now the discrete equations we derive have unbounded memory and are therefore of a class that is more challenging to analyze than in the classical case. One cannot expect insights from the classical case to carry over to the fractional Adams method, as we shall see in the sequel.

To construct the required formula, we use the product trapezoidal quadrature formula with respect to the weight function  $(t_{k+1} - \cdot)^{\alpha-1}$  to replace the integral, where nodes  $t_j$  ( $j = 0, 1, \dots, k+1$ ) are used as before. In other words, we apply the approximation

$$(1.12) \quad \int_0^{t_{k+1}} (t_{k+1} - z)^{\alpha-1} g(z) dz \approx \int_0^{t_{k+1}} (t_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz,$$

where  $\tilde{g}_{k+1}$  is the piecewise linear interpolant for  $g$  with nodes and knots chosen at the  $t_j$ ,  $j = 0, 1, 2, \dots, k+1$ . As stated in [25] (see also [1, 4]) the product integration idea is a rather natural approach in this situation. Using standard techniques from quadrature theory (cf. [13]), we write the integral on the right-hand side of (1.12) as

$$(1.13) \quad \int_0^{t_{k+1}} (t_{k+1} - z)^{\alpha-1} \tilde{g}_{k+1}(z) dz = \sum_{j=0}^{k+1} a_{j,k+1} g(t_j)$$

where

$$(1.14) \quad a_{j,k+1} = \frac{h^\alpha}{\alpha(\alpha+1)} \times \begin{cases} (k^{\alpha+1} - (k-\alpha)(k+1)^\alpha) & \text{if } j = 0, \\ ((k-j+2)^{\alpha+1} + (k-j)^{\alpha+1} - 2(k-j+1)^{\alpha+1}) & \text{if } 1 \leq j \leq k, \\ 1 & \text{if } j = k+1. \end{cases}$$

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

$$(1.15) \quad y_{k+1} = \sum_{j=0}^{\lceil \alpha \rceil - 1} \frac{t_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(\alpha)} \left( \sum_{j=0}^k a_{j,k+1} f(t_j, y_j) + a_{k+1,k+1} f(t_{k+1}, y_{k+1}^P) \right).$$

The remaining problem is the determination of the predictor formula required to calculate  $y_{k+1}^P$ . 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 eq. (1.2) by the product rectangle rule

$$(1.16) \quad \int_0^{t_{k+1}} (t_{k+1} - z)^{\alpha-1} g(z) dz \approx \sum_{j=0}^k b_{j,k+1} g(t_j),$$

where now

$$(1.17) \quad b_{j,k+1} = \frac{h^\alpha}{\alpha} ((k+1-j)^\alpha - (k-j)^\alpha)$$

(see also [13]). Thus, the predictor  $y_{k+1}^P$  is determined by the fractional Adams-Bashforth method

$$(1.18) \quad y_{k+1}^P = \sum_{j=0}^{\lceil \alpha \rceil - 1} \frac{t_{k+1}^j}{j!} y_0^{(j)} + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} f(t_j, y_j).$$

Our basic algorithm, the fractional Adams-Bashforth-Moulton method, is completely described now by eqs. (1.18) and (1.15) with the weights  $a_{j,k+1}$  and  $b_{j,k+1}$  being defined according to (1.14) and (1.17), respectively.

We have thus completed the description of our numerical algorithm. The remainder of this paper will be devoted to the error analysis for this scheme. For this purpose, we shall first (in §2) present some auxiliary results, and then (in §3) we will use these results to give a thorough investigation of the error. Finally, in §4 we will present some numerical examples illustrating the theoretical results.

**2. Auxiliary Results.** Throughout the rest of the paper we assume that the Adams method (with the predictor given by (1.18) and the corrector as in (1.15)) is used to solve the initial value problem (1.1). As usual we demand that the function  $f$  is continuous and fulfils a Lipschitz condition with respect to its second argument with Lipschitz constant  $L$  on a suitable set  $G$ . Then, by [11, Thms. 2.1 and 2.2], a uniquely determined solution  $y$  of the problem exists on some interval  $[0, T]$ , say. It is this solution that we aim to approximate.

For the error analysis it is useful to know additional properties of the solution. Specifically, we require information about the smoothness. From [24, §2] we take the following result (note that  $\alpha$  in that paper corresponds to  $\alpha - 1$  in our work).

