

Modified equations for ODEs

M. P. CALVO, A. MURUA AND J. M. SANZ-SERNA

ABSTRACT. We study the method of modified equations for the analysis of discretizations of ordinary differential equations. We show how to systematically construct modified system of any order. Some applications are presented.

1. Introduction

Modified equations [28], [13] are a means for the analysis of numerical methods for differential equations. Modified equations are strongly related to the idea of *backward error analysis*, explained in all numerical analysis textbooks. Given a problem \mathcal{P} with true solution \mathcal{S} and given an approximate solution $\tilde{\mathcal{S}}$, *forward error analysis* consists of estimating the distance between $\tilde{\mathcal{S}}$ and \mathcal{S} . Backward error analysis consists of showing that $\tilde{\mathcal{S}}$ exactly solves a problem $\tilde{\mathcal{P}}$ which is close to \mathcal{P} . While backward error analysis has played a role of paramount importance in areas like numerical linear algebra, error analysis of numerical methods for evolutionary problems has essentially been of the forward variety (see nevertheless [4], [23], [10]).

However, there are many instances where forward error analysis of numerical simulations of evolutionary problems is doomed to fail. In regimes where true orbits of the system quickly diverge from each other, including chaotic dynamics, any numerical method in realistic circumstances will produce an answer $\tilde{\mathcal{S}}$ very different from the true \mathcal{S} . Hence the outcome of forward analysis would be that any method performs badly, a conclusion at odds with the fact that numerical simulations have been helpful in ascertaining the behaviour of the systems involved. Similarly, classical error bounds are meaningless in long-time simulations performed in order to find the qualitative behaviour of most nontrivial dynamical systems. Therefore there is a clear need for analyses that depart from

1991 *Mathematics Subject Classification*. Primary 65L05; Secondary 70H15, 05C05.

This research has been supported by project DGICYT PB89-0351.

This paper is in final form and no version of it will be submitted for publication elsewhere.

the classical (forward) error bounds for numerical integrators of evolutionary problem.

An idea that has become quite prominent is that of *shadowing*. Originally introduced in a dynamical systems context [2], [5], it has recently gained popularity in numerical analysis applications, see e.g. [1], [3], [8], [9], [12], [17], [18], [19], [20], [21], [22], [26], [27]. In a shadowing approach, the numerically computed orbit with initial value u_0 is compared not with the true orbit from u_0 , but with the shadowing orbit, the exact orbit of the system being simulated corresponding to a slightly perturbed \tilde{u}_0 . Typically it is shown that the distance between the numerical and shadowing orbits is small in some sense, while the distance between the numerical orbit and the true orbit (i.e. the classical error) is unacceptable. The similarity with backward error analysis is evident.

In the shadowing approach, the initial condition is allowed to be changed, while keeping the same evolutionary system. In the modified equation technique the numerical solution is compared with a solution of a perturbed system. The idea of modified equations has been around for some time (see e.g. [28]), mainly in the study of dissipation and dispersion properties of numerical schemes for partial differential equations. However it is only recently that the method has been applied to ordinary differential equations (ODEs), specially to investigate symplectic methods for Hamiltonian systems [24], [25], [14].

In this paper, the attention is restricted to one-step numerical methods for initial value problems for D -dimensional systems of ODEs:

$$(1) \quad \frac{du}{dt} = f(u), \quad u(0) = u_0.$$

For simplicity, we assume that the vector field f is defined in the whole of \mathcal{R}^D and of class C^∞ . Of course the system in (1) may arise from the discretization in space of a system of time-dependent partial differential equations.

Simple examples of numerical methods are Euler's rule

$$(2) \quad u_{n+1} = u_n + hf(u_n),$$

the implicit midpoint rule

$$(3) \quad u_{n+1} = u_n + hf\left(\frac{1}{2}(u_n + u_{n+1})\right),$$

and Runge's second order method

$$(4) \quad u_{n+1} = u_n + hf\left(u_n + \frac{h}{2}f(u_n)\right).$$

Here h denotes the time step and u_n is the numerical solution at time $t_n = nh$.

