



On the method of modified equations. I: Asymptotic analysis of the Euler forward difference method

F.R. Villatoro ^{*}, J.I. Ramos

*Departamento de Lenguajes y Ciencias de la Computación, E.T.S. Ingenieros Industriales,
Universidad de Málaga, Plaza El Ejido, s/n, 29013-Málaga, Spain*

Abstract

The method of modified equations is studied as a technique for the analysis of finite difference equations. The non-uniqueness of the modified equation of a difference method is stressed and three kinds of modified equations are introduced. The first modified or equivalent equation is the natural pseudo-differential operator associated to the original numerical method. Linear and nonlinear combinations of the equivalent equation and their derivatives yield the second modified or second equivalent equation and the third modified or (simply) modified equation, respectively. For linear problems with constant coefficients, the three kinds of modified equations are equivalent among them and to the original difference scheme. For nonlinear problems, the three kinds of modified equations are asymptotically equivalent in the sense that an asymptotic analysis of these equations with the time step as small parameter yields exactly the same results. In this paper, both regular and multiple scales asymptotic techniques are used for the analysis of the Euler forward difference method, and the resulting asymptotic expansions are verified for several nonlinear, autonomous, ordinary differential equations. It is shown that, when the resulting asymptotic expansion is uniformly valid, the asymptotic method yields very accurate results if the solution of the leading order equation is smooth and does not blow up, even for large step sizes. © 1999 Elsevier Science Inc. All rights reserved.

Keywords: Modified equations; Numerical methods; Finite differences; Ordinary differential equations; Asymptotic methods

^{*} Corresponding author. E-mail: villa@lcc.uma.es.

“Modified equations have been a commonly used tool in the study of difference schemes. Because of the lack of any theoretical foundation, this use has been accompanied by constant difficulties and results derived from modified equations have sometimes been regarded with apprehension. As a result, a situation arises where authors either disregard entirely the technique or have an unjustified faith in its scope”.

Griffiths and Sanz Serna, 1986 [1]

1. Introduction

This paper is the first of a series dealing with the method of modified equations as a means for both the analysis of finite difference schemes and the development of new numerical ones.

The technique of modified equations consists of building a differential problem which approximates the given difference method more accurately than the original differential equation, so that the modified equation can be used for the analysis of the difference problem [1]. The modified equation is the original differential equation plus the truncation error terms introduced by the numerical discretization, which can be calculated by Taylor series expansions, so that the modified equation can also be used for the development of more accurate numerical methods by removing the truncation terms in the modified equation. Alternatively, some authors consider that the modified equation represents the differential equation “truly” solved by the difference method [2].

The technique of modified equations has been referred to by several names, e.g., equivalent equations, differential approximations, truncation error methods, augmented systems, etc. Its origin may be attributed to Daly [3], Noh and Protter [4], Yanenko and Shokin [5,6], and Hirt [7]. There also exists a number of related techniques which deal with the analysis of finite difference schemes by taking into account the truncation error terms, e.g., the analysis of the dispersive and dissipative errors in linear finite difference schemes for hyperbolic or parabolic equations [8].

One of the first applications of modified equations was the analysis of the consistency and stability of numerical methods for the initial-value problem of linear partial differential equations. Hirt [7] introduced the technique of modified equations as a heuristic stability analysis, and Warming and Hyett [2] related it with the Fourier–von Neumann method for the linear stability analysis of the initial-value problem of two-level linear difference schemes. The latter also studied the conditions under which a truncated version of the modified equation can be used to recover the stability constraints of a von Neumann analysis, and, therefore, to gain insight into the dissipative and dispersive errors of numerical schemes. They also introduced a systematic

procedure for the construction of the actual differential equation being solved when a numerical solution is obtained by means of finite difference methods, and related the coefficients of the modified equation with the Taylor series expansion of the amplification factor of the scheme.

For nonlinear problems, the method of Warming and Hyett [2] for the construction of modified equations has been extended by Lerat and Peyret [9–11] who have developed a family of difference schemes for hyperbolic equations in conservation-law form based on modified equations. Their schemes have two parameters which allow for a higher order of accuracy, the addition of artificial viscosity, and the elimination of oscillations in flows with shock waves, with a minimal smearing of the discontinuities.

The modified equation approach for nonlinear problems may be derived by Taylor series expansions and, in general, requires the existence of higher order derivatives [10]. Hedstrom [12] has shown that truncated modified equations for dissipative finite difference schemes are correct for the equation $u_t + u_x = 0$ even if discontinuous solutions are considered. He also warned on the use of modified equations for non-dissipative schemes. Goodman and Madja [13] have proved the validity of the truncated modified equation for an upwind difference scheme for flows with shock waves in a nonlinear hyperbolic equation, by using an explicit discrete solution discovered by Peter Lax.

The validity of the modified equation method has been studied by very few authors in the past. Perhaps, the best analysis is that of Griffiths and Sanz-Serna [1] who make a critical mathematical analysis of the technique for initial-value problems in ordinary differential equations. These authors have shown the non-uniqueness of the modified equation of a given finite difference scheme and indicated that the modified equation must be supplemented with the correct initial conditions; therefore, they put a great emphasis on modified problems. The lack of higher order initial conditions, if the modified equation is truncated or if it is applied to boundary-value problems, is one of the main drawbacks of the modified equation approach. If the modified equation is used for the construction of new numerical methods, the need for stable discretizations was emphasized by Griffiths and Sanz-Serna [1].

Another analysis of modified equations is that of Chang [14] who studied the Warming and Hyett [2] method for the calculation of the modified equation of linear hyperbolic or parabolic partial differential equations, showed (although he did not explicitly stated it) that this technique is equivalent to the inversion of a Taylor series expansion, and proved that it cannot be applied to schemes with more than two time levels since spurious solutions are outside the scope of the Warming and Hyett [2] procedure.

Rigorous studies of modified equations for the analysis of the consistency and stability of finite difference schemes have been considered by a number of authors. For example, Yanenko and Shokin [5] have obtained necessary and sufficient conditions for stability based on a truncated version of the modified

equation (in their words, on the validity of the first differential approximation), for simple, majorant and property-K difference schemes for linear, hyperbolic equations with constant or variable coefficients.

The technique of modified equations and its variants have been a common tool widely used for the analysis and development of numerical methods, and additional references can be found in the bibliographies of the papers quoted above. Nowadays, modified equation techniques are described in most textbooks on computational fluid mechanics and in monographs on numerical methods for partial differential equations [15–18], although there is a need for a rigorous justification for the scope of the method, and many authors use them in an incomplete manner.

This paper is the first part in a series dealing with modified equation methods which are analyzed by means of regular and multiple scales asymptotic expansions by using the time step as the small parameter, and whose objective is the assessment of the validity of modified equations for a variety of initial- and boundary-value problems. In the next section of this paper, the technique of modified equations is applied to a non-autonomous, first-order ordinary differential equation which is solved numerically by the Euler forward scheme. The non-uniqueness of the modified equation is justified, and three representative equations, i.e., the first, second and third modified equations, also referred to as equivalent, second equivalent and (simply) modified equations, respectively, in this series are introduced. For linear problems with constant coefficients, the modified equation can be solved exactly and yields the (natural) analytical continuation of the exact solution of the difference equation.

The remaining of this paper deals with the analysis of the first modified or equivalent equation by using asymptotic methods based on the time step as a small parameter. In particular, a straightforward (regular) asymptotic analysis of the equivalent equation is presented in Section 3.1, while some nonlinear, first-order ordinary differential equations for which this asymptotic expansion is uniformly valid are presented in Section 3.2. Surprisingly, this (regular perturbation) asymptotic method seems to work even for time steps larger than both unity and those demanded by the linear stability of the Euler forward method.

In Section 4, some nonlinear ordinary differential equations with non-uniform regular asymptotic expansions are presented as a basis for the subsequent presentation of the multiple scales technique. In Section 4.1, the method of multiple scales is applied to linear problems, and the resulting asymptotic expansions are added to all orders in order to obtain the (natural) analytical continuation of the solution of the Euler forward difference method. This important result validates the use of equivalent equations for linear ordinary differential equations with constant coefficients.

The multiple scales technique is applied to some nonlinear problems in Section 4.2 where it is shown that, when the resulting asymptotic expansion is

uniform, the accuracy of the method of multiple scales is very good. Moreover, in order to accelerate the convergence of the resulting asymptotic expansion, the contribution at each order of all the slow time scales can be summed up, thus obtaining the so-called summed-up asymptotic expansions.

In Section 5, the multiple scales technique is applied to the asymptotic analysis of the equivalent equation of a non-autonomous, linear, ordinary differential equation, in order to illustrate that this method also works for non-autonomous problems. Finally, in Section 6, some conclusions on the validity of the asymptotic analysis of the equivalent (modified) equation for ordinary differential equations are presented.

2. Modified equations for first-order, ordinary differential equations

In order to assess the validity of the method of modified equations, we shall first consider the following first-order, non-autonomous, ordinary differential equation

$$\frac{du(t)}{dt} = F(u(t), t), \quad u(0) = a, \quad (1)$$

where F is a function regular enough, e.g., F is smooth and Lipschitz continuous, so that Eq. (1) is well posed, and the simplest numerical finite difference scheme for this equation, i.e., the Euler forward (explicit) scheme

$$\frac{U^{n+1} - U^n}{k} = F(U^n, t^n), \quad U^0 = a, \quad (2)$$

where $t^n = nk$, k denotes the step size, and U^n is a numerical approximation to the exact solution $u(nk)$.