**THEOREM 2.1.**

(a) Assume that  $f \in C^2(G)$ . Define  $\hat{\nu} := \lceil 1/\alpha \rceil - 1$ . Then there exist a function  $\psi \in C^1[0, T]$  and some  $c_1, \dots, c_{\hat{\nu}} \in \mathbb{R}$  such that the solution  $y$  of (1.1) can be expressed in the form

$$y(t) = \psi(t) + \sum_{\nu=1}^{\hat{\nu}} c_{\nu} t^{\nu\alpha}.$$

(b) Assume that  $f \in C^3(G)$ . Define  $\hat{\nu} := \lceil 2/\alpha \rceil - 1$  and  $\tilde{\nu} := \lceil 1/\alpha \rceil - 1$ . Then there exist a function  $\psi \in C^2[0, T]$  and some  $c_1, \dots, c_{\hat{\nu}} \in \mathbb{R}$  and  $d_1, \dots, d_{\tilde{\nu}} \in \mathbb{R}$  such that the solution  $y$  of (1.1) can be expressed in the form

$$y(t) = \psi(t) + \sum_{\nu=1}^{\hat{\nu}} c_{\nu} t^{\nu\alpha} + \sum_{\nu=1}^{\tilde{\nu}} d_{\nu} t^{1+\nu\alpha}.$$

Moreover it is useful to relate the smoothness properties of a given function to the smoothness properties of its Caputo derivatives. In this context we state a quite simple theorem.

**THEOREM 2.2.** If  $y \in C^m[0, T]$  for some  $m \in \mathbb{N}$  and  $0 < \alpha < m$  then

$$D_*^\alpha y(t) = \sum_{\ell=0}^{m-\lceil\alpha\rceil-1} \frac{y^{(\ell+\lceil\alpha\rceil)}(0)}{\Gamma(\lceil\alpha\rceil - \alpha + \ell + 1)} t^{\lceil\alpha\rceil - \alpha + \ell} + g(t)$$

with some function  $g \in C^{m-\lceil\alpha\rceil}[0, T]$ . Moreover, the  $(m - \lceil\alpha\rceil)$ th derivative of  $g$  satisfies a Lipschitz condition of order  $\lceil\alpha\rceil - \alpha$ .

*Proof.* This is a direct consequence of the definition of the Caputo differential operator and [38, Thm. 3.2].  $\square$

Note that this immediately yields a very elementary but useful corollary that generalizes the classical result for derivatives of integer order.

**COROLLARY 2.3.** Let  $y \in C^m[0, T]$  for some  $m \in \mathbb{N}$  and assume that  $0 < \alpha < m$ . Then  $D_*^\alpha y \in C[0, T]$ .

Very simple counterexamples show that such a result cannot hold for the Riemann-Liouville derivatives. We therefore interpret this corollary as an indication for the practical usefulness of the Caputo derivatives. However, we explicitly point out that we can only prove the continuity of  $D_*^\alpha y$  but not the differentiability. The representation from Theorem 2.2 reveals that differentiability will in general only hold if certain (integer-order) derivatives of  $y$  vanish at the origin. Since the deeper investigation of this topic is outside the scope of this paper, we shall not pursue it any further here.

What we do 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 2.4.

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

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

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

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

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

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

$$\begin{aligned} & \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \\ (2.1) \quad &= \sum_{j=0}^k \int_{jh}^{(j+1)h} (t_{k+1} - t)^{\alpha-1} (z(t) - z(t_j)) dt. \end{aligned}$$

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 (2.1) and derive

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



Here the term in parentheses is simply the remainder of the standard rectangle quadrature formula, applied to the function  $t^\alpha$ , and taken over the interval  $[0, k+1]$ . Since the integrand is monotonic, we may apply some standard results from quadrature theory [3, Thm. 97] to find that this term is bounded by the total variation of the integrand, viz. the quantity  $(k+1)^\alpha$ . Thus,

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

Similarly, to prove (b), we use the monotonicity of  $z$  in (2.1) and derive

$$\begin{aligned} & \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} z(t) dt - \sum_{j=0}^k b_{j,k+1} z(t_j) \right| \\ & \leq \sum_{j=0}^k |z(t_{j+1}) - z(t_j)| \int_{jh}^{(j+1)h} (t_{k+1} - t)^{\alpha-1} dt \\ & = \frac{h^{\alpha+p}}{\alpha} \sum_{j=0}^k ((j+1)^p - j^p) ((k+1-j)^\alpha - (k-j)^\alpha) \\ & \leq \frac{h^{\alpha+p}}{\alpha} \left( 2(k+1)^\alpha - 2k^\alpha + p\alpha \sum_{j=1}^{k-1} j^{p-1} (k-j+q)^{\alpha-1} \right) \\ & \leq \frac{h^{\alpha+p}}{\alpha} \left( 2\alpha(k+q)^{\alpha-1} + p\alpha \sum_{j=1}^{k-1} j^{p-1} (k-j+q)^{\alpha-1} \right) \end{aligned}$$

by additional applications of the Mean Value Theorem. Here  $q = 0$  if  $\alpha \leq 1$ , and  $q = 1$  otherwise. In either case a brief asymptotic analysis using the Euler-MacLaurin formula [42, Thm. 3.7] yields that the term in parentheses is bounded from above by  $C_{\alpha,p}(k+1)^{p+\alpha-1}$  where  $C_{\alpha,p}$  is a constant depending on  $\alpha$  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 2.4; we therefore omit the details.

THEOREM 2.5.

