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ASYMPTOTIC EXPANSIONS AND BACKWARD ANALYSIS FOR NUMERICAL INTEGRATORS

ERNST HAIRER* AND CHRISTIAN LUBICH†

Abstract. For numerical integrators of ordinary differential equations we compare the theory of asymptotic expansions of the global error with backward error analysis. On a formal level both approaches are equivalent. If, however, the arising divergent series are truncated, important features such as the semigroup property, structure perservation and exponentially small estimates over long times are valid only for the backward error analysis. We consider one-step methods as well as multistep methods, and we illustrate the theoretical results on several examples. In particular, we study the preservation of weakly stable limit cycles by symmetric methods.

Key words. Asymptotic expansions, backward error analysis, one-step methods, multistep methods, long-time behavior.

1. Introduction. Together with an autonomous system of ordinary differential equations

$$y' = f(y), \qquad y(0) = y_0 \tag{1.1}$$

we consider a numerical solution sequence

$$y_0, y_1, y_2, y_3, \ldots,$$

obtained either by a one-step method or by a multistep method. We assume that a constant stepsize h is used so that $y_n \approx y(nh)$, where $y(t)$ stands for the exact solution of the problem. The aim of the techniques described in this article is to gain insight into the dynamics of the numerical solution. We discuss the following two techniques:

Asymptotic expansion. This theory was developed by Henrici [17], in the thesis of Gragg [6] and by Stetter [24] in order to justify extrapolation methods. It consists in deriving an asymptotic expansion

$$\widetilde{y}(t) = y(t) + he_1(t) + h^2 e_2(t) + \ldots, \tag{1.2}$$

such that $y_n = \widetilde{y}(nh) + \mathcal{O}(h^{N+1})$, if the series (1.2) is truncated after the h^N-term.

Backward analysis. This technique has its origin in numerical linear algebra. For ordinary differential equations it has been used in the works of Griffiths & Sanz-Serna [7], Feng Kang [5], Sanz-Serna [23], Yoshida [29],

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and many others. The idea of backward error analysis consists in searching for a modified differential equation

$$\widetilde{y}\,' = f(\widetilde{y}\,) + hf_2(\widetilde{y}\,) + h^2 f_3(\widetilde{y}\,) + \ldots, \qquad \widetilde{y}(0) = y_0, \tag{1.3}$$

such that $y_n = \widetilde{y}(nh) + \mathcal{O}(h^{N+1})$ on finite time intervals, if the series (1.3) is truncated after the h^{N-1}-term.

Outside numerical analysis, the problem of interpolation of discrete mappings by a continuous flow has been considered e.g. by Moser [20]. The subject of asymptotic expansions has older roots, as can be seen from the following quotations taken from [3]:

> Wherefore it is highly desirable that it be clearly and rigorously shown why series of this kind, which at first converge very rapidly and then ever more slowly, and at length diverge more and more, nevertheless give a sum close to the true one if not too many terms are taken, and to what degree such a sum can safely be considered as exact. (C.F. Gauss 1799)
>
> Divergent series are in their entirety an invention of the devil and it is a disgrace to base the slightest demonstration on them. (N.H. Abel 1826)

2. One-step methods. We first consider one-step methods written as $y_{n+1} = \Phi_h(y_n)$, and we assume that the function $\Phi_h(y)$ admits an expansion

$$\begin{aligned} \Phi_h(y) = y \;&+\; hf(y) + \frac{h^2}{2!}\, a_2(f'f)(y) \\ &+\; \frac{h^3}{3!}\Big(a_3 f''(f,f)(y) + a_4 f'f'f(y)\Big) + \ldots\ . \end{aligned} \tag{2.1}$$

This assumption is not essential, but all important methods have a Taylor series expansion of such (or similar) form.

Asymptotic expansion. In order to obtain the h-independent coefficient functions $e_j(t)$, we insert the ansatz (1.2) into $\widetilde{y}(t+h) = \Phi_h\big(\widetilde{y}(t)\big)$, we expand all appearing expressions at $h = 0$, and we compare the coefficients of like powers of h. This yields

$$\begin{aligned} &y' = f(y), \qquad y(0) = y_0 \\ &e_1' = f'(y)e_1 + \frac{1}{2!}(a_2 - 1)(f'f)(y), \qquad e_1(0) = 0 \\ &e_j' = f'(y)e_j + g_j(y, e_1, \ldots, e_{j-1}), \qquad e_j(0) = 0, \qquad j = 2, 3, \ldots \end{aligned} \tag{2.2}$$

Here, the expressions g_j also depend on first and higher derivatives of e_i (for $i \le j-2$), but this dependence can be recursively eliminated with the help of the differential equations for e_i.

Backward analysis. Here, we put $y := \widetilde{y}(t)$ for a fixed t and we expand the solution of (1.3) into a Taylor series

$$\begin{aligned} \widetilde{y}(t+h) = y &+ h\big(f(y) + hf_2(y) + h^2 f_3(y) + \ldots\big) \\ &+ \frac{h^2}{2!}\big(f'(y) + hf_2'(y) + \ldots\big)\big(f(y) + hf_2(y) + \ldots\big) + \ldots\ . \end{aligned}$$

Inserting this relation into $\widetilde{y}(t+h) = \Phi_h(y)$, expanding, and comparing like powers of h yields recursion formulas for the coefficient functions $f_j(y)$ of (1.3) such as

$$\begin{aligned} f_2(y) &= \frac{1}{2!}(a_2 - 1)f'f(y) \\ f_3(y) &= \frac{1}{3!}\Big((a_3 - 1)f''(f,f)(y) + (a_4 - 1)f'f'f(y)\Big) \\ &\quad - \frac{1}{2!}\Big(f'f_2(y) + f_2'f(y)\Big). \end{aligned}$$

In both cases the coefficient functions ($e_j(t)$ for the asymptotic expansion and $f_j(y)$ for the backward analysis) are uniquely determined. This implies that, neglecting $\mathcal{O}(h^N)$-terms (for arbitrary N), both approaches yield the same function $\widetilde{y}(t)$. Hence, on a formal level, the theory of asymptotic expansions of the global error and backward error analysis are equivalent. We next investigate the effect of truncation in the series (1.2) and (1.3), respectively.