The method of modified equations replaces the finite difference equation (2) by an ordinary differential equation obtained by Taylor series expansion of $U^{n+i} = U(t^n + ik)$ around t^n . The Taylor series expansion of Eq. (2) can be written as the following pseudo-differential operator equation

$$\frac{e^{kD} - 1}{k} U(t) = F(U(t), t), \quad U(0) = a, \quad (3)$$

where $D = d/dt$ and $U(t)$ is a formal analytical continuation of the discrete sequence U^n so that $U(nk) = U^n$, and Eq. (3) is mathematically well-posed.

Usually, the modified equation is obtained by using the Taylor series expansion of the exponential operator, e.g.,

$$\frac{dU(t)}{dt} + \frac{k}{2} \frac{d^2U(t)}{dt^2} + \frac{k^2}{3!} \frac{d^3U(t)}{dt^3} + O(k^3) = F(U(t), t). \quad (4)$$

Eqs. (3) and (4) are referred to as the first modified or equivalent equation for the Euler forward difference method for Eq. (1). It is important to note that for the well-posedness of the equivalent equation only one initial condition is necessary, although, if the equivalent equation is truncated to any order, additional initial conditions for the higher order derivatives are required [1,14]; otherwise, there would not exist a unique solution to the modified equation. These additional conditions cannot be obtained by using the differential equation consistent with the finite difference scheme, i.e., Eq. (1); rather, it is necessary that these conditions be consistent with the finite difference scheme [1].

The equivalent equation (3) is not the unique formal pseudo-differential operator equation which is formally equivalent to the Euler forward scheme, i.e., Eq. (2), as has been previously stressed by Griffiths and Sanz-Serna [1]. In fact, any equation obtained by linear combinations of the derivatives of the equivalent equation (4) is also formally equivalent to the equivalent equation and to the difference scheme. As an example, consider the following infinite linear combination of Eq. (4),

$$\begin{aligned} & (\text{Eq. (4)}) - \frac{k}{2} \frac{d}{dt}(\text{Eq. (4)}) + \frac{k^2}{12} \frac{d^2}{dt^2}(\text{Eq. (4)}) + \frac{k^3}{24} \frac{d^3}{dt^3}(\text{Eq. (4)}) \\ & + \frac{7k^4}{360} \frac{d^4}{dt^4}(\text{Eq. (4)}) + \frac{k^5}{160} \frac{d^5}{dt^5}(\text{Eq. (4)}) + O(k^6) \end{aligned} \quad (5)$$

where $\text{Eq. (4)} = \text{LHS}(\text{Eq. (4)}) - \text{RHS}(\text{Eq. (4)})$. Eq. (5) yields

$$\begin{aligned} \frac{dU(t)}{dt} = & F(U(t), t) - \frac{k}{2} \frac{dF(U(t), t)}{dt} + \frac{k^2}{12} \frac{d^2F(U(t), t)}{dt^2} \\ & - \frac{k^4}{720} \frac{d^4F(U(t), t)}{dt^4} + O(k^6). \end{aligned} \quad (6)$$

The infinite linear combination corresponding to Eq. (5) can be interpreted as a division of Eq. (3) by the pseudo-differential operator which appears in its left-hand-side, as can be easily verified by using the power series expansion of $\exp(Dk)$. This means that Eq. (6) can be rewritten as

$$\frac{dU(t)}{dt} = \frac{kD}{e^{kD} - 1} F(U(t), t), \quad U(0) = a. \quad (7)$$

In this series, Eqs. (6) and (7) are referred to as the second modified or second equivalent equation for the Euler forward difference method, i.e., Eq. (2). Note that for the well-posedness of the second equivalent equation only one initial condition is necessary, although, if this equation is truncated to any order, additional initial conditions for the higher order derivatives are required as for the first modified equation. Note also that the second equivalent equation includes a nonlinear pseudo-differential operator in its right-hand side and,

therefore, its analysis is more complicated than that of the equivalent equation; however, this analysis may have some advantages which will be studied in the following papers of this series.

If k is a small parameter, the equivalent and the second equivalent equations, i.e., Eqs. (4) and (6), respectively, are highly singular perturbed differential equations whose study by analytical or numerical methods is expected to find some difficulties. Techniques for the avoidance of this singular behaviour have been developed in the past, and are often considered as the main difference between modified equation and truncation error methods [2,18]. It must be noted that the value of k for the Euler forward method is usually controlled by stability considerations and, therefore, it is usually small.

In order to avoid the higher order derivatives in the equivalent and the second equivalent equations, a procedure of formal subtraction has been developed by Warming and Hyett [2]. By using this method, these derivatives can be removed by adding the derivatives of the equivalent or the second equivalent equation. However, this method works well only when the differential operator commutes with the nonlinearity, i.e., it works for linear homogeneous equations with constant coefficients $F(u(t), t) = Au(t)$. Although in the original paper of Warming and Hyett, this method was applied to one-dimensional, linear evolution (hyperbolic or parabolic), partial differential equations, i.e., when $F(u(t), t)$ is a linear differential operator $A(\partial/\partial x)u(t, x)$, this procedure is applied to ordinary differential equations in this paper.

Use of the Warming and Hyett procedure to Eq. (4) with $F(u, t) = Au$ is equivalent to the formal solution of an upper triangular linear system of equations for the derivatives of $U(t)$ considered as formally independent variables, whose rows are Eq. (4) and all its derivatives, or, alternatively, Eq. (6) and all its derivatives. Since the general solution of a triangular linear system can be easily obtained, this approach allows for a mathematical analysis of modified equation techniques for linear partial differential equations like that of Chang [14].

Another interpretation of the Warming and Hyett procedure has been recently given by Ramshaw [19] who applied the implicit function theorem to pseudo-differential operators and showed that the Warming and Hyett procedure is an inversion of the formal power series of the pseudo-differential operator which appears on the left-hand side of the equivalent Eq. (3).

For a linear equation with $F(u(t), t) = Au(t)$, the inversion of the power series of the Euler forward pseudo-differential operator of Eq. (3) yields

$$\begin{aligned} \frac{dU(t)}{dt} &= \frac{1}{k} \ln(1 + Ak)U(t) \\ &= AU(t) - \frac{k}{2}A^2U(t) + \frac{k^2}{3}A^3U(t) + \frac{k^3}{4}A^4U(t) + O(k^4), \quad U(0) = a. \end{aligned} \quad (8)$$

Eq. (8) is a linear partial differential equation if A is a constant-coefficient differential operator, and a linear constant-coefficient ordinary differential equation if A is a constant. For the latter, Eq. (8) can be easily solved to yield

$$U(t) = a \exp\left(\frac{t}{k} \ln(1 + Ak)\right) = a(1 + Ak)^{t/k} \quad (9)$$

which is the “natural” analytical continuation of the solution of Eq. (2), i.e.,

$$U^n = a(1 + Ak)^n. \quad (10)$$

Although the Warming and Hyett procedure [2] is not applicable to linear equations with variable coefficients or to nonlinear ones because derivatives appear in the resulting equation, Lerat and Peyret [10] have extended the scope of this procedure for these cases. Their method subtracts the higher order derivatives by adding products of the derivatives of the nonlinearity times the derivatives of the second equivalent equation. This procedure was originally applied to nonlinear (hyperbolic or parabolic) evolution, partial differential equations but it can also be applied directly to ordinary differential equations. For example, for Eq. (6), it yields

$$\begin{aligned} & (\text{Eq. (6)}) - \frac{k}{2} F_U(\text{Eq. (6)}) + \frac{k^2}{6} (2F_U^2 + F_{U_t})(\text{Eq. (6)}) \\ & + \frac{k^2}{12} F_{UU}(\text{Eq. (6)})^2 + \frac{k^2}{12} F_U \frac{d}{dt}(\text{Eq. (6)}) \\ & - \frac{k^3}{24} (2F_U^3 + F_U F_{U_t} + F F_{UU}) (\text{Eq. (6)}) - \frac{k^3}{24} F_U F_{UU} (\text{Eq. (6)})^2 \\ & - \frac{k^3}{24} F_U^2 \frac{d}{dt}(\text{Eq. (6)}) + O(k^4), \end{aligned} \quad (11)$$

where $\text{Eq. (6)} = \text{LHS}(\text{Eq. (6)}) - \text{RHS}(\text{Eq. (6)})$, the arguments of F have been removed and the subscripts indicate partial derivatives.

After some algebra, Eq. (11) can be written as

$$\begin{aligned} U_t = & F - \frac{k}{2} (F_t + F F_U) + \frac{k^2}{12} (F_{tt} + 4F_t F_U + 4F F_U^2 + 2F F_{U_t} + F^2 F_{UU}) \\ & - \frac{k^3}{12} (F_{tt} F_U + 3F_t F_U^2 + 3F F_U^3 + F_t F_{U_t} \\ & + 3F F_U F_{U_t} + F F_t F_{UU} + 2F^2 F_U F_{UU}) + O(k^4). \end{aligned} \quad (12)$$

Note that, in the resulting equation, the higher order derivatives of the unknown function have been replaced by the corresponding derivatives of the nonlinearity, so that the resulting equation is highly more nonlinear than that of the equivalent or the second equivalent equations, i.e., Eqs. (4) and (6), respectively.

In this series of papers, Eq. (12) is referred to as the third modified or (simply) modified equation for the Euler forward difference method (2).