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

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

(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  $B_{\alpha,\mu}^{\text{Tr}}$  (depending only on  $\alpha$  and  $\mu$ ) and  $M(z, \mu)$  (depending only on  $z$  and  $\mu$ ) such that

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

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

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

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

REMARK 2.1. Notice that in part (c) of Theorem 2.5 it may happen that  $\alpha < 1$  and  $p < 1$ . This implies  $\varrho = p+1$ . Thus, the exponent of  $t_{k+1}$  on the right-hand side of the inequality is equal to  $\alpha - 1$  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 2.4 (b).

**3. Error Analysis for the Adams Method.** In this section we present the main results of this paper, namely the theorems 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  $\alpha < 1$  or  $\alpha > 1$ . Moreover, the smoothness properties of the given function  $f$  and the unknown solution  $y$  play an important role. In view of Theorem 2.1, 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.

**3.1. A general result.** Based on the error estimates of §2 we shall now present a general convergence result for the Adams-Bashforth-Moulton method. In the subsections below we shall specialize this result to particularly important special cases.

LEMMA 3.1. Assume that the solution  $y$  of the initial value problem is such that

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

and

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

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

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

$$(3.1) \quad |y(t_j) - y_j| \leq Ch^q$$

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 (3.1) 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

$$\begin{aligned}
 |y(t_{k+1}) - y_{k+1}^P| &= \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} f(t, y(t)) dt - \sum_{j=0}^k b_{j,k+1} f(t_j, y_j) \right| \\
 &\leq \frac{1}{\Gamma(\alpha)} \left| \int_0^{t_{k+1}} (t_{k+1} - t)^{\alpha-1} D_*^\alpha y(t) dt - \sum_{j=0}^k b_{j,k+1} D_*^\alpha y(t_j) \right| \\
 &\quad + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} |f(t_j, y(t_j)) - f(t_j, y_j)| \\
 (3.2) \quad &\leq \frac{C_1 t_{k+1}^{\gamma_1}}{\Gamma(\alpha)} h^{\delta_1} + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^k b_{j,k+1} LC h^q \leq \frac{C_1 T^{\gamma_1}}{\Gamma(\alpha)} h^{\delta_1} + \frac{CLT^\alpha}{\Gamma(\alpha+1)} h^q.
 \end{aligned}$$

In this derivation, 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

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

On the basis of the bound (3.2) for the predictor error we begin the analysis of the corrector error. We recall the relation (1.14) which we shall use in particular for  $j = k + 1$  and find, arguing in a similar way to above, that

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

in view of the nonnegativity of  $\gamma_1$  and  $\gamma_2$  and the relations  $\delta_2 \leq q$  and  $\delta_1 + \alpha \leq q$ . 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  $Ch^q$ .  $\square$

**3.2. Error bounds under smoothness assumptions on the solution.** First we assume that the given data is such that the solution  $y$  itself is sufficiently differentiable. As mentioned above, the result depends on whether  $\alpha > 1$  or  $\alpha < 1$ .

**THEOREM 3.2.** *Let  $0 < \alpha$  and assume  $D_*^\alpha y \in C^2[0, T]$  for some suitable  $T$ . Then,*

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

Before we come to the proof, we note one particular point: The order of convergence depends on  $\alpha$ , and it is a non-decreasing function of  $\alpha$ . This is due to the fact that we discretize the integral operator in (1.2) which behaves more smoothly (and hence can be approximated with a higher accuracy) as  $\alpha$  increases. In contrast, the method of [10] uses a different approach; it is based on a direct discretization of the differential operator in (1.1). The smoothness properties of this operator (and thus the ease with which it may be approximated) deteriorate as  $\alpha$  increases, and so we find that the convergence order of the method from [10] is a non-increasing function of  $\alpha$ ; in particular no convergence is achieved there for  $\alpha \geq 2$ . It is a distinctive advantage of the Adams scheme presented here that it converges for all  $\alpha > 0$ .

*Proof of Theorem 3.2.* In view of Theorems 2.4 and 2.5, we may apply Lemma 3.1 with  $\gamma_1 = \gamma_2 = \alpha > 0$ ,  $\delta_1 = 1$  and  $\delta_2 = 2$ . Thus we find an  $O(h^q)$  error bound where

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

Note that in a certain sense the theorem above deals with the “optimal” situation: The function that we approximate in our process is  $f(\cdot, y(\cdot)) = D_*^\alpha y$ . 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 [3], that this function is in  $C^2$  on the interval of integration. This is precisely the setting discussed in Theorem 3.2. 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.

There is of course a disadvantage in the formulation of the hypotheses of the theorem: They are stated in terms of the solution  $y$  (or, more precisely, its Caputo derivative of order  $\alpha$ ), which is unknown in general. Even though it is sometimes possible to determine the smoothness properties of  $D_*^\alpha y$  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 the topic of the next subsection.