2.1. Examples. As a first example we consider the blow-up equation

$$y' = y^2, \qquad y(0) = 1 \tag{2.3}$$

with exact solution $y(t) = 1/(1-t)$. It has a singularity at $t = 1$. We apply the explicit Euler discretization $y_{n+1} = y_n + hy_n^2$ with stepsize $h = 0.02$.

For the convenience of the reader we include here a Maple program that computes the first `nn=6` terms of the modified equation.[1]

```
> fcn := y -> y^2:
> nn := 6:
> fcoe[1] := fcn(y):
> for n from 2 by 1 to nn do
>    modeq := sum(h^j*fcoe[j+1], j=0..n-2):
>    diffy[0] := y:
>    for i from 1 by 1 to n do
>       diffy[i] := diff(diffy[i-1],y)*modeq:
>    od:
>    ytilde := sum(h^k*diffy[k]/k!, k=0..n):
>    res := ytilde-y-h*fcn(y):
>    tay := convert(series(res,h=0,n+1),polynom):
```

[1] The differential equation (line 1) and the number of desired terms (line 2) of the modified equation can easily be adapted. For other numerical methods one only has to change the line 11, e.g., for the

implicit Euler method by `> res := ytilde-y-h*fcn(ytilde):`,

trapezoidal rule by `> res := ytilde-y-h*(fcn(y)+fcn(ytilde))/2:`,

implicit midpoint rule by `> res := ytilde-y-h*fcn((y+ytilde)/2):`.

An extension to systems of differential equations is straightforward.

```
>    fcoe[n] := -coeff(tay,h,n):
> od:
> simplify(sum(h^j*fcoe[j+1], j=0..nn-1));
```

The output of this program is the truncated modified equation

$$\widetilde{y}' = \widetilde{y}^2 - h\widetilde{y}^3 + h^2\,\frac{3}{2}\,\widetilde{y}^4 - h^3\,\frac{8}{3}\,\widetilde{y}^5 + h^4\,\frac{31}{6}\,\widetilde{y}^6 - h^5\,\frac{157}{15}\,\widetilde{y}^7 \pm \dots \,. \tag{2.4}$$

To obtain the asymptotic expansion, we insert the ansatz (1.2) into (2.4) and compare like powers of h. This immediately leads to $y' = f(y)$ with $y(0) = y_0 = 1$ and

$$\begin{aligned} e_1' &= 2ye_1 - y^3, \qquad e_1(0) = 0 \\ e_2' &= 2ye_2 + e_1^2 - 3y^2e_1 + \frac{3}{2}\,y^4, \qquad e_2(0) = 0. \end{aligned}$$

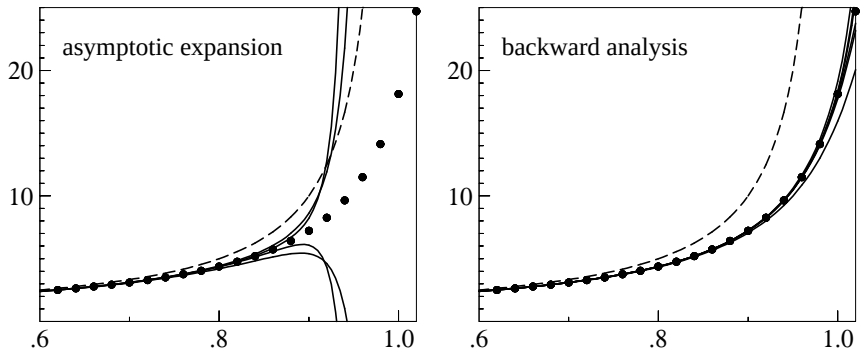

FIG. 1. *Numerical solution (black points) and exact solution (dashed curve) for the blow-up equation (2.3) together with the truncated approximations, obtained by the asymptotic expansion (left picture) and by backward error analysis (right picture)*

In Fig. 1 we present the exact solution $y(t) = 1/(1-t)$ (dashed curve) together with the numerical solution (bullets). The left picture also shows the expansion (1.2) truncated after $1, 2, 3$, and 4 terms. The right picture shows the solutions $\widetilde{y}(t)$ of the modified equation (2.4), when truncated after $1, 2, 3$, and 4 terms. We can observe a significant difference between the two approaches. Whereas all functions $e_j(t)$ of the asymptotic expansion have a singularity at $t = 1$, the solutions $\widetilde{y}(t)$ of the truncated modified equation approximate very well the numerical solution beyond the singularity at $t = 1$ (observe that the numerical solution $y_{n+1} = y_n + hy_n^2$ exists for all times without any finite singularity).

As a second example we consider the linear equation

$$y' = \lambda y, \qquad y(0) = y_0 \tag{2.5}$$

with exact solution $y(t) = e^{\lambda t} y_0$. We apply the implicit midpoint rule with stepsize h, i.e.,

$$y_{n+1} = R(\lambda h)\, y_n, \qquad R(z) = \frac{1 + z/2}{1 - z/2}.$$

This linear problem is an exceptional situation, because the function $\widetilde{y}(t)$ is given in analytic form and the series in (1.2) and (1.3) converge. Indeed, we have

$$\widetilde{y}(t) = \exp\Big(\frac{t}{h}\,\log\big(R(\lambda h)\big)\Big) y_0. \tag{2.6}$$

This function exactly satisfies $\widetilde{y}(nh) = R(\lambda h)^n y_0 = y_n$. Let us study the effect of the truncation of the series (1.2) and (1.3), respectively, on the function $\widetilde{y}(t)$.