To our knowledge, it is difficult to interpret the Lerat and Peyret procedure [10] as a formal operation on pseudo-differential operators due to the loss of commutativity between the nonlinearity and the linear pseudo-differential operator in the right-hand-side of the second equivalent equation (7). As the Warming and Hyett procedure [2], the Lerat and Peyret one can be interpreted as a nonlinear inversion of the formal power series of the pseudo-differential operator in the left-hand-side of the equivalent equation (3) or in the right-hand-side of the second equivalent equation (7). It should be noted that, for a rigorous application of this technique, differentiability conditions on the nonlinearity and, also, on the corresponding solution of the original ordinary differential equation (1) are required. Furthermore, with this power series interpretation, the Lerat and Peyret procedure can be easily automated if computer algebra systems are used.

3. Asymptotic analysis of the equivalent equation for autonomous problems

The equivalent equation (3) can be used for the analysis of the Euler forward numerical scheme. Since this equivalent equation is nonlinear, it is almost impossible in most cases to find its analytical solution, and, therefore, theoretical progress can only be made by means of asymptotic or perturbation methods [20].

In order to simplify the following asymptotic analysis, we shall consider the equivalent equation of the following first-order, autonomous, ordinary differential equation

$$\frac{du(t)}{dt} = F(u(t)), \quad u(0) = a. \quad (13)$$

If the solution $u(t)$ of the original equation (13) is known, an asymptotic expansion for the solution $U(t)$ of the equivalent equation (4) in terms of $u(t)$ and a small parameter $\epsilon \geq 0$ can be developed as follows. Consider the following asymptotic expansion

$$U(t; \epsilon) = u_0(t) + \mu_1(\epsilon)u_1(t) + \mu_2(\epsilon)u_2(t) + \text{h.o.t.}, \quad (14)$$

where $u_0(t) = u(t)$, and $\mu_i(\epsilon)$ are functions to be determined, $u_i(t)$ are $O(1)$ functions, and h.o.t. stands for higher order terms in ϵ .

Substitution of Eq. (14) into the equivalent equation (4) yields a distinguished limit [20] only if $\mu_i(\epsilon) = \epsilon^i$ and $\epsilon = k$, since any other limit requires additional initial conditions. These additional initial conditions cannot be directly obtained from Eq. (13) by differentiation, since, in fact, these initial conditions are the values of higher order derivatives of the analytical continuation of the numerical solution at $t = 0$, i.e., they must be consistent with the

equivalent equation, but not necessarily with the differentiation of Eq. (13) at $t = 0$.

Although the asymptotic character of the successive terms obtained in this section can be easily verified [20], one may check whether or not the ratio of two successive terms tends to zero as k tends to zero. If it tends to zero, then the expansion is asymptotic.

3.1. Straightforward (regular) asymptotic expansion

Substitution of Eq. (14) into the equivalent equation (4) and equating terms of the same degree in k yield the nonlinear equation (13) to leading order $O(1)$, whose solution can be reduced to quadratures, i.e.,

$$\int_a^u \frac{du}{F(u)} = t. \quad (15)$$

To $O(k)$, the following linear equation is obtained

$$\mathcal{L}(u_1) \equiv \frac{du_1}{dt} - \frac{dF(u)}{du} u_1 = -\frac{1}{2} \frac{d^2 u}{dt^2} = -\frac{1}{2} \frac{dF(u)}{du} F(u), \quad u_1(0) = 0, \quad (16)$$

whose solution can be easily obtained by using an integrating factor as

$$u_1 = -\frac{F(u)}{2} \int_0^t \frac{dF(u(t))}{du} dt = -\frac{F(u)}{2} \int_{F(a)}^{F(u)} \frac{dF}{F} = -\frac{F(u)}{2} \ln \frac{F(u)}{F(a)}. \quad (17)$$

The asymptotic expansion (14) with Eqs. (15) and (17) is uniformly valid if the nonlinearity, i.e., $F(u)$, is such that u_1 remains bounded and if it exists a k such that $k|u_1| \ll |u_0|$ uniformly in time. If this is not the case, non-uniform behaviour appears, and a regular perturbation method is not adequate. A multiple scales technique can be used to correct these non-uniformities, as shown in the next section. Here, however, we deal only with nonlinear problems which result in uniform straightforward asymptotic expansions.

The second-order correction, $O(k^2)$, is as follows

$$\mathcal{L}(u_2) = -\frac{1}{2} \frac{d^2 u_1}{dt^2} - \frac{1}{6} \frac{d^3 u}{dt^3} + \frac{d^2 F(u)}{du^2} \frac{u_1^2}{2}, \quad u_2(0) = 0. \quad (18)$$

By using Eqs. (15)–(17), the solution of Eq. (18) is, after some algebra,

$$u_2 = \frac{F(u)}{24} \left[2 \left(G(u) + \frac{dF(u)}{du} - \frac{dF(a)}{du} \right) + \frac{dF(u)}{du} \ln \frac{F(u)}{F(a)} \left(6 + 3 \ln \frac{F(u)}{F(a)} \right) \right], \quad (19)$$

where

$$G(u) = \int_a^u \left(\frac{dF(w)}{dw} \right)^2 \frac{dw}{F(w)}. \quad (20)$$

Following the same procedure, the following equation can be obtained to $O(k^3)$

$$\begin{aligned} \mathcal{L}(u_3) &= -\frac{1}{2} \frac{d^2 u_2}{dt^2} - \frac{1}{6} \frac{d^3 u_1}{dt^3} - \frac{1}{24} \frac{d^4 u}{dt^4} + \frac{d^2 F(u)}{du^2} u_1 u_2 + \frac{d^3 F(u)}{du^3} \frac{u_1^3}{6}, \\ u_3(0) &= 0, \end{aligned} \quad (21)$$

whose solution is, after some algebra,

$$\begin{aligned} u_3 = & - \left(\frac{1}{6} + \frac{5L(u)}{12} + \frac{L(u)^2}{4} + \frac{L(u)^3}{24} \right) F(u) F'(u)^2 \\ & - \left(\frac{G(u)}{12} + \frac{G(u)L(u)}{24} - \frac{F'(a)}{12} - \frac{L(u)F'(a)}{12} \right) F(u) F'(u) \\ & - \left(\frac{G(u)^2}{48} + \frac{H(u)}{12} - \frac{F'(a)^2}{12} \right) F(u) \\ & - \left(\frac{L(u)}{12} + \frac{L(u)^2}{8} + \frac{L(u)^3}{24} \right) F(u)^2 F''(u), \end{aligned} \quad (22)$$

where the primes denote differentiation,

$$H(u) = \int_a^u \left(\frac{dF(w)}{dw} \right)^3 \frac{dw}{F(w)}, \quad (23)$$

$$L(u) = \ln \frac{F(u)}{F(a)}. \quad (24)$$

Higher order terms in the asymptotic expansion can also be easily calculated.

If the same straightforward asymptotic analysis of the Euler forward numerical scheme presented in this section is employed in the second equivalent equation (7) or the modified equation (12), the equations for each asymptotic correction or term are exactly the same as those derived above. Therefore, the equivalent equation, the second equivalent equation and the modified equation are asymptotically equivalent.

3.2. Examples of straightforward asymptotic expansions

Let us consider some applications of the asymptotic expansion (14) for the solution of Eq. (2) as described in the previous section.

Example 1. For Eq. (13) with the nonlinearity

$$F(u) = \frac{1}{1+u} \quad (25)$$

and the initial condition $u(0) = a > 0$, the following asymptotic expansion results to second order

$$U(t) = u(t) + ku_1(t) + k^2u_2(t) + O(k^3), \quad (26)$$

where

$$u(t) = -1 + \sqrt{T_A}, \quad T_A = (1+a)^2 + 2t, \quad (27)$$

$$u_1(t) = \frac{\ln(T_A) - 2 \ln(1+a)}{4\sqrt{T_A}}, \quad (28)$$

$$u_2(t) = \frac{4(2 + \ln(1+a))(\ln(T_A) - \ln(1+a)) - \ln^2(T_A)}{32T_A^{3/2}} + \frac{t}{4(1+a)^2 T_A^{3/2}}. \quad (29)$$

We have also determined the asymptotic terms up to third order; however, the resulting expressions are omitted here. In order to assess the correctness and accuracy of the asymptotic expansion, Eq. (26) has been compared with the numerical solution of the Euler forward method, i.e., Eq. (2), herein after referred to as the Euler numerical solution, for several k , rather than with the exact solution of the ordinary differential equation because our emphasis is on the validity of the modified equation approach, i.e., the solution of the Euler forward method can be considered as the exact solution of the discretized equivalent equation. Note that we are comparing the numerical solution of Eq. (2) with the analytical ones from the asymptotic expansions. In the next papers in this series, comparisons will be presented between the solution of the Euler forward method and the numerical solutions to modified equations.

Fig. 1 shows the difference between the exact solution and the asymptotic expansion, i.e., Eq. (26), to third order for $a = 1$ and two different values of k . It must be pointed out that, although the numerical solution is an accurate approximation to the solution of the original ordinary differential equation only for $k \ll 1/|F_U(u(t))|$, Fig. 1 (top) shows that the asymptotic expansion for the solution of the equivalent equation represents accurately the numerical solution even for $k = 2.5$.