Before we come to those results however, we want to give some more information under assumptions similar to those of the previous theorem. 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  $D_*^\alpha y$ . If this were true, and most of the numerical results shown in §4 indicate this, we could construct a Richardson extrapolation algorithm [42] based on

the Adams scheme. The use of this extrapolation procedure then would permit us to obtain more accurate numerical approximations for the desired solution.

CONJECTURE 3.1. *Let  $\alpha > 0$  and assume that  $D_*^\alpha y \in C^k[0, T]$  for some  $k \geq 3$  and some suitable  $T$ . Then,*

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

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

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

Our belief in the truth of this conjecture is not only supported by the numerical results but also by the results of de Hoog and Weiss [9, §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  $D_*^\alpha y$ . Now we want to replace this by similar assumptions on  $y$  itself. In view of Theorem 2.2 we must be aware of the fact that smoothness of  $y$  in general implies non-smoothness of  $D_*^\alpha y$  (the function that we have to approximate), so some difficulties are likely. Fortunately Theorem 2.2 also informs us about the precise nature of the singularities in the derivatives of  $D_*^\alpha y$ . We can exploit this information to obtain the following results.

THEOREM 3.3. *Let  $\alpha > 1$  and assume that  $y \in C^{1+\lceil\alpha\rceil}[0, T]$  for some suitable  $T$ . Then,*

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

*Proof.* By Theorem 2.2 we find that  $D_*^\alpha y(x) = cx^{\lceil\alpha\rceil} + g(x)$  where  $g \in C^1[0, T]$  and  $g'$  fulfils a Lipschitz condition of order  $\lceil\alpha\rceil - \alpha$ . Thus, according to Theorems 2.4 and 2.5 we can apply Lemma 3.1 with  $\gamma_1 = 0$ ,  $\gamma_2 = \alpha - 1 > 0$ ,  $\delta_1 = 1$  and  $\delta_2 = 1 + \lceil\alpha\rceil - \alpha$ . Because of  $\alpha > 1$  we then find that  $\delta_1 + \alpha = 1 + \alpha > 2 > \delta_2$ , and hence  $\min\{\delta_1 + \alpha, \delta_2\} = \delta_2$ . So the overall error bound is  $O(h^{\delta_2})$ .  $\square$

Notice that a reformulation of Theorem 3.3 yields that, if  $1 < \alpha = k_1 + k_2$  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  $\alpha$  plays the decisive role for the order of the error. In particular, we find slow convergence if the fractional part of  $\alpha$  is large. Consequently, under these assumptions we cannot expect the convergence order to be a monotone function of  $\alpha$  any more. Nevertheless we can prove that the method converges for all  $\alpha > 0$ :

THEOREM 3.4. *Let  $0 < \alpha < 1$  and assume that  $y \in C^2[0, T]$  for some suitable  $T$ . Then, for  $1 \leq j \leq N$  we have*

$$(3.3) \quad |y(t_j) - y_j| \leq C t_j^{\alpha-1} \times \begin{cases} h^{1+\alpha} & \text{if } 0 < \alpha < 1/2, \\ h^{2-\alpha} & \text{if } 1/2 \leq \alpha < 1, \end{cases}$$

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

We obtain two immediate consequences.

COROLLARY 3.5. *Under the assumptions of Theorem 3.4, we have*

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

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

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

*Proof of Theorem 3.4.* The first steps of the proof are as in the proof of Theorem 3.3. The key difference is that now  $\gamma_2 < 0$  (note that we still have  $\gamma_2 = \alpha - 1$ , but now  $\alpha < 1$ ). Thus we cannot apply Lemma 3.1. Instead we modify its proof so that it fits to our requirements: We keep the inductive structure and remember that our claim is now (3.3) rather than (3.1). With this change in the induction hypothesis we proceed much as in the proof of Lemma 3.1. 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  $0 \leq b_{j,k+1} \leq h^\alpha (k-j)^{\alpha-1}$  and  $0 \leq a_{j,k+1} \leq ch^\alpha (k-j)^{\alpha-1}$  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  $S_k := \sum_{j=1}^{k-1} j^{\gamma_2} (k-j)^{\alpha-1}$ . Under our assumptions, both the exponents  $\gamma_2$  and  $\alpha - 1$  are in the interval  $(0, 1)$ , and then it is easily seen that  $S_k = O(k^{\gamma_2+\alpha})$ . Using this relation we can complete the proof of Theorem 3.4 by following along the lines of the rest of the proof of Lemma 3.1.  $\square$

### 3.3. Error bounds under smoothness assumptions on the given data.

We conclude the section on 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 cases  $\alpha > 1$  and later discuss properties of the numerical scheme when  $\alpha < 1$ .

THEOREM 3.6. *Let  $\alpha > 1$ . Then, if  $f \in C^3(G)$ ,*

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

*Proof.* We begin by discussing the case  $\alpha \geq 2$ . Then, according to the results of Miller and Feldstein [31, §4], we find that  $y \in C^2[0, T]$ . Thus, in view of the smoothness assumption on  $f$  and the chain rule,  $D_*^\alpha y := f(\cdot, y(\cdot)) \in C^2[0, T]$  too, and the claim follows by virtue of Theorem 3.2.