Differentiation of (2.6) yields the modified differential equation $\widetilde{y}' = \frac{1}{h}\log\big(R(\lambda h)\big) \cdot \widetilde{y}$. If we expand this equation into powers of h, and if we truncate it after N terms, we obtain as solution

$$\widetilde{y}_N(t) = \exp\Big(\lambda t\big(1 + \lambda^2 h^2 b_1 + \lambda^4 h^4 b_2 + \ldots + \lambda^{2N} h^{2N} b_N\big)\Big) y_0, \tag{2.7}$$

and we see that the relative error due to this truncation is

$$\Big(\widetilde{y}(t) - \widetilde{y}_N(t)\Big) \Big/ \widetilde{y}(t) \approx \text{const} \cdot \lambda t (\lambda h)^{2N+2} \tag{2.8}$$

provided that λh and $\lambda t (\lambda h)^{2N+2}$ are sufficiently small.

On the other hand, in the theory of asymptotic expansions, the series for $\widetilde{y}(t)$ or equivalently that of (2.7) is truncated after N terms which gives

$$\widetilde{y}_N(t) = e^{\lambda t}\Big(1 + \lambda^2 h^2 c_1(\lambda t) + \ldots + \lambda^{2N} h^{2N} c_N(\lambda t)\Big) y_0, \tag{2.9}$$

where $c_j(0) = 0$ and $c_j(t)$ is a polynomial of degree j. The relative error of this truncation behaves asymptotically like

$$\Big(\widetilde{y}(t) - \widetilde{y}_N(t)\Big) \Big/ \widetilde{y}(t) \approx \text{const} \cdot (\lambda t)^{N+1} (\lambda h)^{2N+2} \big/ (N+1)!\ .$$

The truncation error (2.8) of the backward error analysis grows linearly in time, whereas that of the asymptotic expansion grows polynomially with high degree. This phenomenon is illustrated in Fig. 2, where we have plotted the relative errors $\big(y_n - \widetilde{y}_N(nh)\big)/y_n$ as functions of time for the values $\lambda = 1$ and $h = 1$. Again we observe that the numerical solution is much better approximated by the backward error analysis than by the asymptotic expansion of the global error.

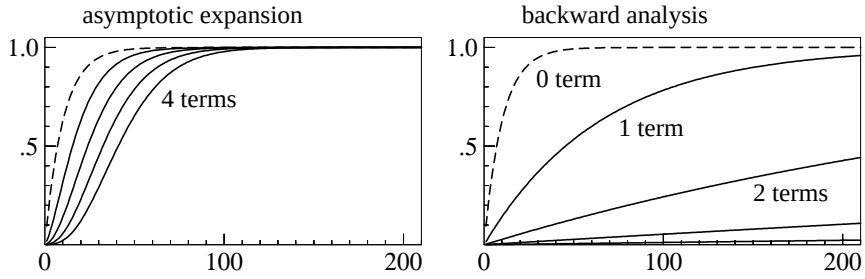

FIG. 2. *Relative error* $(y_n - \widetilde{y}_N(nh))/y_n$ *of the implicit midpoint rule applied to the linear problem* $y' = \lambda y$ *with* $\lambda = 1$ *and stepsize* $h = 1$

2.2. Properties of backward analysis. We summarize here some important features of backward error analysis, which are indispensable for the study of the dynamics of numerical solutions over long time intervals. For this we consider the truncated modified equation

$$\widetilde{y}\,' = f(\widetilde{y}\,) + hf_2(\widetilde{y}\,) + \ldots + h^{N-1}f_N(\widetilde{y}\,), \qquad \widetilde{y}(0) = y_0 \tag{2.10}$$

and we denote its solution by $\widetilde{y}_N(t)$, or by $\widetilde{y}_N(t, y_0)$ if we want to indicate its dependence on the initial value.

Semigroup property. Since the differential equation (2.10) is autonomous, we have $\widetilde{y}_N(t+s, y_0) = \widetilde{y}_N\big(t, \widetilde{y}_N(s, y_0)\big)$. This property makes it possible to study the global error $y_n - \widetilde{y}_N(nh)$ by looking at the error made in one step and by studying its propagation in time.

Structure preservation. If a suitable integrator is used, the modified equation (2.10) shares the same properties as the original problem. For example, if the problem (1.1) is Hamiltonian and if the numerical method is symplectic, the modified system (2.10) is also Hamiltonian [1, 8]. If (1.1) is a reversible system and if the numerical method is symmetric, the modified system is also reversible [16]. Moreover, if the vector field of (1.1) lies in some Lie algebra and if the method is a so-called "geometric integrator", the vector field of the modified equation lies in the same Lie algebra (see, e.g., Reich [22]).

Exponentially small estimates. If the vector field $f(y)$ is real analytic and if the truncation index N in (2.10) is chosen as $N \approx \text{const}\,/h$ with a suitable constant, then it holds (with some $\gamma > 0$)

$$y_1 - \widetilde{y}_N(h) = \mathcal{O}(e^{-\gamma/h}).$$

Different proofs of such an estimate can be found in Benettin & Giorgilli [1], Hairer & Lubich [13], and Reich [22]. These papers also give interesting applications of backward error analysis to the study of the long-time behavior of numerical solutions.