A numerical method is consistent of order $p \geq 1$ if, for all u in \mathcal{R}^D ,

$$(5) \quad \psi_{h,f}(u) - \phi_{h,f}(u) = O(h^{p+1}), \quad h \rightarrow 0,$$

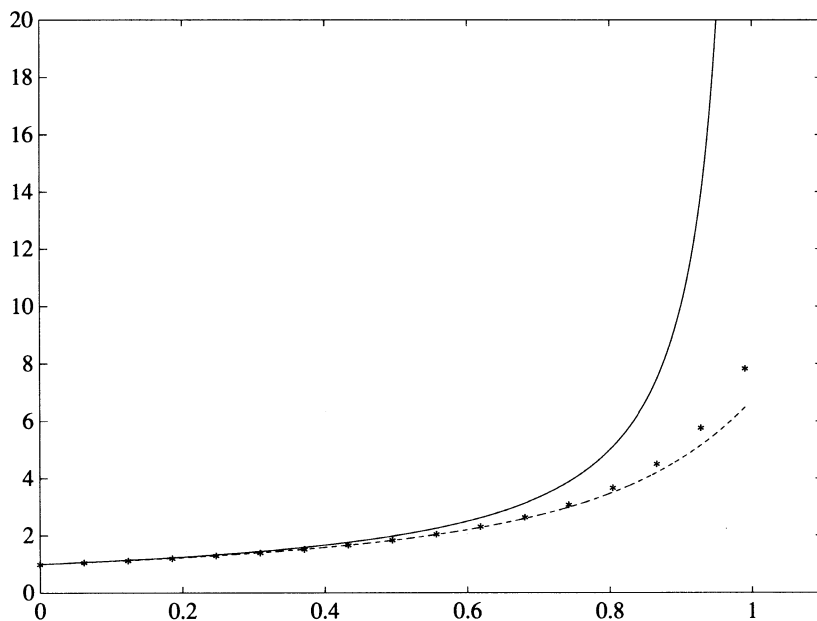


FIGURE 1. True solution $u = u(t)$ (solid), Euler solution (stars) and modified solution (dashes) for $du/dt = u^2$.

where $\psi_{h,f}(u)$ and $\phi_{h,f}(u)$ respectively denote the numerical and theoretical solutions after one step of length h taken from the initial condition u (so that $\phi_{h,f}$ is the flow of (1)). From the local error estimate (5), it follows [6], [15] that, as $h \rightarrow 0$, the global errors $u_n - u(t_n)$ are $O(h^p)$, uniformly in bounded time intervals $0 \leq t_n \leq t_{max}$ contained in the interval of existence of the true solution $u(t)$ (convergence of order p). The order is 2 for (3) and (4) and only 1 for (2).

We now present a simple example of the application of the method of modified equations. We integrate in the interval $0 \leq t \leq T = 0.99$ the equation $du/dt = f(u) = u^2$ with initial condition $u(0) = 1$ (solution $u(t) = 1/(1-t)$). The solid line in Figure 1 represents the true solution, while the stars depict the numerical solution for Euler's rule with $h = T/16$. We see that there is little agreement between the behaviour of the numerical and theoretical solutions. Can we find a differential equation whose solution with initial condition $u_0 = 1$ behaves as the numerically computed points? To be more precise, we try to find a modified equation $du/dt = \tilde{f}(u)$ such that, for all u ,

$$\psi_{h,f}(u) - \phi_{h,\tilde{f}}(u) = O(h^3),$$

i.e. such that Euler's rule, consistent of the first order with the problem being integrated, is consistent of the *second* order with the modified equation. By going from local to global errors, the computed points u_n will lie at distance $O(h^2)$ from the solution of the modified equation with initial value u_0 . To find

\tilde{f} we start with an ansatz $\tilde{f}(u) = u^2 + hF(u)$, where F is a function of u to be determined. Note that \tilde{f} depends on h . Expanding in powers of h the flow $\phi_{h,\tilde{f}}(u)$, it is found that it differs from $\psi_{h,f}(u) = u + hu^2$ in $O(h^3)$ terms if $F = -u^3$, which leads to the modified $\tilde{f} = u^2 - hu^3$. The solution of the modified equation is shown in Figure 1 by a dotted line. It is clear that the numerical solution is better described by the modified equation than by the original equation being solved. It is now possible to look for an even better \tilde{f} , $\tilde{f}_2(u) = u^2 - hu^3 + h^2F_2(u)$, to have consistency of the third order and more generally for vector fields $\tilde{f}_N(u) = u^2 - hu^3 + h^2F_2(u) + \dots + h^{N-1}F_{N-1}(u)$ leading to consistency of order N . We then say that $du/dt = \tilde{f}_N(u)$ is a modified equation of order N .

In §2 of this paper we show how to systematically construct modified systems of any order for one-step methods. The formulae we present are due to Hairer [14]; however our methodology for the derivation of those formulae is different from and easier than that presented in the original paper. An example of the application of modified equation techniques is given in §3.