For the case  $1 < \alpha < 2$ , we want to apply Lemma 3.1 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 [31, §5] from which we derive that  $y(t) = ct^\alpha + \psi(t)$  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  $\alpha > 2$  above we can then deduce  $D_*^\alpha y \in C^1[0, T]$  too, and by Theorem 2.4(a), we find that we may choose  $\gamma_1 = \alpha$  and  $\delta_1 = 1$ . Moreover, the structural information on  $y$  combined with the identity  $D_*^\alpha y = f(\cdot, y(\cdot))$  and the chain rule, yields that  $D^2[D_*^\alpha y](t) = \hat{c}t^{\alpha-2} + \hat{\psi}(t)$  with some  $\hat{c} \in \mathbb{R}$  and some  $\hat{\psi} \in C[0, T]$ . Thus,  $y(t) = \tilde{c}t^\alpha + \tilde{\psi}(t)$  with some  $\tilde{c} \in \mathbb{R}$  and some  $\tilde{\psi} \in C^2[0, T]$ , and by Theorem 2.5(a) and (c) the correct values for the remaining quantities are  $\gamma_2 = \min\{\alpha, 2\alpha - 2\} = 2\alpha - 2 \geq 0$  and  $\delta_2 = 2$ . The claim then follows from Lemma 3.1.  $\square$

In the case  $\alpha < 1$  the situation seems to be less clear. According to Theorem 2.1 smoothness conditions on  $f$  imply that the exact solution is of the form

$$y(t) = \psi(t) + \sum_{\nu=1}^{\bar{\nu}} c_{\nu} t^{\nu\alpha} + \sum_{\nu=1}^{\bar{\nu}} d_{\nu} t^{1+\nu\alpha}$$

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 [24] 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  $O(h^{2\alpha})$  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 what we see in the experiment reported in Table 4.5 and other computations that we have performed, we believe the following conjecture to be true.

CONJECTURE 3.2. *Let  $0 < \alpha < 1$ . Then, if  $f \in C^2(G)$ , for every  $\epsilon > 0$  we have*

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

**4. Numerical Examples.** In this section we present some numerical examples to illustrate the error bounds derived above. We shall distinguish various cases according to the smoothness properties of the functions involved. We only considered examples where  $0 < \alpha < 2$  since the case  $\alpha \geq 2$  does not seem to be of major practical interest.

All computations were done in double precision arithmetic on a Pentium PC.

**4.1. Equations where  $D_*^\alpha y$  is smooth.** Our first example deals with the case that the unknown solution  $y$  has a smooth derivative of order  $\alpha$ . This is the case described in Theorem 3.2. Specifically we shall look at the equation

$$(4.1) \quad D_*^\alpha y(t) = \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3 \frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4} \Gamma(\alpha+1) + \left( \frac{3}{2} t^{\alpha/2} - t^4 \right)^3 - [y(t)]^{3/2}.$$

The initial conditions were chosen to be homogeneous ( $y(0) = 0$ ,  $y'(0) = 0$ ; the latter only in the case  $\alpha > 1$ ). The exact solution of this initial value problem is

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

and hence

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

i.e.  $D_*^\alpha y \in C^2[0, T]$  for arbitrary  $T > 0$  if  $\alpha \leq 4$ , and thus the conditions of Theorem 3.2 are fulfilled. Moreover, assuming that Conjecture 3.1 holds, the application of Richardson extrapolation is also justified. We display some of the results in Tables 4.1 and 4.2. In each case, the leftmost column shows the step size used; the following

column gives the error of our scheme at  $t = 1$ , 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  $1 + \alpha$ ,  $2$ ,  $2 + \alpha$ ,  $3 + \alpha$ ,  $4$ ,  $4 + \alpha$ ,  $\dots$  in the case  $0 < \alpha < 1$  and  $2$ ,  $1 + \alpha$ ,  $2 + \alpha$ ,  $4$ ,  $3 + \alpha$ ,  $4 + \alpha$ ,  $\dots$  for  $1 < \alpha < 2$ . The numerical data in the following tables show that these values are reproduced approximately at least for  $\alpha > 1$  (see Table 4.1). In the case  $0 < \alpha < 1$ , displayed in Table 4.2, the situation seems to be less obvious. Apparently, we need to use much smaller values for  $h$  than in the case  $\alpha > 1$  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.

As usual, the notation  $-5.53(-3)$  stands for  $-5.53 \cdot 10^{-3}$ , etc.

TABLE 4.1  
Errors for eq. (4.1) with  $\alpha = 1.25$ , taken at  $t = 1$ .

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 4.2  
Errors for eq. (4.1) with  $\alpha = 0.25$ , taken at  $t = 1$ .