One may ask which of these properties remain valid for the truncated asymptotic expansions. Since for the functions $e_j(t)$ we usually have $e_j(h) \neq 0$, we get different expansions according to as we start at y_0 or at $y_1 = \Phi_h(y_0)$. Hence, the semigroup property does not hold for asymptotic expansions. For the example $y' = \lambda y$ with $\lambda = i$ (the harmonic oscillator) we consider the symplectic midpoint rule as in subsection 2.1. The function $\widetilde{y}_N(t)$ obtained by backward error analysis satisfies $|\widetilde{y}_N(t)| = |y_0|$ as the exact solution $y(t) = e^{it}y_0$ does. For the function $\widetilde{y}_N(t)$, obtained by truncation of the asymptotic expansion, this property is lost. Hence, we do not have structure preservation for the asymptotic expansions. Exponentially small estimates for the local error $y_1 - \widetilde{y}_N(h)$ are not very useful in the context of asymptotic expansions, because the semigroup property does not hold.

The above properties of backward error analysis assume that the one-step method is applied with constant stepsize, and it is known from numerical experiments that a standard use of variable stepsizes destroys the favorable longtime behavior. In some situations (e.g., planetary orbits with large eccentricity) the use of variable stepsizes is indispensable for an efficient integration. There, it is possible to reparametrize time [19, 25, 16, 18] or to scale the Hamiltonian [9, 22] so that the use of constant stepsizes for the new problem corresponds to a variable stepsize integration of the original one.

3. Multistep methods. It is well-known that multistep methods have many advantages when constant stepsizes are used. They can be implemented very efficiently, and it is easy to construct high order, explicit, symmetric methods. It is therefore of interest to investigate the longtime behavior of multistep methods.

3.1. Numerical phenomena. We describe two situations where certain multistep methods exhibit an excellent longtime behavior, similar to symmetric or symplectic one-step methods.

Preservation of weakly stable limit cycles. We consider the nonlinear oscillator (Van der Pol equation)

$$q'' = -q + \varepsilon(1 - q^2)q', \qquad \varepsilon = 0.01, \tag{3.1}$$

which has a stable limit cycle close to the circle of radius 2. It is known (Stoffer [26], Hairer & Lubich [14]) that symmetric or symplectic one-step methods give qualitatively correct numerical solutions even when the stepsize is much larger than ε. Fig. 3 shows the numerical solutions obtained by three different multistep methods. For the strictly stable explicit Adams method (A) the numerical solution spirals outwards and tends to a wrong limit cycle. The explicit midpoint rule (B) shows large oscillations around the correct solution. Method (C), which is symmetric and whose growth parameters are all positive, spirals inwards to an asymptotically correct

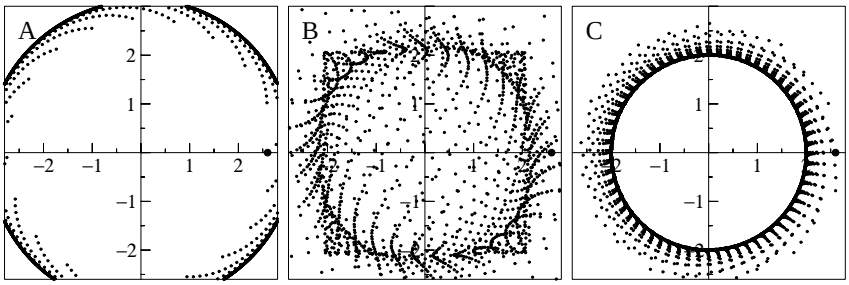

FIG. 3. *Numerical solution of the following second order multistep methods applied to Van der Pol's equation (3.1) with initial value* $(q_0, q_0') = (2.6, 0)$ *and with constant stepsize* $h = 0.3$*: (A) the 2-step explicit Adams method; (B) the explicit midpoint rule; and (C) the symmetric method* $y_{n+1} = y_{n-1} + h(\beta f_{n+1} + 2(1-\beta)f_n + \beta f_{n-1})$ *with* $\beta = 0.7$*. The starting value* y_1 *is computed by the explicit Euler method.*

limit cycle. We shall explain this phenomenon in Sect. 4 with the help of a backward error analysis for multistep methods.

Outer solar system. The movement of the five outer planets around the sun is described by the system

$$p' = -H_q(p,q), \qquad q' = H_p(p,q), \tag{3.2}$$

where the Hamiltonian is given by

$$H(p,q) = \frac{1}{2}\sum_{i=0}^{5} m_i^{-1} p_i^T p_i - \sum_{i=1}^{5}\sum_{j=0}^{i-1} \frac{K\, m_i\, m_j}{\|q_i - q_j\|}$$

with $p_i, q_i \in \mathbb{R}^3$. We consider initial values from September 5, 1994 [2]. Fig. 4 presents the numerical results of three different multistep methods. Only method (C) shows the correct behavior. It is the partitioned method

$$\begin{aligned} \sum_{i=0}^{k} \alpha_i p_{n+i} &= -h \sum_{i=0}^{k} \beta_i H_q(p_{n+i}, q_{n+i}) \\ \sum_{i=0}^{k} \widehat{\alpha}_i q_{n+i} &= h \sum_{i=0}^{k} \widehat{\beta}_i H_p(p_{n+i}, q_{n+i}) \end{aligned} \tag{3.3}$$

where the generating polynomials are

$$\begin{aligned} \rho(\zeta) &= (\zeta-1)(\zeta^2 - 2\cos(4\pi/9)\zeta + 1)(\zeta^2 - 2\cos(8\pi/9)\zeta + 1) \\ \widehat{\rho}(\zeta) &= (\zeta-1)(\zeta^2 - 2\cos(2\pi/9)\zeta + 1)(\zeta^2 - 2\cos(6\pi/9)\zeta + 1) \end{aligned}$$

and $\sigma(\zeta)$, $\widehat{\sigma}(\zeta)$ are such that the resulting method is explicit, symmetric and of order 4. It is important that $\rho(\zeta)$ and $\widehat{\rho}(\zeta)$ have no common zero other than $\zeta_1 = 1$.