2. Constructing modified equations

It is well known [6], [15] that (rooted) trees are an important tool in the analysis of one-step methods. The trees with four or fewer nodes are depicted in Figure 2. The symbol τ_1 denotes the only tree with one node. It is common to denote by $[\tau^1, \tau^2, \dots, \tau^m]$ the tree that consists of the root and m leaving edges to which the trees $\tau^1, \tau^2, \dots, \tau^m$ are attached. Thus in Figure 2, $\tau_2 = [\tau_1]$, $\tau_{31} = [\tau_1, \tau_1]$, $\tau_{32} = [\tau_2]$, etc. For each tree τ , the integers $\rho(\tau)$ and $\alpha(\tau)$ respectively denote its order (number of nodes) and number of monotonic labellings. These functions can be computed recursively by the formulae $\rho(\tau_1) = \alpha(\tau_1) = 1$ and, for $\tau = [\tau^1, \dots, \tau^m]$,

$$\begin{aligned} \rho(\tau) &= 1 + \rho(\tau^1) + \dots + \rho(\tau^m), \\ \alpha(\tau) &= \frac{(\rho(\tau) - 1)!}{\rho(\tau^1)! \dots \rho(\tau^m)!} \alpha(\tau^1) \dots \alpha(\tau^m) \frac{1}{\mu_1! \mu_2! \dots}. \end{aligned}$$

The integers μ_i count the number of equal trees among τ^1, \dots, τ^m . Finally, in connection with the system in (1), an \mathcal{R}^D -valued function $F(\tau)(u)$ (elementary differential) is associated with each tree τ . The recursive definition of the $F(\tau)(u)$'s is $F(\tau_1)(u) = f(u)$ and for $\tau = [\tau^1, \dots, \tau^m]$

$$F(\tau)(u) = f^{(m)}(u)(F(\tau^1)(u), \dots, F(\tau^m)(u)),$$

where $f^{(m)}(u)$ represents the m -th Frechet derivative of f evaluated at u .

With these notations, the formal Taylor expansion of the flow $\phi_{h,f}$ in powers of h is given by

$$\phi_{h,f}(u) = u + \sum_{\tau \in T} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \alpha(\tau) F(\tau)(u),$$

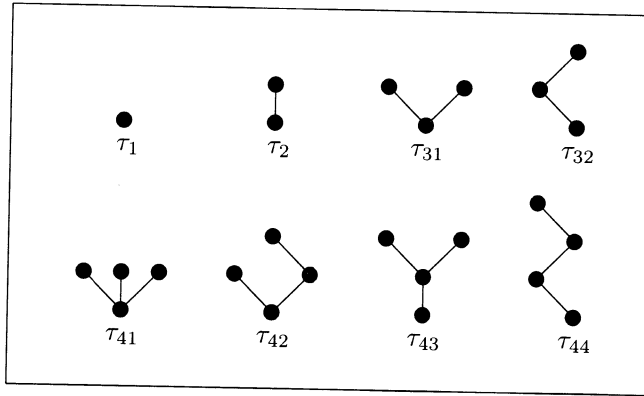


FIGURE 2. Trees of order ≤ 4 .

where T denotes the set of all trees.

Numerical methods can be Taylor expanded in a similar way. Methods (2), (3) and (4) are particular instances of Runge-Kutta methods. A general Runge-Kutta method is specified by an integer $s \geq 1$ (the number of stages) and real coefficients $a_{ij}, b_i, i, j = 1, \dots, s$. Its application to (1) results in the formulae

$$U_i = u_n + h \sum_{j=1}^s a_{ij} f(U_j),$$

$$u_{n+1} = u_n + h \sum_{i=1}^s b_i f(U_i).$$

For Euler's rule $s = 1, a_{11} = 0, b_1 = 1$; for the midpoint rule $s = 1, a_{11} = 1/2, b_1 = 1$; for the method (4), $s = 2, a_{21} = 1/2, b_2 = 1$ and the remaining coefficients are 0. The Taylor expansion of a Runge-Kutta method is

$$\psi_{h,f}(u) = u + \sum_{\tau \in T} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \alpha(\tau) \left(\gamma(\tau) \sum_{i=1}^s b_i \Phi_i(\tau) \right) F(\tau)(u),$$

where the recursive definitions of γ and Φ_i are $\gamma(\tau_1) = 1, \Phi_i(\tau_1) = 1$ and

$$\gamma(t) = \rho(\tau) \gamma(\tau^1) \dots \gamma(\tau^m),$$

$$\Phi_i(\tau) = \sum_{j_1, \dots, j_m} a_{ij_1} \Phi_{j_1}(\tau^1) \dots a_{ij_m} \Phi_{j_m}(\tau^m).$$