The behaviour of the errors shown in Fig. 1 illustrates the uniformity of the asymptotic expansion up to the third-order; this result can also be understood from a careful analysis of Eqs. (27)–(29). The asymptotic solution indicates that the finite difference solution grows faster than the solution of the original differential equation, although the asymptotic growth rate of the two solutions is nearly the same for large times.

Example 2. Another nonlinear case for which an explicit solution of the leading order differential equation in the asymptotic expansion can be obtained is

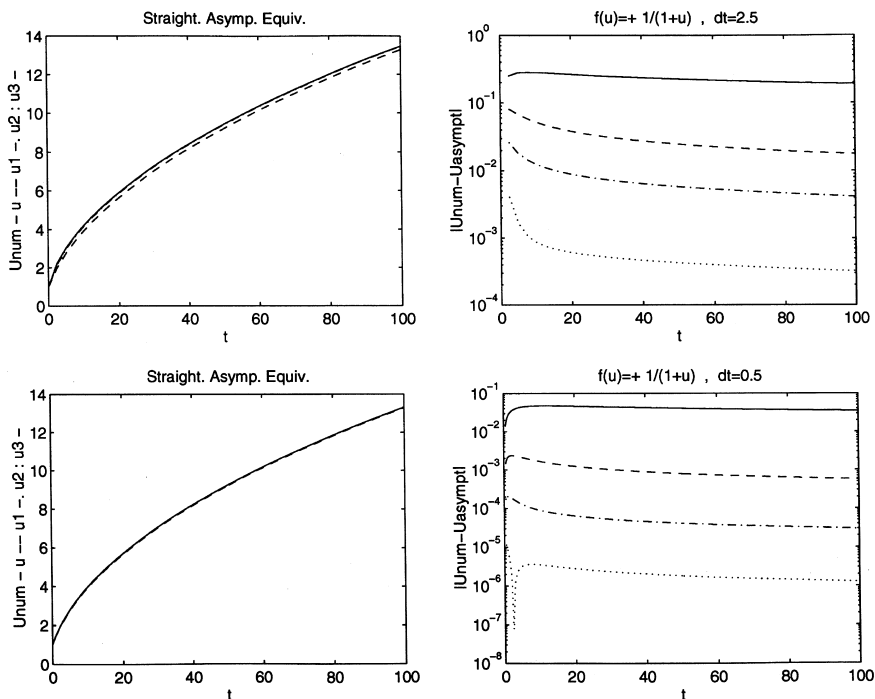


Fig. 1. Straightforward asymptotic expansion for the solution of the equivalent equation with $F(u) = 1/(1+u)$ (left) and absolute errors with respect to the Euler numerical solution (right) for $k = 2.5$ (top) and $k = 0.5$ (bottom) and $a = 1$. In the left plots, the Euler numerical solution and the asymptotic expansion including the leading, first, second and third order terms are denoted by solid, dashed, dash-dotted and dotted lines, respectively. In the right plots, the absolute errors of the asymptotic expansion with the leading, first, second and third order terms are denoted by solid, dashed, dash-dotted and dotted lines, respectively.

$$F(u) = -u^2 \quad (30)$$

whose asymptotic expansion (cf. Eq. (26)) yields

$$u(t) = 1/T_A, \quad T_A = \frac{1}{a} + t, \quad (31)$$

$$u_1(t) = -\frac{\ln(aT_A)}{T_A^2}, \quad (32)$$

$$u_2(t) = \frac{1 - aT_A - 2 \ln(aT_A) + 2 \ln^2(aT_A)}{2T_A^3}. \quad (33)$$

This asymptotic expansion with its corresponding errors is compared with the Euler numerical solution in Fig. 2. The resulting asymptotic expansion is

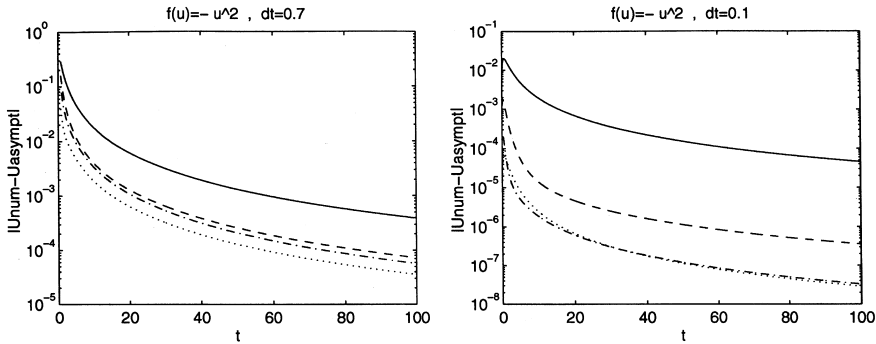


Fig. 2. Straightforward asymptotic expansion for the solution of the equivalent equation with $F(u) = -u^2$ and $k = 0.7$ (left) and $k = 0.1$ (right), and $a = 1$. The labels are the same as those of Fig. 1.

uniform, and the error is small even for k near unity. This asymptotic expansion indicates that the numerical solution decreases faster than the solution of the original differential equation, but both converge asymptotically to zero.

Example 3. Similar results have been obtained for the following nonlinearity

$$F(u) = -u^3 \quad (34)$$

which yields the following asymptotic expansion (Eq. (26))

$$u(t) = a/\sqrt{(T_A)}, \quad T_A = 1 + 2a^2t, \quad (35)$$

$$u_1(t) = \frac{3a(1 - T_A) \ln(T_A)}{8t\sqrt{T_A^3}}, \quad (36)$$

$$u_2(t) = -\frac{5a^5}{8T_A^{3/2}} - \frac{a^5(-20 + 36 \ln(T_A) - 27 \ln^2(T_A))}{32T_A^{5/2}}. \quad (37)$$

For this nonlinearity, the straightforward asymptotic expansion of Eq. (26) yields a uniformly valid solution with small errors even for $k = 0.25$, as shown in Fig. 3 (right). In Fig. 3 (left), it is shown that the Euler method has a large slope near $t = 0$ when k approaches 1, and this slope introduces a boundary layer with must be accounted for; therefore, the straightforward asymptotic methods used in the previous section do not work in this case as illustrated.

4. Multiple scales asymptotic analysis

Since the equivalent equation (4) for small time steps can be interpreted as a singular perturbation problem due to the appearance of higher order derivatives multiplied by the step size, non-uniformities are expected to occur for

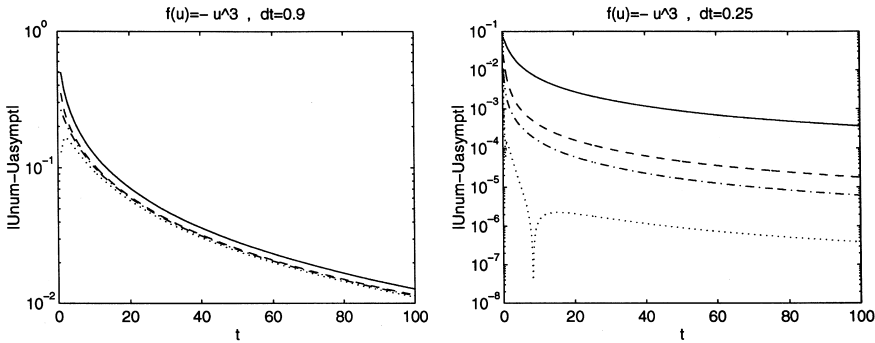


Fig. 3. Straightforward asymptotic expansion for the solution of the equivalent equation with $F(u) = -u^3$, $k = 0.9$ (left), $k = 0.25$ (right) and $a = 1$. The labels are the same as those of Fig. 1.

most nonlinear problems. In this section, we shall first present some nonlinear ordinary differential equations whose straightforward asymptotic expansions are non-uniform, and then introduce the method of multiple scales to avoid them in some cases.

Let us first consider the nonlinear function

$$F(u) = -u(1 + u) \quad (38)$$

whose regular asymptotic expansion (cf. Eq. (26)) is such that

$$u(t) = \frac{e^{-t}}{2 - e^{-t}}, \quad (39)$$

$$u_1(t) = \frac{-e^{-t} 2 \ln(2 - e^{-t}) + t}{(e^{-t} - 2)^2}, \quad (40)$$

$$u_2(t) = \frac{e^{-t}}{12(e^{-t} - 2)^3} \left(24 + 16t - 6t^2 - e^{-t}(24 - 4t + 3t^2) + 12(2 + e^{-t})((1 - t)L(t) - L(t)^2) \right), \quad (41)$$

where

$$L(t) = \ln(2 - e^{-t}). \quad (42)$$

For this nonlinear function (cf. Eq. (38)), the regular asymptotic expansion is non-uniformly valid since, for times $t = O(1/k)$, the linear dependence in the numerator of Eq. (40) dominates, and the condition $|u(t)| \ll k|u_1(t)|$ is not met. Fig. 4 (left) shows this secular behaviour since, as time increases, the relative error of the asymptotic expansion increases as the number of terms is increased.