[2] The data for this problem can be obtained on request.

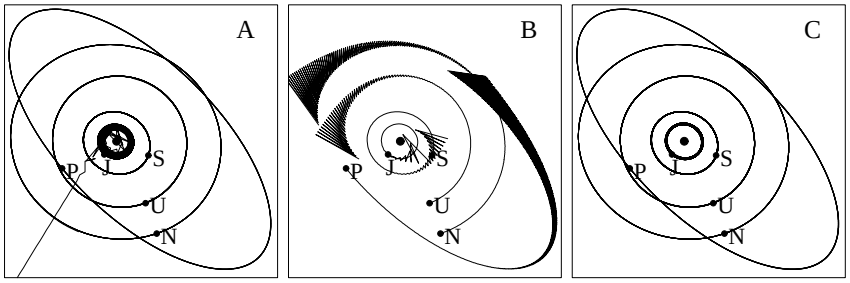

FIG. 4. *Numerical trajectories of the five outer planets, obtained with (A) the 4-step explicit Adams method; (B) the symmetric method* $y_{n+4} - y_n = h(8f_{n+3} - 4f_{n+2} + 8f_{n+1})/3$*; and (C) the partitioned multistep method (3.3), all applied with constant stepsize* $h = 100$ *(earth days).*

For the moment we cannot rigorously explain this behavior. We hope that an extension of the backward error analysis to partitioned multistep methods (see [10]) will allow us to prove the observed long-time behavior.

3.2. Asymptotic expansion. We recall here the form of the asymptotic expansion of the global error. It will serve as a motivation for the ansatz of the backward error analysis of multistep methods. For the differential equation $y' = f(y)$ we consider the multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f(y_{n+i}), \tag{3.4}$$

whose generating polynomials are $\rho(\zeta) = \sum_{i=0}^{k} \alpha_i \zeta^i$ and $\sigma(\zeta) = \sum_{i=0}^{k} \beta_i \zeta^i$. For ease of presentation, we assume that the roots of $\rho(\zeta)$, denoted by $\zeta_1 = 1, \zeta_2, \ldots, \zeta_k$, are distinct and different from zero. For stability all these roots have to satisfy $|\zeta_\ell| \le 1$. We then consider the index set

$$\mathcal{I} = \big\{ \zeta = \zeta_2^{m_2} \cdot \ldots \cdot \zeta_k^{m_k} \;\big|\; m_i \ge 0, \zeta \ne 1 \big\} = \big\{ \zeta_2, \ldots, \zeta_k, \zeta_{k+1}, \ldots \big\}$$

and we often write $\ell \in \mathcal{I}$ in order to indicate $\zeta_\ell \in \mathcal{I}$. Gragg [6] (see also [12]) proved that the numerical solution of the multistep method (3.4) admits for arbitrary N an expansion of the form

$$y_n = y(nh) + \sum_{j=1}^{N} \Big(\sum_{\ell \in \mathcal{I} \cup \{1\}} \zeta_\ell^n e_{j\ell}(nh) \Big) h^j + \mathcal{O}(h^{N+1}). \tag{3.5}$$

Here $y(t)$ is the solution of (1.1), and the functions $e_{j\ell}(t)$ for $1 \le \ell \le k$ are a solution of the differential equation

$$e'_{j\ell} = \lambda_\ell f'(y) e_{j\ell} + \mathit{fcn}\,\big(y, \{e_{im}\}_{\substack{1 \le i < j \\ 1 \le m \le k}}\big), \tag{3.6}$$

where $\lambda_\ell = \sigma(\zeta_\ell)/\big(\zeta_\ell\rho'(\zeta_\ell)\big)$ is the growth parameter (as introduced by Dahlquist [4]) and the inhomogeneity in (3.6) is given recursively. The functions $e_{j\ell}(t)$ for $\ell \ge k+1$ are given by algebraic relations of the form

$$e_{j\ell} = \mathit{fcn}\,\big(y, \{e_{im}\}_{\substack{1\le i<j\\ 1\le m\le k}}\big). \tag{3.7}$$

The initial values for (3.6) have to be computed from the starting values $y_0, y_1, \ldots, y_{k-1}$. Gragg [6] assumes that these starting values possess a Taylor series expansion of the form $y_j = y_j(h) = y_{j0} + hy_{j1} + h^2 y_{j2} + \ldots$, and he shows that the validity of (3.5) for $n \in \{0, 1, \ldots, k-1\}$ uniquely determines the initial values $e_{j\ell}(0)$ for $1 \le \ell \le k$ as functions of $\{y_{j0}, y_{j1}, y_{j2}, \ldots\}$ for $j = 0, 1, \ldots, k-1$.

3.3. Backward analysis. We collect all functions in (3.5) that are multiplied by ζ_ℓ^n into one function, and therefore search for a *formal* representation of the numerical solution of (3.4) as

$$y_n = \widetilde{y}(nh) + \sum_{\ell\in\mathcal{I}} \zeta_\ell^n z_\ell(nh). \tag{3.8}$$