In view of the Taylor expansions above, Hairer and Wanner [16] introduced the notion of a B-series. Given a real valued mapping a defined in the union of T and the set $\{\emptyset\}$, a B-series $B(a, u)$ is a formal power series

$$a(\emptyset)u + \sum_{\tau \in T} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \alpha(\tau) a(\tau) F(\tau)(u).$$

Thus the true flow $\phi_{h,f}$ corresponds to $a \equiv 1$, while for a Runge-Kutta method $a(\emptyset) = 1$ and

$$a(\tau) = \gamma(\tau) \sum_{i=1}^s b_i \Phi_i(\tau).$$

These ideas are not confined to Runge-Kutta methods. The Taylor expansion of most one-step methods used in practice is also a B-series. In the remainder of the section we assume that we are dealing with a method $\psi_{h,f}(u)$ corresponding to a suitable B-series $B(a, u)$, without specifying the exact nature of the method. We suppose that the method is at least of order 1, i.e.

$$(6) \quad a(\emptyset) = 1, \quad a(\tau_1) = 1.$$

Our aim is to construct a formal power series \tilde{f}

$$(7) \quad \sum_{\tau \in T} \frac{h^{\rho(\tau)-1}}{\rho(\tau)!} \alpha(\tau) b(\tau) F(\tau)(u)$$

so that for each integer $N \geq 1$

$$(8) \quad \frac{du}{dt} = \tilde{f}_N(u) = \sum_{1 \leq \rho(\tau) \leq N} \frac{h^{\rho(\tau)-1}}{\rho(\tau)!} \alpha(\tau) b(\tau) F(\tau)(u)$$

provides a modified equation of order N .

An essential tool for our purposes is the formula for composition of B-series, see Theorem 11.6 in [15]. If a and b are B-series coefficients with $a(\emptyset) = 1$ then the composition $B(b, B(a, y))$ is again a B-series $B(ab, y)$ whose coefficients $ab(\tau)$ can be found in a systematic way from the a 's and b 's. The formulae for the first $ab(\tau)$ are

$$(9) \quad ab(\emptyset) = b(\emptyset),$$

$$(10) \quad ab(\tau_1) = b(\emptyset)a(\tau_1) + b(\tau_1),$$

$$(11) \quad ab(\tau_2) = b(\emptyset)a(\tau_2) + 2b(\tau_1)a(\tau_1) + b(\tau_2),$$

$$(12) \quad ab(\tau_{31}) = b(\emptyset)a(\tau_{31}) + 3b(\tau_1)a(\tau_1)^2 + 3b(\tau_2)a(\tau) + b(\tau_{31}),$$

$$(13) \quad ab(\tau_{32}) = b(\emptyset)a(\tau_{32}) + 3b(\tau_1)a(\tau_2) + 3b(\tau_2)a(\tau) + b(\tau_{32}).$$

We introduce a real parameter λ and write the flow of the vector field in (7) as a B-series

$$\phi_{\lambda h, \tilde{f}}(u) = u + \sum_{\tau \in T} \frac{h^{\rho(\tau)}}{\rho(\tau)!} \alpha(\tau) a_\lambda(\tau) F(\tau)(u).$$

Next we substitute this series into the equation

$$\frac{d}{dt} \phi_{t, \tilde{f}} = \tilde{f}(\phi_{t, \tilde{f}});$$

in doing so the B-series of the right hand side is computed by the formula for composing B-series. In this way we find that the $a_\lambda(\tau)$ satisfy, for each tree τ ,

$$(14) \quad \frac{d}{d\lambda} a_\lambda(\tau) = (a_\lambda b)(\tau).$$

Furthermore at $\lambda = 0$, $\phi_{0,\tilde{f}}(u) = u$ and hence, for each τ ,

$$(15) \quad a_0(\tau) = 0.$$

The relations (14)–(15) allow the computation of the $a_\lambda(\tau)$'s in terms of the $b(\tau)$'s when the latter are known. In our setting, the b coefficients are determined to ensure that, for each τ , at $\lambda = 1$

$$(16) \quad a_1(\tau) = a(\tau),$$

to impose that, as formal power series, $\phi_{h,\tilde{f}}$ and $\psi_{h,f}$ coincide.