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	

**4.2. Equations where  $y$  is smooth.** Next we come to the case that the unknown solution  $y$  itself is a smooth function. This is the case described in Theorems 3.3 and 3.4 and in Corollary 3.5. Specifically we shall look at the very simple linear equation

$$(4.2) \quad D_*^\alpha y(t) = \begin{cases} \frac{2}{\Gamma(3-\alpha)} t^{2-\alpha} - y(t) + t^2 - t & \text{for } \alpha > 1, \\ \frac{2}{\Gamma(3-\alpha)} t^{2-\alpha} - \frac{1}{\Gamma(2-\alpha)} t^{1-\alpha} - y(t) + t^2 - t & \text{for } \alpha \leq 1. \end{cases}$$



The initial values were chosen as  $y(0) = 0$  and (for  $\alpha > 1$ ) as  $y'(0) = -1$ . The true solution is

$$y(t) = t^2 - t.$$

In Tables 4.3 and 4.4 we show the errors of the Adams method at the point  $t = 1$  for various step sizes and various values of  $\alpha$ . In each case, the last row again states the experimental order of convergence. No extrapolation has been attempted. The theoretical findings of Theorems 3.4 (more precisely stated in the second part of Corollary 3.5) and 3.3 are reproduced approximately: In Table 4.3 we find an EOC close to  $1 + \alpha$  in the first three columns (corresponding to the case  $\alpha \leq 1/2$ ) and an EOC near  $2 - \alpha$  in the other columns where  $1/2 < \alpha < 1$ . Similarly, in Table 4.4 we see that the EOC is always close to  $2 - k_2$  where  $k_2 = \alpha - [\alpha]$  is the fractional part of  $\alpha$ .

TABLE 4.3  
Errors for eq. (4.2) with  $\alpha < 1$ , taken at  $t = 1$ .

$h$	$\alpha = 0.1$	$\alpha = 0.3$	$\alpha = 0.5$	$\alpha = 0.7$	$\alpha = 0.9$
1/10	-1.03(-1)	-3.14(-2)	-1.44(-2)	-1.05(-2)	-1.49(-2)
1/20	-4.95(-2)	-1.10(-2)	-4.52(-3)	-3.38(-3)	-6.08(-3)
1/40	-2.09(-2)	-3.91(-3)	-1.46(-3)	-1.14(-3)	-2.62(-3)
1/80	-8.65(-3)	-1.42(-3)	-4.81(-4)	-3.99(-4)	-1.16(-3)
1/160	-3.59(-3)	-5.26(-4)	-1.62(-4)	-1.44(-4)	-5.28(-4)
1/320	-1.51(-3)	-1.98(-4)	-5.52(-5)	-5.31(-5)	-2.42(-4)
EOC	1.25	1.41	1.55	1.44	1.12

TABLE 4.4  
Errors for eq. (4.2) with  $\alpha > 1$ , taken at  $t = 1$ .

$h$	$\alpha = 1.25$	$\alpha = 1.5$	$\alpha = 1.85$
1/10	6.74(-4)	9.14(-3)	4.69(-2)
1/20	3.63(-4)	3.42(-3)	2.15(-2)
1/40	1.43(-4)	1.25(-3)	9.75(-3)
1/80	5.00(-5)	4.49(-4)	4.41(-3)
1/160	1.65(-5)	1.61(-4)	1.99(-3)
1/320	5.28(-6)	5.71(-5)	8.98(-4)
EOC	1.65	1.49	1.15

**4.3. Equations where  $f$  is smooth.** Finally we present an example where the given function  $f$  (the right-hand side of the differential equation) is smooth. This allows us to illustrate the theorems of Subsection 3.3. Once again our example is a linear equation. This time it is homogeneous and has the form

$$(4.3) \quad D_*^\alpha y(t) = -y(t), \quad y(0) = 1, \quad y'(0) = 0$$

(the second of the initial conditions only for  $\alpha > 1$  of course). It is well known that the exact solution is

$$y(t) = E_\alpha(-t^\alpha)$$

where

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}$$

is the Mittag-Leffler function of order  $\alpha$ . Obviously, neither  $y$  nor  $D_*^\alpha y$  is smooth, and hence we cannot apply the results of Subsection 3.2.

In Table 4.5 we state some numerical results for this problem in the case  $\alpha < 1$ . As in the previous subsection, the data given in the tables is the error of the Adams scheme at the point  $t = 1$ . We can see from the last line that the order of convergence is always close to  $1 + \alpha$  as indicated by Conjecture 3.2. In contrast, Table 4.6 displays the case  $\alpha > 1$ ; here the results confirm the  $O(h^2)$  behaviour stated in Theorem 3.6.

TABLE 4.5  
Errors for eq. (4.3) with  $\alpha < 1$ , taken at  $t = 1$ .