We are interested to represent the functions $\widetilde{y}(t)$ and $z_\ell(t)$ as the solution of an autonomous system of differential (and algebraic) equations. This can be achieved by inserting (3.8) into (3.4), by Taylor series expansions, and by equating expressions of like powers of h. The details of this construction are given in [10]. The result is a system of the form

$$\begin{aligned}
&\widetilde{y}\,' = f(\widetilde{y}) + \mathit{fcn}_1(h, \widetilde{y}, z_2, \ldots, z_k)\\
&z_\ell' = \lambda_\ell f'(\widetilde{y}) z_\ell + \mathit{fcn}_\ell(h, \widetilde{y}, z_2, \ldots, z_k) \quad \text{for } \ell = 2, \ldots, k\\
&z_\ell = h\ \mathit{fcn}_\ell(h, \widetilde{y}, z_2, \ldots, z_k) \quad \text{for } \ell \ge k+1,
\end{aligned} \tag{3.9}$$

where $\lambda_\ell = \sigma(\zeta_\ell)/\big(\zeta_\ell\rho'(\zeta_\ell)\big)$ is the growth parameter of (3.4) corresponding to ζ_ℓ, and $\mathit{fcn}_\ell(h, \widetilde{y}, z_2, \ldots, z_k)$ are formal series in powers of h. We call the differential equation for $\widetilde{y}$ *principal modified equation* and those for z_ℓ *parasitic modified equations*. It turns out that the functions fcn_ℓ are linear combinations of expressions like

$$\begin{aligned}
&h^3 c_1 f'''(\widetilde{y})\big(f(\widetilde{y}), f(\widetilde{y}), f(\widetilde{y})\big)\\
&h^0 c_2 f''(\widetilde{y})\big(z_2, z_3\big)\\
&h^3 c_3 f'(\widetilde{y}) f''(\widetilde{y})\big(f'(\widetilde{y}) z_2, f(\widetilde{y})\big).
\end{aligned} \tag{3.10}$$

These are meaningful compositions of derivatives of $f(y)$ with $z_2, \ldots, z_k$ appearing as factors. The coefficients c_j only depend on the multistep method, and the exponent in h^r equals the number of appearances of the symbol f minus 1. Moreover, an expression that is independent of $z_2, \ldots, z_k$ automatically belongs to fcn_1. If an expression contains $z_{i_1}, \ldots, z_{i_m}$ as factors, it belongs to fcn_ℓ where the index ℓ is determined by $\zeta_\ell = \zeta_{i_1} \cdot \ldots \cdot$

ζ_{i_m}. As a consequence, the first expression of (3.10) belongs to fcn_1, the last one to fcn_2, and the second one belongs to fcn_1 if $\zeta_2\zeta_3 = 1$ or to fcn_ℓ if $\zeta_2\zeta_3 = \zeta_\ell$. It follows that the expressions in fcn_1 either are independent of $z_2, \dots, z_k$ or they are at least quadratic in $z_2, \dots, z_k$.

Let us briefly discuss the truncation of the formal series in (3.9), which is necessary for a rigorous backward error analysis. Consider for example the case $\zeta_2 = -1$ so that $\zeta_2^2 = 1$. The expressions $f''(\widetilde{y}\,)(z_2, z_2)$, $f^{(4)}(\widetilde{y}\,)(z_2, z_2, z_2, z_2)$, $f^{(6)}(\widetilde{y}\,)(z_2, z_2, z_2, z_2, z_2, z_2), \dots$ usually all appear in fcn_1. Hence, in contrast to the theory for one-step methods, there appears an infinite number of expressions in fcn_ℓ corresponding to the same power of h. Fortunately, it turns out that for real analytic $f(y)$ the sum of these expressions converges absolutely [10], so that only the terms containing $h^N, h^{N+1}, \dots$ as a factor will be removed. We denote the solution of the resulting system again by $\widetilde{y}(t)$ and $z_\ell(t)$.

Semigroup property. The initial values for the differential part in the modified equation (3.9) can be obtained from the starting approximations $y_0, y_1, \dots, y_{k-1}$ as follows: we expand the solution $\widetilde{y}(ih), z_\ell(ih)$ of the truncated system (3.9) into powers of h, and we insert the result into (3.8) for $n \in \{0, 1, \dots, k-1\}$. This gives a nonlinear system for $\widetilde{y}(0), z_2(0), \dots, z_k(0)$ which, by the implicit function theorem, yields a locally unique solution. This unique correspondence between the starting approximations $y_0, y_1, \dots, y_{k-1}$ and the initial values for (3.9) implies that the values $\{y_n\}$ defined by (3.8) (where $\widetilde{y}(t)$ and $z_\ell(t)$ are the solution of the truncated modified system) satisfy the semigroup property.

Structure preservation. If the starting values $y_0, y_1, \dots, y_{k-1}$ are such that $z_2(0) = z_3(0) = \dots = z_k(0) = 0$, then we have $z_\ell(t) \equiv 0$ for all ℓ and the (truncated) principal modified equation becomes independent of $z_2, \dots, z_k$, i.e.,

$$\widetilde{y}\,' = f(\widetilde{y}\,) + hf_1(\widetilde{y}\,) + h^2 f_2(\widetilde{y}\,) + \dots \tag{3.11}$$

This is the key element for defining structure preserving properties:

a) We call a multistep method *symplectic* if, applied to a Hamiltonian system, the modified equation (3.11) is Hamiltonian. Unfortunately, multistep methods cannot be symplectic (see [28, 11]).

b) We call a multistep method *symmetric* if, applied to a reversible system, the modified equation (3.11) is reversible. This turns out to be equivalent to the usual definition of symmetric multistep methods.