The relations (14)–(16) make it possible to recursively compute the b coefficients. Let us illustrate this. For τ_1 we obtain from (14) and (10), $(d/d\lambda)a_\lambda(\tau_1) = b(\tau_1)$, so that, according to (15), $a_\lambda(\tau_1) = \lambda b(\tau_1)$. If we now impose (16), we obtain the relation $b(\tau_1) = a(\tau_1)$. We conclude, from the consistency assumption (6), that $b(\tau_1) = 1$, and therefore, as expected, \tilde{f} differs from f in $O(h)$ terms.

If we now go through the same steps for the next tree τ_2 , we successively obtain

$$\begin{aligned} \frac{d}{d\lambda} a_\lambda(\tau_2) &= 2b(\tau_1)a_\lambda(\tau_1) + b(\tau_2) \\ &= 2\lambda b(\tau_1)^2 + b(\tau_2), \\ a_\lambda(\tau_2) &= \lambda^2 b(\tau_1)^2 + \lambda b(\tau_2), \\ a(\tau_2) &= b(\tau_1)^2 + b(\tau_2). \end{aligned}$$

The last equation yields $b(\tau_2)$. Note that for a method of order ≥ 2 , $a(\tau_2) = 1$, which, in tandem with $b(\tau_1) = 1$, leads to $b(\tau_2) = 0$ and \tilde{f} and f differ in $O(h^2)$ terms.

Similarly the equations for finding $b(\tau_{32})$ and $b(\tau_{31})$ turn out to be

$$\begin{aligned} a(\tau_{31}) &= b(\tau_1)^3 + \frac{3}{2}b(\tau_2)b(\tau_1) + b(\tau_{31}), \\ a(\tau_{32}) &= b(\tau_1)^3 + 3b(\tau_2)b(\tau_1) + b(\tau_{32}). \end{aligned}$$

From here $b(\tau_{31}) = b(\tau_{32}) = 0$ for methods of order ≥ 3 .

We summarize our findings in the following theorem, due to Hairer [14].

THEOREM 1. *Assume that an order p , $p \geq 1$, one-step method can be formally Taylor expanded into a B-series $B(a, u)$. There is a unique B-series (7), differing from $f(u)$ in $O(h^p)$ terms, such that, for each integer $N \geq 1$, (8) provides a modified system of order N . The coefficients b can be recursively found as functions of the coefficients a .*

We emphasize that the formal power series (7) in general does not converge. Lack of space prevents us from discussing further this point and the interested reader is referred to [24] and to Chapter 10 in [25].

3. An application

We now illustrate the use of modified equations in ODEs. We consider the pendulum system, that we write in terms of the components p and q of u as

$$\frac{dp}{dt} = -\sin q, \quad \frac{dq}{dt} = p.$$

This is a Hamiltonian problem [24], [25] with Hamiltonian function (energy) $H = (1/2)p^2 + 1 - \cos q$. Let (p_0, q_0) be an initial condition with energy H_0 , $0 < H_0 < 2$, leading to a periodic solution. In phase plane the trajectory corresponds to the level set $H = H_0$; the period T_0 of the solution is an increasing function of H_0 . Furthermore, we respectively denote by f_0 and g_0 the vector field f evaluated at (p_0, q_0) and the energy gradient at (p_0, q_0) . The vectors f_0 and g_0 are mutually orthogonal by conservation of energy.

This initial value problem is integrated by a one-step method of order p with step length h , that for simplicity we assume to be of the form $h = T_0/\nu$, with ν a positive integer. Let $e_M(h)$ be the global error $u_n - u(t_n)$ after $n = M\nu$ steps, i.e. after simulating M periods of the solution. Then it is not too difficult to show (see [7]) that

$$(17) \quad e_M(h) = M e_1(h) + \frac{1}{2}(M^2 - M)(g_0, e_1(h)) \delta_0 f_0 + O(h^{2p}), \quad h \rightarrow 0,$$

where (\cdot, \cdot) means inner product and δ_0 denotes the derivative of the period T with respect to the energy H evaluated at the initial condition. Therefore, ignoring the $O(h^{2p})$ remainder, the error $e_M(h)$ grows quadratically with M . The leading M^2 growth is in the direction of f_0 , i.e. tangent to the solution at the initial point, thus corresponding to a *phase error*. However linear error growth with M is possible: if $(g_0, e_1(h)) = O(h^{2p})$ (i.e. the error after one period is almost orthogonal to the energy gradient), then