$h$	$\alpha = 0.1$	$\alpha = 0.3$	$\alpha = 0.5$	$\alpha = 0.7$	$\alpha = 0.9$
1/10	-5.42(-3)	-1.86(-3)	-1.30(-3)	-9.91(-4)	-7.51(-4)
1/20	-1.22(-3)	-5.85(-4)	-3.93(-4)	-2.81(-4)	-1.91(-4)
1/40	-4.40(-4)	-1.97(-4)	-1.26(-4)	-8.28(-5)	-4.99(-5)
1/80	-1.68(-4)	-6.90(-5)	-4.18(-5)	-2.50(-5)	-1.32(-5)
1/160	-6.65(-5)	-2.49(-5)	-1.42(-5)	-7.63(-6)	-3.54(-6)
1/320	-2.68(-5)	-9.18(-6)	-4.86(-6)	-2.35(-6)	-9.48(-7)
EOC	1.31	1.44	1.54	1.70	1.90

TABLE 4.6  
Errors for eq. (4.3) with  $\alpha > 1$ , taken at  $t = 1$ .

$h$	$\alpha = 1.25$	$\alpha = 1.5$	$\alpha = 1.85$
1/10	-5.61(-4)	-5.46(-4)	-4.40(-4)
1/20	-1.27(-4)	-1.28(-4)	-1.07(-4)
1/40	-2.90(-5)	-3.04(-5)	-2.65(-5)
1/80	-6.68(-6)	-7.33(-6)	-6.57(-6)
1/160	-1.55(-6)	-1.78(-6)	-1.63(-6)
1/320	-3.63(-7)	-4.37(-7)	-4.07(-7)
EOC	2.09	2.03	2.00

#### REFERENCES

- [1] C. T. H. BAKER, *The Numerical Treatment of Integral Equations*, Clarendon Press, Oxford, 1977.
- [2] D. A. BENSON, *The Fractional Advection-Dispersion Equation: Development and Application*, PhD thesis, University of Nevada Reno, 1998.
- [3] H. BRASS, *Quadraturverfahren*, Vandenhoeck & Ruprecht, Göttingen, 1977.
- [4] H. BRUNNER, *A survey of recent advances in the numerical treatment of Volterra integral and integro-differential equations*, J. Comput. Appl. Math., 8 (1982), pp. 213–229.
- [5] M. CAPUTO, *Linear models of dissipation whose  $Q$  is almost frequency independent–II*, Geophys. J. Royal Astronom. Soc., 13 (1967), pp. 529–539.
- [6] M. CAPUTO AND F. MAINARDI, *Linear models of dissipation in anelastic solids*, Rivista del Nuovo Cimento, 1 (1971), pp. 161–198.
- [7] ———, *A new dissipation model based on memory mechanism*, Pure and Appl. Geophys., 91 (1971), pp. 134–147.