Exponentially small estimates. Let $\widetilde{y}(x)$ and $z_\ell(x)$ be the solution of the principal and parasitic modified equations, truncated after the h^N terms, and assume that the multistep method is weakly stable, symmetric, and that all zeros ζ_ℓ of $\rho(\zeta)$ are roots of unity. If $N = \text{const}\,/h$ with a

suitable constant, then the expressions (3.8) satisfy

$$\sum_{i=0}^{k} \alpha_i y_{n+i} - h \sum_{i=0}^{k} \beta_i f(y_{n+i}) = \mathcal{O}(e^{-\gamma/h}). \tag{3.12}$$

A proof of this estimate is given in [10]. Using the unique correspondence between starting values $y_0, \dots, y_{k-1}$ of the multistep method and the initial values $\widetilde{y}_0, z_{20}, \dots, z_{k0}$ of the truncated modified differential equation (see above) this means that the following diagram commutes up to terms of order $\mathcal{O}(e^{-\gamma/h})$:

$$\begin{array}{ccc} y_0, \dots, y_{k-1} & \longleftrightarrow & \widetilde{y}_0, z_{20}, \dots, z_{k0} \\ & & \Big\downarrow \text{flow of (3.9)} \\ \Big\downarrow \text{multistep method (3.4)} & & \widetilde{y}(h), \zeta_2 z_2(h), \dots, \zeta_k z_k(h) \\ & & = \quad (\text{up to } \mathcal{O}(e^{-\gamma/h})) \\ y_1, \dots, y_k & \longleftrightarrow & \widetilde{y}_1, z_{21}, \dots, z_{k1} \end{array} \tag{3.13}$$

The study of the long-time behavior of multistep methods can be done along the following lines: (i) study the solutions of the principal and parasitic modified differential equation, (ii) bound the size of the solutions $z_\ell(t)$; they should be small and of size $\mathcal{O}(h^p)$, (iii) study the propagation of the exponentially small perturbations. An illustration of this technique will be given in Sect. 4.

4. Application: Preservation of weakly stable limit cycles. As an illustration, we show how backward analysis explains the behavior of numerical integrators applied to systems with a weakly stable periodic orbit. We consider Van der Pol's equation

$$q' = p\,, \qquad p' = -q + \varepsilon(1 - q^2)p \qquad (0 < \varepsilon \ll 1)\,. \tag{4.1}$$

4.1. One-step methods. We consider applying a one-step method of order p whose stability function satisfies

$$|R(i\eta)| = 1 \quad \text{for} \quad \eta \in \mathbb{R}.$$

For

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{4.2}$$

we then have

$$\frac{1}{h} \log R(hA) = \omega A \qquad \text{with} \quad \omega = 1 + \mathcal{O}(h^p)\,.$$

Therefore, the modified differential equation (1.3) for this method applied to (4.1) becomes

$$\widetilde{q}\,' = \omega\widetilde{p}\;, \qquad \widetilde{p}\,' = -\omega\widetilde{q} + \varepsilon(1-\widetilde{q}^{\,2})\widetilde{p} + \mathcal{O}(\varepsilon\delta)\;, \tag{4.3}$$

where $\delta = h^p$ and the $\mathcal{O}(\varepsilon\delta)$ term represents a function of $(\widetilde{q},\widetilde{p}\,)$ which together with its derivatives is bounded by $\mathrm{const}\cdot\varepsilon\delta$. With the symplectic change to polar coordinates $\widetilde{q} = \sqrt{2a}\sin\varphi$, $\widetilde{p} = \sqrt{2a}\cos\varphi$, the system becomes

$$\begin{aligned} a' &= \varepsilon\, 2a(1-2a\sin^2\varphi)\cos^2\varphi + \mathcal{O}(\varepsilon\delta) \\ \varphi' &= \omega - \varepsilon(1-2a\sin^2\varphi)\cos\varphi\sin\varphi + \mathcal{O}(\varepsilon\delta)\;. \end{aligned} \tag{4.4}$$

The dependence on the angle φ in the leading terms can be eliminated by a coordinate transform which is $\mathcal{O}(\varepsilon)$-close to the identity (cf. [2, 26]). In the new variables $(\widehat{a},\widehat{\varphi})$ the system becomes of a form where the coefficients of ε are the averages over φ of the previous coefficients:

$$\begin{aligned} \widehat{a}\,' &= \varepsilon\,\widehat{a}(1-\tfrac{1}{2}\widehat{a}) + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\varepsilon\delta) \\ \widehat{\varphi}\,' &= \omega + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\varepsilon\delta)\;. \end{aligned} \tag{4.5}$$

Ignoring the $\mathcal{O}(\ldots)$ terms, it is seen that this system has the weakly stable periodic orbit $\widehat{a} = 2$, which is $\mathcal{O}(\varepsilon)$ close to the circle $\widetilde{q}^{\,2} + \widetilde{p}^{\,2} = 4$ in the original variables. By an invariant manifold theorem [21], it follows that the periodic orbit persists under the $\mathcal{O}(\varepsilon^2) + \mathcal{O}(\varepsilon\delta)$ perturbation, and that the limit cycle of the modified equations (4.3) is $\mathcal{O}(h^p)$-close to the limit cycle of Van der Pol's equation. By the same invariant manifold theorem and the finite-time estimates between the numerical solution and the solution of the modified equation, it finally follows that the numerical method has a weakly attractive invariant closed curve that is $\mathcal{O}(e^{-\gamma/h})$ close to the limit cycle of the modified equation. See [14, 26, 27] for more details and for extensions of such a result to the preservation of weakly attractive invariant tori of more general dissipatively perturbed Hamiltonian systems.