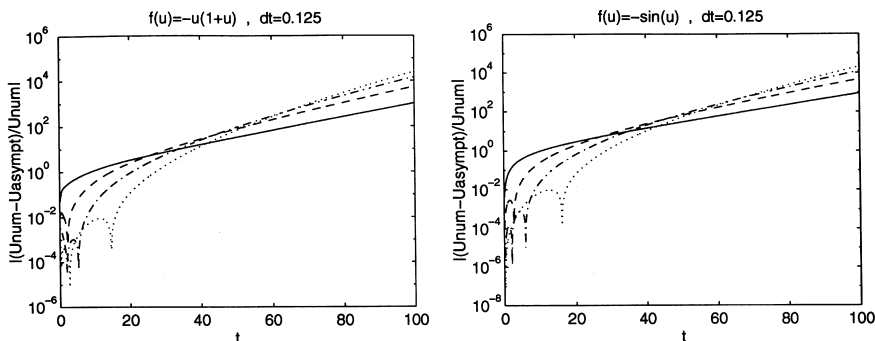


Fig. 4. Relative errors of the straightforward asymptotic expansion for the solution of the equivalent equation for $F(u) = -u(1+u)$ (left) and $F(u) = -\sin(u)$ (right), both for $k = 0.125$ and $a = 1$. The labels are the same as those of Fig. 1.

Another nonlinearity which results in a non-uniform asymptotic expansion is

$$F(u) = -\sin u \quad (43)$$

which yields the asymptotic expansion (26), where

$$\begin{aligned} u(t) &= 2 \arctan(e^{-t} \tan(1/2)), \\ u_1(t) &= -e^{-t} \sin(1) \frac{\ln(D(t)/2) + t}{D(t)}, \end{aligned} \quad (44)$$

$$D(t) = 1 + \cos(1) + (1 - \cos(1)) e^{-2t} \quad (45)$$

and higher order terms have been omitted for brevity, but are illustrated in Fig. 4 (right). This asymptotic expansion is non-uniform, i.e., the first order term (cf. Eq. (44)) is not uniformly valid at $t = 1/k$. The errors of the asymptotic expansion are shown in Fig. 4 (right), and confirm the appearance of secular behaviour for this nonlinearity.

4.1. Multiple scales technique for linear autonomous equations

In the previous section, it was shown that regular or straightforward asymptotic expansions may not provide uniformly valid solutions; therefore, other techniques may be required. Here, we shall consider the multiple scales method. However, since the non-uniform behaviour depends strongly on the nonlinearity, it is, in general, difficult to carry out a multiple scales analysis for arbitrary nonlinear equations. Therefore, in order to illustrate the procedure, we shall first consider a linear equation for which a regular expansion breaks down but which illustrates the different time scales that must be introduced in the method of multiple scales.

A straightforward asymptotic expansion (cf. Eq. (26)) applied to a linear equation with $F(u) = \pm u$ yields

$$U(t) = e^{\pm t} \left(1 - \frac{k}{2}t + \frac{k^2}{24}(\pm 8t + 3t^2) - \frac{k^3}{48}(12t \pm 8t^2 + t^3) + O(k^4) \right), \quad (46)$$

which is non-uniformly valid because higher order corrections are not smaller than lower order ones.

In order to obtain a uniformly valid asymptotic expansion and avoid non-uniformities, one must cope with the appearance of the many time scales suggested by Eq. (46). A multiple variable expansion procedure introduces a series of slower time scales, i.e., it assumes the expansion

$$U(t; k) = \sum_{i=0}^N u_i(t_0, t_1, \dots, t_{N-i})k^i + O(k^{N+1}), \quad (47)$$

where, as suggested by Eq. (46),

$$t_0 = t, \quad t_1 = kt, \quad t_2 = k^2t, \quad t_3 = k^3t, \dots, \quad (48)$$

$$\frac{d}{dt} = \frac{\partial}{\partial t_0} + k \frac{\partial}{\partial t_1} + k^2 \frac{\partial}{\partial t_2} + O(k^3). \quad (49)$$

Use of Eqs. (47)–(49) into the linear equivalent equation (4) and equating terms of equal powers in k , yield, to leading order $O(1)$, the following linear ordinary differential equation

$$\frac{\partial u_0}{\partial t_0} = \pm u_0, \quad u_0(t_0 = 0) = a, \quad (50)$$

whose solution is

$$u_0 = A_1(t_1, t_2, \dots) e^{\pm t_0}, \quad (51)$$

where A_1 depends on the slower time scales and $A_1(0, 0, \dots) = a$.

To first order, $O(k)$, the following linear equation is obtained

$$\frac{\partial u_1}{\partial t_0} \mp u_1 = -\frac{\partial u_0}{\partial t_1} - \frac{1}{2} \frac{\partial^2 u_0}{\partial t_0^2}, \quad u_1(t_0 = 0) = 0, \quad (52)$$

whose solution is

$$u_1 = -\frac{t_0}{2} e^{\pm t_0} \left(A_1 + 2 \frac{\partial A_1}{\partial t_1} \right), \quad (53)$$

which is unbounded in t_0 unless

$$\frac{\partial A_1}{\partial t_1} = -\frac{A_1}{2}, \quad A_1(t_1 = 0) = a, \quad (54)$$

the solution of which is

$$A_1 = A_2(t_2, \dots) e^{-t_1/2}, \quad A_2(0, \dots) = a, \quad (55)$$

and results in

$$u_0 = A_2(t_2, \dots) e^{\pm t_0 - t_1/2}, \quad u_1 = 0. \quad (56)$$

To second order, the following linear equation is obtained

$$\frac{\partial u_2}{\partial t_0} \mp u_2 = -\frac{1}{6} \frac{\partial^3 u_0}{\partial t_0^3} - \frac{\partial^2 u_0}{\partial t_1 \partial t_0}, \quad u_2(t_0 = 0) = 0, \quad (57)$$

which yields

$$A_2(t_2) = A_3(t_3, \dots) e^{\pm t_2/3}, \quad A_3(0, \dots) = a, \quad (58)$$

and, therefore,

$$u = A_3(t_3, \dots) \exp(\pm t_0 - t_1/2 \pm t_2/3). \quad (59)$$

This procedure can be easily continued to higher orders, resulting in the following asymptotic expansion

$$u = a \exp\left(\pm t - k \frac{t}{2} \pm k^2 \frac{t}{3} - k^3 \frac{t}{4} \pm k^4 \frac{t}{5}\right) + O(k^5), \quad (60)$$

which can be summed up to all orders to yield Eq. (9), i.e., the exact solution of the linear finite Euler forward scheme, i.e., Eq. (2).

The relative errors of the uniform asymptotic expansion (Eq. (60)) are illustrated in Fig. 5 where the uniformity of the expansion and the boundedness of the relative errors can be observed. It must be pointed out that the number of terms that must be kept in an asymptotic multi-time scales expansion depends on the time interval that one considers, i.e., the larger the time interval, the larger is the number of time scales that need to be introduced.

For a general linear equation with $F(u) = Au + B$, the following straightforward asymptotic expansion may be obtained

$$u(t) = -\frac{B}{A} + (A+B)e^{At} \left(\frac{1}{A} - \frac{k}{2}At + k^2 \left(A^2 \frac{t}{3} + A^3 \frac{t^2}{8} \right) - k^3 \left(A^3 \frac{t}{4} + A^4 \frac{t^2}{6} + A^5 \frac{t^3}{48} \right) + O(k^4) \right), \quad (61)$$

and, if a multiple scales technique is used, the following asymptotic expansion can be found

$$u = \left(a + \frac{B}{A} \right) \exp \left(At - kA^2 \frac{t}{2} + k^2 A^3 \frac{t}{3} - k^3 A^4 \frac{t}{4} \right) - \frac{B}{A} + O(k^4), \quad (62)$$

which can be summed up to all orders to yield

$$U(t) = \left(a + \frac{B}{A} \right) (1 + Ak)^{t/k} - \frac{B}{A}, \quad (63)$$

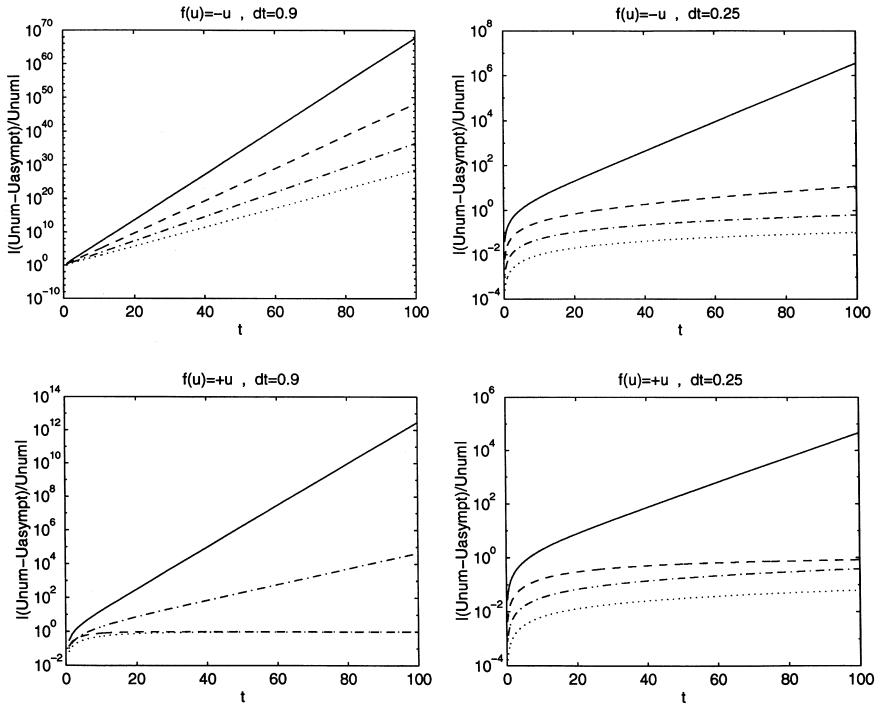


Fig. 5. Relative errors between the Euler numerical solution and the multiple scales asymptotic expansion for the solution of the equivalent equation with $F(u) = -u$ (top) and $F(u) = +u$ (bottom), with $k = 0.9$ (left), and $k = 0.25$ (right).

i.e., the exact solution of the equivalent equation of the Euler forward scheme, i.e., Eq. (2).