$$e_M(h) = M e_1(h) + O(h^{2p}), \quad h \rightarrow 0.$$

To sum up, the way global errors build up is determined by the *direction* of the error $e_1(h)$. This is not surprising: if after one period the error $e_1(h)$ has a significant component in the direction of g_0 , then the numerical solution has jumped in phase plane to a neighbouring trajectory corresponding to a different (say larger) value of the energy. Thereafter, the method, when evaluating the vector field f , picks up wrong information as to the solution period and is led to believe that the motion is faster than it really is. As the integration proceeds the numerical solution keeps jumping to higher and higher energy levels and getting unduly speeded up. This is the mechanism leading to quadratic growth in the *phase error*. On the other hand, if $e_1(h)$ is essentially in the direction of

f_0 , then there is no energy error: the method is basically describing the right trajectory with a slightly distorted average velocity and errors grow linearly. These considerations apply to all nonlinear oscillators with one degree of freedom [7] and even to some partial differential equations [11].

We now use the method of modified equations to investigate the direction of $e_1(h)$. We begin with the midpoint rule (3). The modified system with $N = 4$ is found to be

$$\begin{aligned}\frac{dp}{dt} &= -\sin q + \frac{h^2}{24}(\sin 2q - p^2 \sin q), \\ \frac{dq}{dt} &= p - \frac{h^2}{12}p \cos q.\end{aligned}$$

There are no $O(h^3)$ terms: the b coefficients corresponding to trees of order 4 vanish, a consequence of the symmetry of the midpoint rule [14]. The modified system is the Hamiltonian system with Hamiltonian function

$$\tilde{H} = \frac{1}{2}p^2 + (1 - \cos q) + \frac{h^2}{48}(-2p^2 \cos q + \cos 2q - 1).$$

The Hamiltonian character of the modified system is linked to the symplecticness of the midpoint rule [24], [25], [14]. The modified solution \tilde{u} conserves \tilde{H} exactly and hence, Taylor expanding,

$$\begin{aligned}0 = \tilde{H}(\tilde{u}(T_0)) - \tilde{H}(u_0) &= (\tilde{g}_0, \tilde{u}(T_0) - u_0) + O(|\tilde{u}(T_0) - u_0|^2) \\ (18) \qquad \qquad \qquad &= (\tilde{g}_0, \tilde{u}(T_0) - u_0) + O(h^4).\end{aligned}$$

Here \tilde{g}_0 is the gradient of \tilde{H} at the initial point u_0 and we have used that

$$(19) \qquad \tilde{u}(T_0) - u_0 = \tilde{u}(T_0) - u(T_0) = O(h^2),$$

due to the periodicity of the true solution and to the fact that the true and modified vector fields differ in $O(h^2)$ terms. From (18)–(19), along with $\tilde{g}_0 - g_0 = O(h^2)$, we obtain

$$(20) \qquad (g_0, \tilde{u}(T_0) - u_0) = O(h^4),$$

and finally, since \tilde{u} and the numerical solution differ in $O(h^4)$ terms,

$$(21) \qquad (g_0, e_1(h)) = O(h^4).$$

We take this to (17) and conclude that for the midpoint rule

$$e_M(h) = c_0 M h^2 f_0 + O(h^4), \quad h \rightarrow 0,$$

where c_0 is a constant depending on the initial condition, but independent of M and h . This is illustrated in Figure 3, where the initial condition is $p_0 = 0$, $q_0 = \pi/3$ and $h = T_0/400$. The dash-dot line gives the Euclidean norm of the error as a function of M . The linear growth is clear.