4.2. Multistep methods. We now explain the numerical behavior shown in Fig. 3. We consider the symmetric two-step scheme

$$y_{n+1} = y_{n-1} + h(\beta f_{n+1} + 2(1-\beta)f_n + \beta f_{n-1})\;.$$

For $z \in \mathbb{C}$ near 0, we factor the characteristic polynomial

$$\zeta^2 - 1 - z\big(\beta\zeta^2 + 2(1-\beta)\zeta + \beta\big) = (1-z\beta)\,\big(\zeta - \zeta_1(z)\big)\,\big(\zeta - \zeta_2(z)\big)$$

with $\zeta_1(0) = 1$, $\zeta_2(0) = -1$. Because of the symmetry of the method we have

$$|\zeta_1(i\eta)| = |\zeta_2(i\eta)| = 1 \qquad \text{for} \quad \eta \in \mathbb{R}.$$

The numerical solution of the method applied to $y' = Ay$, with A of (4.2), is of the form

$$y_n = \zeta_1(hA)^n v_1 + \zeta_2(hA)^n v_2 = \widetilde{y}(nh) + (-1)^n z_2(nh) \ ,$$

where $\widetilde{y}(t)$ and $z_2(t)$ are solutions of the differential equations

$$\begin{array}{rcll} \widetilde{y}\,' & = & \frac{1}{h}\log\big(\zeta_1(hA)\big)\,\widetilde{y} = \omega A\widetilde{y}, & \omega = 1 + \mathcal{O}(h^2) \\ z_2' & = & \frac{1}{h}\log\big(-\zeta_2(hA)\big)\,z_2 = \mu A z_2, & \mu = \lambda_2 + \mathcal{O}(h^2). \end{array} \tag{4.6}$$

Here $\lambda_2 = (3\beta - 2)/2$ is the growth parameter of the root -1.

We write $(\widetilde{q}(t), \widetilde{p}(t))$ and $(Q(t), P(t))$ in the roles of $\widetilde{y}(t)$ and $z_2(t)$ of the modified differential equations (3.9). The equations for $(\widetilde{q}(t), \widetilde{p}(t))$ are (4.3) with ω of (4.6), with $\delta = h^2 + Q^2 + P^2$ and with $\mathcal{O}(\varepsilon\delta)$ perturbation functions depending on $(\widetilde{q}, \widetilde{p}, Q, P)$. The differential equations for $(Q(t), P(t))$ are of the form

$$\begin{array}{rcl} Q' & = & \mu P + \mathcal{O}(\varepsilon\delta) \\ P' & = & \mu\big(-Q - 2\varepsilon\widetilde{q}\,\widetilde{p}\,Q + \varepsilon(1 - \widetilde{q}^{\,2})P\big) + \mathcal{O}(\varepsilon\delta) \ . \end{array} \tag{4.7}$$

We express $(\widetilde{q}, \widetilde{p}\,)$ in the variables $(\widehat{a}, \widehat{\varphi})$ of (4.5), and search for a transformation

$$\begin{pmatrix} Q \\ P \end{pmatrix} = \Big(I + \varepsilon S(\widehat{a}, \widehat{\varphi})\Big) \begin{pmatrix} \widehat{Q} \\ \widehat{P} \end{pmatrix}$$

which eliminates the dependence on $\widehat{\varphi}$ in the leading terms of (4.7). We obtain

$$\begin{pmatrix} \widehat{Q}' \\ \widehat{P}' \end{pmatrix} = \mu \begin{pmatrix} 0 & 1 \\ -1 & \varepsilon(1 - \widehat{a}) \end{pmatrix} \begin{pmatrix} \widehat{Q} \\ \widehat{P} \end{pmatrix} + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\varepsilon\delta) \tag{4.8}$$

provided that S satisfies

$$\partial S/\partial\widehat{\varphi} = \mu(AS - SA + B) \ ,$$

where $B = B(\widehat{a}, \widehat{\varphi})$ contains the difference between the coefficients of ε in (4.7) and their angular averages. This equation can be solved for S by Fourier expansion whenever $\mu \neq k/2$ with $k \in \mathbb{Z}$.

For $\widehat{a} = 2$, the matrix in (4.8) has eigenvalues $-\frac{1}{2}\mu(\varepsilon \pm i\sqrt{4 - \varepsilon^2})$. Ignoring the $\mathcal{O}(\ldots)$ perturbation terms, the system (4.8) therefore has 0 as a weakly attractive equilibrium if and only if $\mu > 0$, that is, for $\beta > 2/3$ in the numerical scheme. The $\mathcal{O}(\varepsilon^2) + \mathcal{O}(\varepsilon\delta)$ terms are again taken into account by an invariant manifold theorem, provided that $Q(0) = \mathcal{O}(h)$ and $P(0) = \mathcal{O}(h)$, which is satisfied if the starting values of the multistep method are $\mathcal{O}(h)$ close to each other. The invariant manifold theorem of

[21] yields that for $\beta > 2/3$ the combined system (4.5) and (4.8) has a weakly attractive invariant curve $(\widehat{a}, \widehat{Q}, \widehat{P})$ parametrized by $\widehat{\varphi}$, whose first component is $\mathcal{O}(h^p)$ close to the exact limit cycle of Van der Pol's equation, and whose further components are of size $\mathcal{O}(h^p)$.

Using the diagram (3.13), it is seen that the numerical solution of Van der Pol's equation is of the form

$$\begin{pmatrix} q_n \\ p_n \end{pmatrix} = \begin{pmatrix} \widetilde{q}_n \\ \widetilde{p}_n \end{pmatrix} + \begin{pmatrix} Q_n \\ P_n \end{pmatrix} \ ,$$

where the mapping $(\widetilde{q}_0, \widetilde{p}_0, Q_0, P_0) \mapsto (\widetilde{q}_1, \widetilde{p}_1, -Q_1, -P_1)$ differs only by $\mathcal{O}(\varepsilon e^{-\gamma/h})$ (in the $\mathcal{C}^1$ sense) from the time-h flow of the modified differential equations (4.3) and (4.7). The additional factor ϵ as compared to (3.13) results from the fact that no truncation is necessary in the linear modified differential equations (4.6). The invariant manifold theorem finally shows the existence of a weakly attractive invariant curve of the above mapping that is exponentially close to the limit cycle of the modified equations. All combined, this shows that, for $\beta > 2/3$, the numerical method has a weakly attractive curve that is $\mathcal{O}(h^p)$ close to the limit cycle of Van der Pol's equation. This explains the favorable numerical behavior in Fig. 3C.

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