Eqs. (60) and (62) provide an assessment of the validity of the method of modified equations based on the equivalent equation for linear problems with constant coefficients, i.e., the equivalent equation is a rigorous analogue of the finite difference scheme. This implies that the consistency and stability of finite difference schemes can be obtained by using the equivalent equation. However, it must be noted that, if only the first terms of an asymptotic expansion of the equivalent equation are retained, the resulting truncated equation can be used only for special kinds of equations, since a finite number of terms of the modified equation cannot be of general use for stability analysis. For example, Yanenko and Shokin [5,21] have obtained some conditions, e.g., simplicity or majorancy, that the truncated equivalent equations must satisfy in order to have the same stability characteristics as the (original) numerical method.

4.2. Multiple scales technique for nonlinear autonomous equations

For nonlinear equations, a multiple scales asymptotic analysis of the equivalent equation usually encounters some difficulties associated with the lack of an explicit expression for the exact solution to the leading order differential equation although this solution can be reduced to quadratures (cf. Eq. (15)).

In order to illustrate the multiple scales technique for nonlinear problems, we shall first consider a nonlinearity with results in an explicit solution to the leading order equation (15), e.g., $F(u) = -\sin(u)$, and for which a straightforward asymptotic expansion is nonuniform as illustrated in Fig. 4 (right) and Section 3.2.

If Eqs. (47)–(49) are substituted into the equivalent equation (4) with the nonlinearity $F(u) = -\sin(u)$, and terms of equal powers in k are equated, the following nonlinear differential equation is obtained to leading order

$$\frac{\partial u_0}{\partial t_0} = F(u_0) = -\sin(u_0), \quad u_0(t_0 = 0) = a, \quad (64)$$

whose solution is

$$u_0 = 2 \arctan(E_A), \quad E_A = A_1(t_1, t_2, \dots) e^{-t_0}, \quad (65)$$

where A_1 depends on slower time scales, $A_1(0, 0, \dots) = \tan(a/2)$, and a is not a multiple of π ; otherwise, the solution to Eq. (64) would be a constant.

To $O(k)$, the following linear equation results

$$\mathcal{L}(u_1) \equiv \frac{\partial u_1}{\partial t_0} - \frac{dF(u_0)}{du} u_1 = -\frac{\partial u_0}{\partial t_1} - \frac{1}{2} \frac{\partial^2 u_0}{\partial t_0^2}, \quad u_1(t_0 = 0) = 0, \quad (66)$$

which reduces to

$$\mathcal{L}(u_1) \equiv \frac{\partial u_1}{\partial t_0} + \frac{1 - E_A^2}{1 + E_A^2} u_1 = -E_A \frac{1 - E_A^2}{(1 + E_A^2)^2} - \frac{2}{A} \frac{\partial A_1}{\partial t_1} \frac{E_A}{1 + E_A^2}. \quad (67)$$

The solution of Eq. (67) is

$$u_1 = \frac{e^{-t_0} B - E_A \ln(1 + E_A^2)}{1 + E_A^2} - t_0 \frac{E_A + 2 e^{-t_0} \partial A_1 / \partial t_1}{1 + E_A^2}, \quad (68)$$

which clearly indicates the appearance of non-uniform behaviour for $t_0 = O(1/k)$.

In order to avoid non-uniformities, A_1 must satisfy

$$2 \frac{\partial A_1}{\partial t_1} + A_1 = 0, \quad A_1(t_1 = 0) = \tan(a/2), \quad (69)$$

whose solution yields

$$A_1(t_1, t_2, \dots) = A_2(t_2, \dots) e^{-t_1/2}. \quad (70)$$

Introducing Eq. (70) into Eqs. (65) and (68) yields

$$E_A = A_2(t_2, \dots) e^{-t_0 - t_1/2}, \quad (71)$$

and

$$u_1 = \frac{E_B - E_A \ln(1 + E_A^2)}{1 + E_A^2}, \quad (72)$$

where $E_B = B_1(t_1, \dots) \exp(-t_0)$, $B_1(0, 0, \dots) = A_1(0, \dots) \ln(1 + A_1(0, \dots)^2)$ and $A_2(0, \dots) = \tan(a/2)$.

To second order, one can easily obtain

$$\begin{aligned} \mathcal{L}(u_2) = & -\frac{1}{2} \frac{\partial^2 u_1}{\partial t_0^2} - \frac{1}{6} \frac{\partial^3 u_0}{\partial t_0^3} - \frac{\partial u_1}{\partial t_1} - \frac{\partial u_0}{\partial t_2} - \frac{\partial^2 u_0}{\partial t_1 \partial t_0} + \frac{d^2 F(u_0)}{du^2} \frac{u_1^2}{2}, \\ u_2(t_0 = 0) = & 0, \end{aligned} \quad (73)$$

whose solution is, after using Eqs. (65) and (72),

$$\begin{aligned} u_2 = & \frac{E_C}{1 + E_A^2} + \frac{4E_A^2 + 3E_B^2 + 6E_A E_B}{6E_A(1 + E_A^2)^2} \\ & - \frac{(1 - E_A^2)(E_B + E_A) \ln(1 + E_A^2)}{2(1 + E_A^2)^2} + \frac{E_A(1 - E_A^2) \ln^2(1 + E_A^2)}{4(1 + E_A^2)^2}, \end{aligned} \quad (74)$$

where now

$$E_A = A_3(t_3, \dots) \exp(-t_0 - t_1/2 - t_2/3), \quad (75)$$

$$E_B = B_3(t_2, \dots) \exp(-t_0 - t_1/2), \quad (76)$$

$$E_C = C_3(t_1, \dots) \exp(-t_0), \quad (77)$$

and the initial conditions for A_3 , B_3 and C_3 can be easily obtained but are omitted here.

To third order,

$$\begin{aligned} \mathcal{L}(u_3) = & -\frac{1}{2} \frac{\partial^2 u_2}{\partial t_0^2} - \frac{1}{6} \frac{\partial^3 u_1}{\partial t_0^3} - \frac{1}{24} \frac{\partial^4 u_0}{\partial t_0^4} - \frac{\partial u_2}{\partial t_1} - \frac{\partial u_1}{\partial t_2} - \frac{\partial u_0}{\partial t_3} - \frac{\partial^2 u_1}{\partial t_1 \partial t_0} - \frac{\partial^2 u_0}{\partial t_2 \partial t_0} \\ & - \frac{1}{2} \frac{\partial^2 u_0}{\partial t_1^2} - \frac{1}{2} \frac{\partial u_0}{\partial t_1 \partial t_0^2} + \frac{d^2 F(u_0)}{du^2} u_1 u_2 + \frac{d^3 F(u_0)}{du^3} \frac{u_1^3}{6}, \\ u_3(t_0 = 0) = & 0, \end{aligned} \quad (78)$$

whose solution can be readily obtained but is omitted here. We, therefore, have Eqs. (65) and (72) with

$$E_A = A_3(t_3, \dots) \exp(-t_0 - t_1/2 - t_2/3 - t_3/4), \quad (79)$$

$$E_B = B_2(t_2, \dots) \exp(-t_0 - t_1/2 - t_2/3), \quad (80)$$

$$E_C = C_1(t_1, \dots) \exp(-t_0 - t_1/2). \quad (81)$$

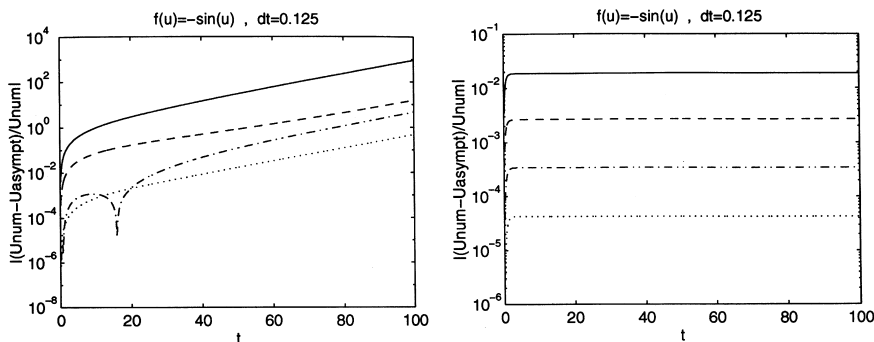


Fig. 6. Relative errors between the exact numerical solution and the multiple scales asymptotic expansion (left) and the summed-up asymptotic expansion (right) of the solution of the equivalent equation for $F(u) = -\sin(u)$, with $k = 0.125$ and $a = 1$. The relative errors of the asymptotic expansion including the leading, first, second and third order terms are denoted by solid, dashed, dash-dotted and dotted lines, respectively.

The errors of the resulting asymptotic expansion are illustrated in Fig. 6. In particular, Fig. 6 (left) shows that no secular behaviour is observed for this nonlinearity and for k sufficiently small. However, the accuracy of this uniform asymptotic expansion decreases for $k \geq 0.5$. For this nonlinearity, the resulting asymptotic expansion is uniform, although its relative error grows in time as illustrated in Fig. 6 (left); however, the asymptotic solution is not of any use as k is near to unity.