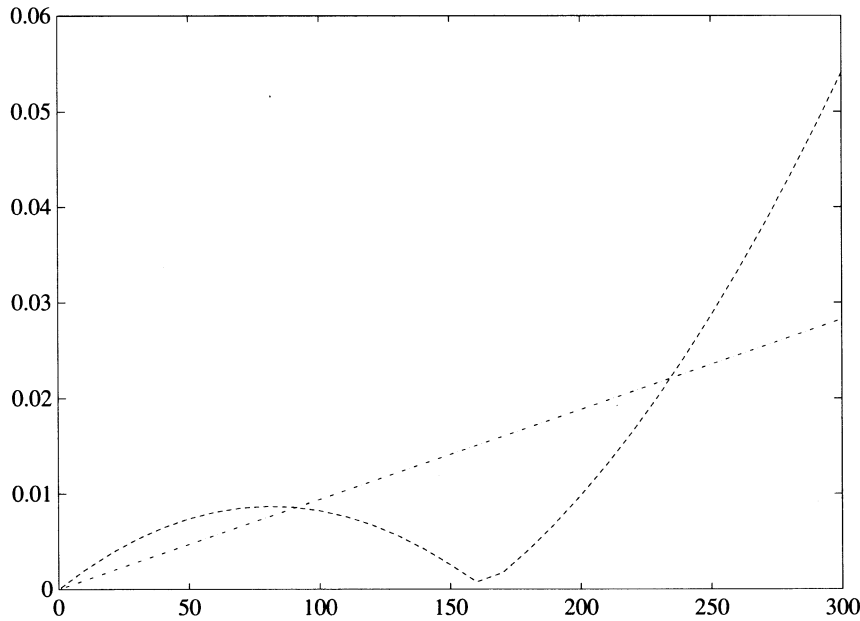


FIGURE 3. Euclidean norm of the error against time measured in periods. The dash-dot line corresponds to the midpoint rule and the dash line to Runge's method.

We next use the method (4). The modified equations with $N = 3$ turn out to be

$$\begin{aligned}\frac{dp}{dt} &= -\sin q - \frac{h^2}{24}(p^2 \sin q + 2 \sin 2q), \\ \frac{dq}{dt} &= p + \frac{h^2}{6}p \cos q,\end{aligned}$$

and for $N = 4$ we find

$$\begin{aligned}\frac{dp}{dt} &= -\sin q - \frac{h^2}{24}(p^2 \sin q + 2 \sin 2q) + \frac{h^3}{8}p \cos^2 q, \\ \frac{dq}{dt} &= p + \frac{h^2}{6}p \cos q + \frac{h^3}{16}(p^2 \sin q + \sin 2q).\end{aligned}$$

The modified system of order $N = 3$ is not Hamiltonian but has the reversibility property of being invariant under the change of p into $-p$ and t into $-t$. It has the following invariant of motion

$$I = \frac{p^2}{2(1 + (h^2/6) \cos q)^{\frac{1}{2}}} + \int_0^q \frac{\sin \xi + (h^2/3) \sin 2\xi}{(1 + (h^2/6) \cos \xi)^{\frac{3}{2}}} d\xi.$$

This quantity plays now the role played by \tilde{H} in the midpoint rule analysis, so that (20) still holds. However since we are dealing with a modified system of

order 3 we only conclude that

$$(22) \quad (g_0, e_1(h)) = O(h^3),$$

(rather than (21)), and (17) implies

$$e_M(h) = C_0 M f_0 h^2 + O(h^3), \quad h \rightarrow 0.$$

To explicitly obtain the h^3 term in the asymptotic expansion of $e_M(h)$ we have to resort to the modified problem with $N = 4$. Now, this is a system with negative dissipation. Straightforward differentiation reveals that along its solutions the $O(h^3)$ quantity dI/dt remains positive for $|q| \leq \pi/2$, leading to $O(h^3)$ outward spiraling. From here we see that the inner product in (22) is actually of size $O(h^3)$ and no better. Then

$$e_M(h) = C_0 M f_0 h^2 + (D_0 M^2 + E_0 M) f_0 h^3 + F_0 M g_0 h^3 + O(h^4), \quad h \rightarrow 0,$$

where C_0 , D_0 , E_0 and F_0 are real constants independent of h and M , with C_0 , D_0 and F_0 different from 0.

The dotted line in Figure 3 gives the actual error norm for the value $h = T_0/400$ used before. For M large, $M^2 h^3$ dominates over $M h^2$ and what we see is the quadratic growth of the $O(h^3)$ terms in the expansion. For M small (say less than 20) $M^2 h^3$ is negligible relatively to the leading $M h^2$ term and we see linear growth. We infer from the figure that for M near 160 the $M h^2$ and $M^2 h^3$ contributions are of equal size and cancel each other.

REFERENCES

1. F. Alouges and A. Debussche, *On the qualitative behavior of the orbits of a parabolic differential equation and its discretization in the neighborhood of a hyperbolic fixed point*, Numer. Funct. Anal and Optimiz. **12** (1991), 253–269.
2. D. V. Anosov, *Geodesic flows and closed Riemannian manifolds with negative curvature*, Proc. Steklov Inst. Math. **90** (1967).
3. W.-J. Beyn, *On the numerical approximation of phase portraits near stationary points*, SIAM J. Numer. Anal. **24** (1987), 1095–1113.
4. ———, *Numerical methods for dynamical systems*, Advances in Numerical Analysis, Vol. I (W. Light ed.), Clarendon, Oxford, 1991, pp. 175–236.
5. R. Bowen, *ω -limit sets for axiom A-diffeomorphisms*, J. Diff. Eq. **18** (1975), 333–339.
6. J. C. Butcher, *The Numerical Analysis of Ordinary Differential Equations*, “John Wiley”, Chichester, 1987.
7. M. P. Calvo and J. M. Sanz-Serna, *The development of variable-step symplectic integrators, with application to the two-body problem*, SIAM J. Sci. Comput. **14** (1993), 936–952.
8. S. N. Chow and K. J. Palmer, *On the numerical computation of orbits of dynamical systems: the one-dimensional case*, Dynamics and Diff. Eqn. **3** (1991), 361–380.
9. S. N. Chow and E. S. Van Vleck, *A shadowing lemma approach to global error analysis for initial value ODEs*, Report No. 92-12, Department of Mathematics and Statistics, Simon Fraser University.
10. T. Eirola, *Aspects of backward error analysis of numerical ODEs*, J. Comput. Appl. Math. **45** (1993), 65–73.