- [8] J.-T. CHERN, *Finite Element Modeling of Viscoelastic Materials on the Theory of Fractional Calculus*, PhD thesis, Pennsylvania State University, 1993.
- [9] F. DE HOOG AND R. WEISS, *Asymptotic expansions for product integration*, Math. Comp., 27 (1973), pp. 295–306.
- [10] K. DIETHELM, *An algorithm for the numerical solution of differential equations of fractional order*, Elec. Transact. Numer. Anal., 5 (1997), pp. 1–6.
- [11] K. DIETHELM AND N. J. FORD, *Analysis of fractional differential equations*, J. Math. Anal. Appl., 265 (2002), pp. 229–248.
- [12] ———, *Numerical solution of the Bagley-Torvik equation*, BIT, to appear (2002).
- [13] K. DIETHELM AND A. D. FREED, *The FracPECE subroutine for the numerical solution of differential equations of fractional order*, in Forschung und wissenschaftliches Rechnen: Beiträge zum Heinz-Billing-Preis 1998, S. Heinzel and T. Plesser, eds., Göttingen, 1999, Gesellschaft für wissenschaftliche Datenverarbeitung, pp. 57–71.
- [14] ———, *On the solution of nonlinear fractional differential equations used in the modeling of viscoplasticity*, in Scientific Computing in Chemical Engineering II — Computational Fluid Dynamics, Reaction Engineering, and Molecular Properties, F. Keil, W. Mackens, H. Voß and J. Werther, eds., Heidelberg, 1999, Springer, pp. 217–224.
- [15] A. D. FREED AND K. DIETHELM, *Viscoelastic and Viscoplastic Material Modeling Using the Classical and Fractional Calculi: A Study of the Caputo Derivative*, in preparation.
- [16] L. GAUL, P. KLEIN, AND S. KEMPFLE, *Damping description involving fractional operators*, Mech. Systems Signal Processing, 5 (1991), pp. 81–88.
- [17] W. G. GLÖCKLE AND T. F. NONNENMACHER, *A fractional calculus approach to self-similar protein dynamics*, Biophysical J., 68 (1995), pp. 46–53.
- [18] R. GORENFLO, G. DE FABRITIIS, AND F. MAINARDI, *Discrete random walk models for symmetric Lévy-Feller diffusion processes*, Physica A, 269 (1999), pp. 79–89.
- [19] R. GORENFLO AND F. MAINARDI, *Fractional calculus: Integral and differential equations of fractional order*, in Fractals and Fractional Calculus in Continuum Mechanics, A. Carpinteri and F. Mainardi, eds., Wien, 1997, Springer, pp. 223–276.
- [20] R. GORENFLO, F. MAINARDI, AND E. SCALAS, *From continuous-time random walks to fractional diffusion*, Physica A, (to appear).
- [21] R. GORENFLO AND R. RUTMAN, *On ultraslow and intermediate processes*, in Transform Methods and Special Functions, Sofia 1994, P. Rusev, I. Dimovski, and V. Kiryakova, eds., Singapore, 1995, Science Culture Technology, pp. 61–81.
- [22] E. HAIRER, S. P. NØRSETT, AND G. WANNER, *Solving Ordinary Differential Equations I: Non-stiff Problems*, Springer, Berlin, Heidelberg, New York, 2nd revised ed., 1993.
- [23] E. HAIRER AND G. WANNER, *Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems*, Springer, Berlin, Heidelberg, New York, 1991.
- [24] C. LUBICH, *Runge-Kutta theory for Volterra and Abel integral equations of the second kind*, Math. Comp., 41 (1983), pp. 87–102.
- [25] ———, *Fractional linear multistep methods for Abel-Volterra integral equations of the second kind*, Math. Comp., 45 (1985), pp. 463–469.
- [26] F. MAINARDI, *Fractional calculus: Some basic problems in continuum and statistical mechanics*, in Fractals and Fractional Calculus in Continuum Mechanics, A. Carpinteri and F. Mainardi, eds., Wien, 1997, Springer, pp. 291–348.
- [27] F. MAINARDI, M. RABERTO, R. GORENFLO, AND E. SCALAS, *Fractional calculus and continuous-time finance II: The waiting-time distribution*, Physica A, 287 (2000), pp. 468–481.
- [28] R. J. MARKS, II AND M. W. HALL, *Differintegral interpolation from a bandlimited signal's samples*, IEEE Transact. Acoust. Speech Signal Process., 29 (1981), pp. 872–877.
- [29] D. MATIGNON AND G. MONTSENY, eds., *Fractional Differential Systems: Models, Methods, and Applications*, vol. 5 of ESAIM Proceedings, SMAI, Paris, 1998. <http://www.emath.fr/Maths/Proc/Vol.5/index.htm>.
- [30] R. METZLER, W. SCHICK, H.-G. KILIAN, AND T. F. NONNENMACHER, *Relaxation in filled polymers: A fractional calculus approach*, J. Chem. Phys., 103 (1995), pp. 7180–7186.
- [31] R. K. MILLER AND A. FELDSTEIN, *Smoothness of solutions of Volterra integral equations with weakly singular kernels*, SIAM J. Math. Anal., 2 (1971), pp. 242–258.
- [32] T. F. NONNENMACHER AND R. METZLER, *On the Riemann-Liouville fractional calculus and some recent applications*, Fractals, 3 (1995), pp. 557–566.
- [33] K. B. OLDHAM AND J. SPANIER, *The Fractional Calculus*, Academic Press, New York, 1974.
- [34] W. E. OLMSTEAD AND R. A. HANDELSMAN, *Diffusion in a semi-infinite region with nonlinear surface dissipation*, SIAM Review, 18 (1976), pp. 275–291.
- [35] I. PODLUBNY, *Fractional-order systems and fractional-order controllers*, Tech. Report UEF-03-94, Slovak Acad. Sci., 1994.

- [36] ———, *Fractional Differential Equations*, Academic Press, San Diego, 1999.
- [37] I. PODLUBNY, L. DORCAK, AND J. MISANEK, *Application of fractional-order derivatives to calculation of heat load intensity change in blast furnace walls*, Transact. Tech. Univ. Košice, 5 (1995), pp. 137–144.
- [38] S. G. SAMKO, A. A. KILBAS, AND O. I. MARICHEV, *Fractional Integrals and Derivatives: Theory and Applications*, Gordon and Breach, Yverdon, 1993.
- [39] E. SCALAS, R. GORENFLO, AND F. MAINARDI, *Fractional calculus and continuous-time finance*, Physica A, 284 (2000), pp. 376–384.
- [40] S. SHAW, M. K. WARBY, AND J. R. WHITEMAN, *A comparison of hereditary integral and internal variable approaches to numerical linear solid elasticity*, tech. report, Brunel University, 1997.
- [41] P. J. TORVIK AND R. L. BAGLEY, *On the appearance of the fractional derivative in the behavior of real materials*, J. Appl. Mech., 51 (1984), pp. 294–298.
- [42] G. WALZ, *Asymptotics and Extrapolation*, Akademie-Verlag, Berlin, 1996.
- [43] S. C. WOON, *Analytic continuation of operators. Applications: From number theory and group theory to quantum field and string theories*, Rev. Math. Phys., 11 (1999), pp. 463–501.