If further asymptotic terms are determined, the exponents in Eqs. (79)–(81) can be summed up to yield

$$E_A = \tan(a/2)(1-k)^{t/k}, \quad (82)$$

$$E_B = \tan(a/2) \ln(1 + \tan(a/2))(1-k)^{t/k}, \quad (83)$$

$$E_C = C_1(0, 0, \dots)(1-k)^{t/k}. \quad (84)$$

This kind of asymptotic method where the contributions of the slow time variables in each term are summed up to all orders, is referred to, in this work, as summed-up asymptotic expansion. The resulting asymptotic series resembles, but it is not equal to, the so-called superasymptotics introduced by Stokes [22] in 1847. Fig. 6 (right) shows that the summed-up asymptotic solution is completely uniform and results in an almost constant error.

Another example of an asymptotic expansion without non-uniformities corresponds to $F(u) = -u(1+u)$ for which Eq. (14) becomes

$$\begin{aligned}
u_0(t) &= \frac{E_A}{1 - E_A}, \\
u_1(t) &= \frac{E_B - E_A \ln(1 - E_A)}{(E_A - 1)^2}, \\
u_2(t) &= \frac{E_C}{(E_A - 1)^2} - \frac{2E_A E_B + E_A^2 + 2E_B^2}{2(E_A - 1)^3} \\
&\quad + \frac{(1 + E_A)(E_A - 2E_B) \ln(1 - E_A)}{2(E_A - 1)^3} + \frac{E_A(1 + E_A) \ln^2(1 - E_A)}{2(E_A - 1)^3}, \quad (85)
\end{aligned}$$

where higher order terms have been omitted, E_A , E_B and E_C are given by Eqs. (79)–(84), and the initial conditions are

$$\begin{aligned}
A_i(0, 0, \dots) &= \frac{a}{1 + a}, \\
B_i(0, 0, \dots) &= A_i(0, \dots) \ln(1 - A_i(0, \dots)). \quad (86)
\end{aligned}$$

This asymptotic solution is illustrated in Fig. 7 (left) which shows that the asymptotic expansion is uniform behaviour, although its error grows with time.

By using Eqs. (82)–(84), one can obtain a summed-up asymptotic expansion which is very accurate and exhibits a constant error for large times as indicated in Fig. 7 (right).

We have also studied other nonlinearities and obtained results similar to the ones presented in this section [23]. Note that the use of the multiple scales technique for the nonlinearities considered in Section 3.2 for which the regular asymptotic expansion appears to be uniform in the corresponding figures for the errors, i.e., $1/(1 + u)$, $-u^2$ and $-u^3$, yields the same asymptotic expansion

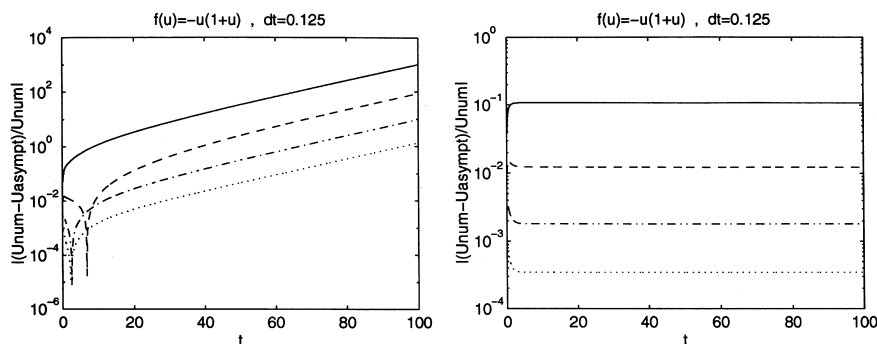


Fig. 7. Relative errors between the exact numerical solution and the multiple scales asymptotic expansion (left) and the summed-up asymptotic expansion (right) of the solution of the equivalent equation for $F(u) = -u(1 + u)$, with $k = 0.125$ and $a = 1$. The labels are the same as those in Fig. 6.

as that presented in Section 3.2, since non-uniform behaviour does not occur when the leading order term of the asymptotic expansion does not blow up. However, when the leading order term blows up, the multiple scales technique used in this section cannot be employed to avoid non-uniformities as time approaches the blow-up time.

It should be stated that, if the multiple scales asymptotic analysis is based on the second equivalent or the modified equation, the resulting asymptotic expansion is exactly the same as the one obtained here by using the equivalent equation.

5. Multiple scales technique for non-autonomous problems

Both the straightforward and the multiple scales asymptotic techniques used in the previous sections for autonomous problems can also be applied to non-autonomous ones, although it is more difficult to obtain the exact solution to the leading order equation in the asymptotic expansion.

For the sake of illustration, we shall consider a non-autonomous linear equation with $F(u, t) = \pm \sin(t)u$ and $u(t = 0) = a$, for which Eq. (14) yields

$$u_0 = E_A, \quad u_1 = E_A \frac{\sin(t)}{4} (\cos(t) \mp 2), \quad (87)$$

$$u_2 = 6E_C + \frac{E_A}{2304} (-495 \mp 456 \cos(t) - 432 \cos(2t) \pm 136 \cos(3t) - 9 \cos(4t)), \quad (88)$$

$$u_3 = E_A \frac{\sin(t)}{18432} (\pm 444 + 582 \cos(t) \pm 2560 \cos(2t) + 979 \cos(3t) \pm 100 \cos(4t) - 3 \cos(5t)) + E_C \frac{\sin(t)}{2} (\cos(t) \mp 2), \quad (89)$$

where

$$E_A = a \exp(\pm 1 \mp \cos(t) - t_1/4 - 3t_3/32),$$

$$E_C = \frac{117 \pm 40}{1728} a \exp(\pm 1 \mp \cos(t) - t_1/4).$$

The relative errors of the resulting asymptotic expansion are illustrated in Fig. 8 which shows that for the linearity with both signs and sufficiently small time steps, the error of the second- and fourth-order asymptotic expansions oscillates around zero, whereas it slowly grows in time for the leading and second order ones (cf. Fig. 8 (bottom)). In both cases, the resulting asymptotic expansion is uniform. Fig. 8 (top) indicates that, for time steps as large as

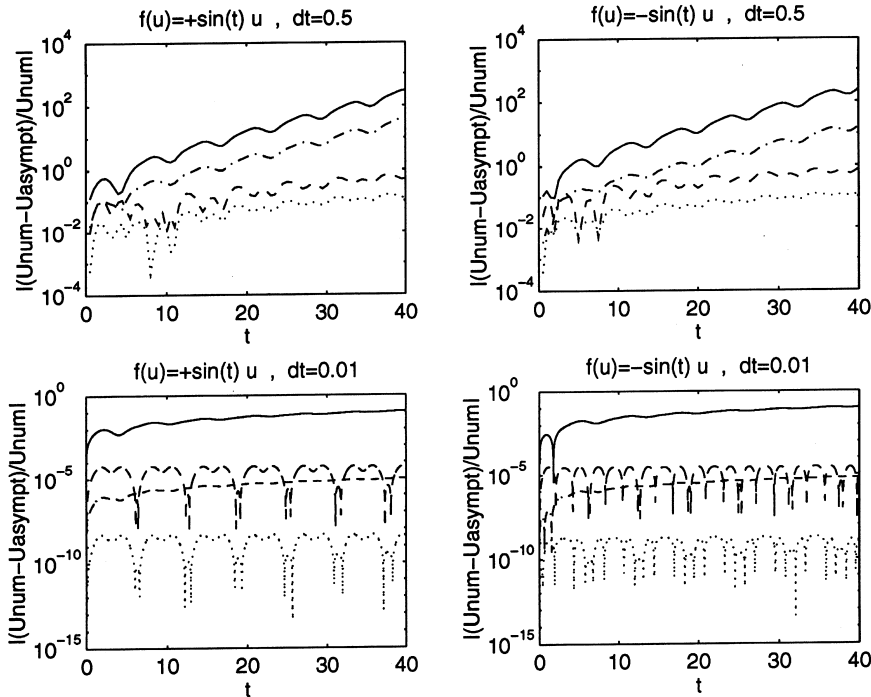


Fig. 8. Relative errors between the Euler numerical solution and the multiple scales asymptotic expansion for the solution of the equivalent equation for $F(u) = +\sin(t)u$ (left) and $F(u) = -\sin(t)u$ (right), $k = 0.5$ (top) $k = 0.01$ (bottom). The labels are the same as those in Fig. 6.

$k = 0.5$, the error of the asymptotic expansion grows with time and the slope of the error decreases as the number of terms in the asymptotic expansion is increased.