11. J. de Frutos and J. M. Sanz-Serna, *Error growth and invariant quantities in numerical methods: a case study*, Report 1993/4, May 1993, Applied Mathematics and Computation Reports, Universidad de Valladolid.
12. C. Grebogi, S. M. Hammel, J. A. Yorke and T. Sauer, *Shadowing of physical trajectories in chaotic dynamics: containment and refinement*, Phys. Rev. Lett. **65** (1990), 1527–1530.
13. D. F. Griffiths and J. M. Sanz-Serna, *On the scope of the method of modified equations*, SIAM J. Sci. Comput. **7** (1986), 994–1008.
14. E. Hairer, *Backward analysis of numerical integrators and symplectic methods* (submitted).
15. E. Hairer, S. P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations I, Nonstiff Problems*, “Springer”, Berlin, 1987.
16. E. Hairer and G. Wanner, *On the Butcher group and general multivalued methods*, Computing **13** (1974), 1–15.
17. J. K. Hale, *Dynamics and numerics*, The Dynamics of Numerics and the Numerics of Dynamics (D. S. Broomhead and A. Iserles, eds.), Clarendon, Oxford, 1992, pp. 243–253.
18. S. M. Hammel, J. A. Yorke and C. Grebogi, *Do numerical orbits of chaotic dynamical processes represent true orbits?*, J. Complexity **3** (1987), 136–145.
19. ———, *Numerical orbits of chaotic processes represent true orbits*, Bull. Am. Math. Soc. **19** (1988), 465–469.
20. S. Larsson and J. M. Sanz-Serna, *The behavior of finite element solutions of semilinear parabolic problems near stationary points*, SIAM J. Numer. Anal. (to appear).
21. Ch. Lubich, K. Nipp and D. Stoffer, *Runge-Kutta solutions of stiff differential equations near stationary points*, Report No. 93-01, April 1993, Seminar für Angewandte Mathematik, Eidgenössische Technische Hochschule, Zürich.
22. H. E. Nusse and J. A. Yorke, *Is every approximate trajectory of some process near an exact trajectory of a nearby process?*, Commun. Math. Phys. **114** (1988), 381–347.
23. J. M. Sanz-Serna, *Numerical ordinary differential equations vs. dynamical systems*, The Dynamics of Numerics and the Numerics of Dynamics (D. S. Broomhead and A. Iserles, eds.), Clarendon, Oxford, 1992, pp. 81–106.
24. ———, *Symplectic integrators for Hamiltonian problems: an overview*, Acta Numerica **1** (1992), 243–286.
25. J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian problems*, “Chapman and Hall”, London, 1993.
26. J. M. Sanz-Serna and S. Larsson, *Shadows, chaos and saddles*, Appl. Numer. Math. (to appear).
27. T. Sauer and J. A. Yorke, *Rigorous verification of trajectories for the computer simulation of dynamical systems*, Nonlinearity **4** (1991), 961–979.
28. R. F. Warming and B. J. Hyett, *The modified equation approach to the stability and accuracy of finite difference methods*, J. Comput. Phys. **14** (1974), 159–179.

DEPARTAMENTO DE MATEMÁTICA APLICADA Y COMPUTACIÓN, UNIVERSIDAD DE VALLADOLID,
VALLADOLID, SPAIN

E-mail address: maripaz@cpd.uva.es

FACULTAD DE INFORMÁTICA, APARTADO 649, 20080 SAN SEBASTIÁN, SPAIN

E-mail address: ccpmuura@sisb00.si.ehu.es

DEPARTAMENTO DE MATEMÁTICA APLICADA Y COMPUTACIÓN, UNIVERSIDAD DE VALLADOLID,
VALLADOLID, SPAIN

E-mail address: sanzserna@cpd.uva.es