The technique of summed-up asymptotic expansions can also be applied to Eq. (47) with Eq. (87). However, since it has not been possible to obtain an analytical expression for the terms which appear in the exponents of E_A and E_C as in Eqs. (82)–(84), a summed-up asymptotic expansion was obtained by taking

$$E_C = \frac{117 \pm 40}{1728} E_A, \quad (90)$$

where $E_A(t, t_1, t_3, \dots)$ is given by Eq. (90). Fig. 9 shows the relative errors for the summed-up asymptotic expansion and indicates that, for sufficiently small k , the expansion is uniformly valid and both the magnitude and the slope of the error substantially decrease (Fig. 9 (bottom)). For k larger than about 0.1, the error of the second order asymptotic expansion grows in time as illustrated in

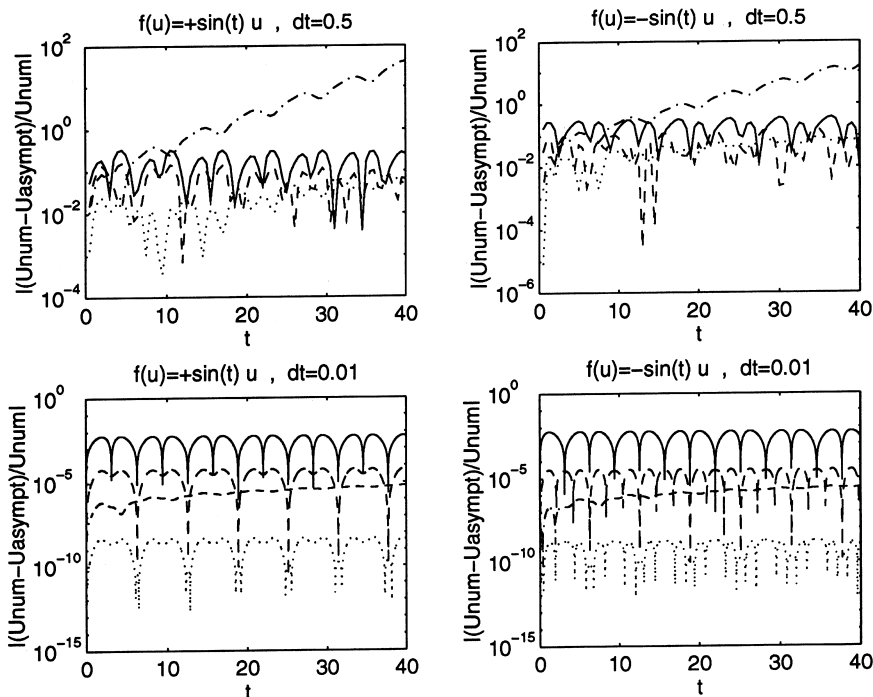


Fig. 9. Relative errors between the Euler numerical solution and the summed-up asymptotic expansion for the solution of the equivalent equation for $F(u) = +\sin(t)u$ (left) and $F(u) = -\sin(t)u$ (right), $k = 0.5$ (top) $k = 0.01$ (bottom). The labels are the same as those in Fig. 6.

Fig. 9 (top); however, the error decreases as additional terms are included in the expansion, and a uniform behaviour results.

6. Conclusions

Asymptotic methods have been employed to analyze the modified equation method resulting from the discretization of ordinary differential equations by means of the Euler forward numerical technique. The non-uniqueness of the differential equation truly represented by the difference equation has been illustrated, and three kinds of modified equations have been introduced. These modified equations are related to the interpretation of the finite difference method as a pseudo-differential one.

The first modified or equivalent equation has been obtained by expanding the truncation error terms of the difference method, and involves higher order derivatives multiplied by powers of the step size. Any linear combination of the

equivalent equation and its formal derivatives yields a new modified equation which is asymptotically equivalent to the numerical scheme provided that the step size is sufficiently small and higher order derivatives exist; in particular, the second modified or second equivalent equation has been introduced by dividing the right-hand-side of the equivalent equation by the pseudo-differential operator appearing in the left-hand-side of the equivalent equation. Any nonlinear combination of the equivalent equation and its derivatives, whose coefficients are polynomial functions of the nonlinearity and its derivatives, also yields a modified equation which is asymptotically equivalent to the (first) equivalent equation; in particular, the third modified or (simply) modified equation has been introduced and may be derived by inversion of the Taylor series expansion of the pseudo-differential operator appearing on the right hand-side of the (first) equivalent equation.

A regular asymptotic analysis based on the step size as small parameter has been presented for the analysis of modified equations corresponding to initial-value problems of autonomous ordinary differential equations, and its results indicate that, depending on the nonlinearity, the resulting asymptotic expansion may be uniform and very accurate even for very large step sizes.

In order to eliminate the non-uniform behaviour of regular expansions for modified equations, the technique of multiple scales has been first used for linear equations with constant coefficients. The resulting asymptotic expansion has been summed-up to all orders, and the results indicate that the solution of the equivalent equation, second equivalent equation and modified equation are all equal to the natural analytical continuation of the finite difference solution. Therefore, the modified equation method has been shown to be valid for linear equations with constant coefficients.

For nonlinear problems, some examples of nonlinearities for which the method of multiple scales yields uniform asymptotic expansions, have been presented, although this is not always the case for general nonlinearities. It has been illustrated that, when the asymptotic expansion is uniform, the resulting asymptotic expansion has been shown to be very accurate. However, for nonlinear problems whose leading order term either grows with time or blows up in finite time, non-uniform results are obtained.

The asymptotic analysis of the Euler forward method for autonomous problems can be easily extended to non-autonomous ones. For the simple linear problem considered here, it has been found that the asymptotic analysis presented in this paper provide very accurate results.

The main conclusion of the present paper is that the equivalent, the second equivalent and the modified equations, and, therefore, other modified equations obtained by similar methods, are asymptotically equivalent; moreover, they are also equivalent to the Euler forward difference scheme. This asymptotic equivalence means that an asymptotic analysis based on the step size as small parameter yields exactly the same results for all the modified equations

provided that higher order derivatives exist and are bounded. Furthermore, the results presented in this paper indicate that the asymptotic analysis of general consistent, two-level, both explicit and implicit, stable, finite difference schemes may be obtained by means of asymptotic methods for the corresponding modified equation by using the step size as a small parameter.

Acknowledgements

The research reported in this paper was supported by Project PB94-1494 from the D.G.I.C.Y.T. of Spain.

References

- [1] D.F. Griffiths, J.M. Sanz-Serna, On the scope of the method of modified equations, *SIAM J. Sci. Statist. Comput.* 7 (1986) 994–1008.
- [2] R.F. Warming, B.J. Hyett, The modified equation approach to the stability and accuracy analysis of finite-difference methods, *J. Comput. Phys.* 14 (1974) 159–179.
- [3] B.J. Daly, The stability properties of a coupled pair of nonlinear partial differential equations, *Math. Comput.* 17 (1963) 346–360.
- [4] W.F. Noh, M.H. Protter, Difference methods and the equations of hydrodynamics, *J. Math. Mech.* 12 (1963) 143–191.
- [5] N.N. Yanenko, Yu.I. Shokin, First differential approximation method and approximate viscosity of difference schemes, *Phys. Fluids* 12 (Suppl.) (1969) 28–33.
- [6] N.N. Yanenko, Yu.I. Shokin, On the group classification of difference schemes for systems of equations in gas dynamics, in: M. Holt (Eds.), *Proceedings of the Second International Conference on Numerical Methods in Fluid Mechanics*, Springer, New York, 1971.
- [7] C.W. Hirt, Heuristic stability theory for finite difference equations, *J. Comput. Phys.* 2 (1968) 339–355.
- [8] R.D. Richtmyer, K.W. Morton, *Difference Methods for Initial Value Problems*, Wiley/Interscience, New York, 1967.
- [9] A. Lerat, R. Peyret, Sur l'origine des oscillations apparaissant dans les profils de choc calculés par des méthodes aux différences, *Compt. Rend. Acad. Sci. Paris A* 277 (1973) 363–366.
- [10] A. Lerat, R. Peyret, Noncentered schemes and shock propagation problems, *Computers Fluids* 2 (1974) 35–52.
- [11] A. Lerat, R. Peyret, Propriétés dispersives et dissipatives d'une classe de schémas aux différences pour les systèmes hyperboliques nonlinéaires, *Rech. Aérospace* 2 (1975) 61–79.
- [12] G.W. Hedstrom, Models of difference schemes for $u_t + u_x = 0$ by partial differential equations, *Math. Comput.* 29 (1975) 969–977.
- [13] J. Goodman, A. Majda, The validity of the modified equation for nonlinear shock waves, *J. Comput. Phys.* 58 (1985) 336–348.
- [14] S.-Ch. Chang, A critical analysis of the modified equation technique of Warming and Hyett, *J. Comput. Phys.* 86 (1990) 107–126.
- [15] G.E. Forsyth, W.R. Wasow, *Finite Difference Methods for Partial Differential Equations*, Wiley, New York, 1960.
- [16] P.J. Roache, *Computational Fluid Dynamics*, Hermosa Publishers, Albuquerque, NM, 1972.
- [17] R. Peyret, T.D. Taylor, *Computational Methods for Fluid Flow*, Springer, New York, 1983.

- [18] C. Hirsch, Numerical Computation of Internal and External Flows, vol. 1, Wiley, New York, 1988.
- [19] J.D. Ramshaw, Numerical viscosities of difference schemes, Commun. Num. Methods Eng. 10 (1994) 927–931.
- [20] J. Kevorkian, J.D. Cole, Perturbation Methods in Applied Mathematics, Springer, New York, 1981.
- [21] Yu.I. Shokin, The Method of Differential Approximations, Springer, New York, 1983.
- [22] R.B. Dingle, Asymptotic Expansions: Their Derivation and Interpretation, Academic Press, New York, 1973.
- [23] F.R. Villatoro, J.I. Ramos, On the method of modified equations. I. Asymptotic analysis of the Euler forward difference method, Technical Report No. ITI-98-1, Departamento de Lenguajes y Ciencias de la Computación, E.T.S. Ingenieros Industriales, Universidad de Málaga, Spain (1997).