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Accurate long-term integration of dynamical systems

M.P. Calvo [a,*], E. Hairer [b,1]

[a] *Departamento de Matemática Aplicada y Computación, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain*

[b] *Département de Mathématiques, Université de Genève, Case Postale 240, CH-1211 Genève 24, Switzerland*

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Abstract

Symplectic or symmetric integration methods do not only preserve geometrical structures of the flow of the differential equation, but they have also favourable properties concerning their global error when the integration is performed over a very long time. The subject of this paper is to provide new insight into this phenomenon. For problems with periodic solution and for integrable systems we prove that the error growth is only linear for symplectic and symmetric methods, compared to a quadratic error growth in the general case. Furthermore, for symmetric collocation methods we explain a variable-stepsize implementation which does not destroy the above-mentioned properties.

Keywords: Symmetric Runge–Kutta methods; Symplectic methods; Long-term integration; Hamiltonian problems; Reversible systems

1. Introduction

Let us consider systems of differential equations

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

where perturbations in the solution are propagated at most linearly. Denoting the solution in dependence of its initial values by $y(t, t_0, y_0)$, this means that for $t \geqslant t_0$

$$\left\| \frac{\partial y}{\partial y_0}(t, t_0, y_0) \right\| \leqslant M_0 + M_1 \, | t - t_0 |. \tag{1.2}$$

* Corresponding author. E-mail: maripaz@cpd.uva.es.

[1] E-mail: hairer@divsun.unige.ch.

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Typical examples are problems whose solutions are periodic with a period depending in a nontrivial way on the initial value y_0 (Hamiltonian problems with one degree of freedom, e.g., the pendulum or the two-body problem, and also problems like the Volterra–Lotka equations). Since the perturbed solution is periodic too, the two orbits will be everywhere close in the phase space. The fact that their periods are different produces a time-shift which is responsable for the linear growth in (1.2).

Another important class of problems are integrable systems (see [9]). By introducing suitable coordinates they can be transformed into $u_k' = 0$, $v_k' = f_k(u_1, \ldots, u_n)$ for $k = 1, \ldots, n$. Its solution $u_k(t) = u_{k0}$, $v_k(t) = v_{k0} + (t - t_0) f_k(u_{10}, \ldots, u_{n0})$ obviously satisfies (1.2). Backtransformation to the original coordinates yields (1.2) for the originally considered problem.

Quadratic error growth of numerical integrators

For the numerical solution of $y' = f(y)$ we are mainly interested in one-step methods such as Runge–Kutta methods. We shall study the growth of the global error over a long time interval. Standard estimates of the global error typically contain the factor $\exp(L(t_n - t_0))$, where L is a Lipschitz constant of $f(y)$. Here we are interested in the situation where $L(t_n - t_0)$ is large, so that these estimates are useless.

Let the sequence $\{y_i\}$ be an approximation to $\{y(t_i)\}$ obtained by applying a one-step method to Eq. (1.1). The local error is assumed to satisfy

$$\| y(t_{i+1}, t_i, y_i) - y_{i+1} \| \leqslant C h_i^{p+1}, \tag{1.3}$$

where $h_i = t_{i+1} - t_i$. Since $y(t, t_i, y_i) = y(t, t_{i+1}, y(t_{i+1}, t_i, y_i))$, it follows from (1.2) and (1.3) and the mean value theorem that the propagated error satisfies

$$\| y(t, t_i, y_i) - y(t, t_{i+1}, y_{i+1}) \| \leqslant (M_0 + M_1(t - t_{i+1})) C h_i^{p+1}. \tag{1.4}$$

Putting $t = t_n$ and summing up from $i = 0$ to $i = n - 1$ (where we assume $t_0 = 0$) we obtain with $h = \max_i h_i$ that

$$\| y(t_n, 0, y_0) - y_n \| \leqslant \left(M_0 t_n + M_1 \frac{t_n^2}{2} \right) C h^p. \tag{1.5}$$

This shows that the error grows in general *quadratically* in t_n, independent of whether we use constant or variable stepsizes.

Numerical experiment

Let us consider the modified Kepler problem as presented in [11]. It has two degrees of freedom and its Hamiltonian is given by

$$H(p, q) = \frac{p_1^2 + p_2^2}{2} - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\varepsilon}{2\sqrt{(q_1^2 + q_2^2)^3}} \tag{1.6}$$

with $\varepsilon = 0.01$. As initial values we take

$$p_1(0) = 0, \qquad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \qquad q_1(0) = 1 - e, \qquad q_2(0) = 0 \tag{1.7}$$

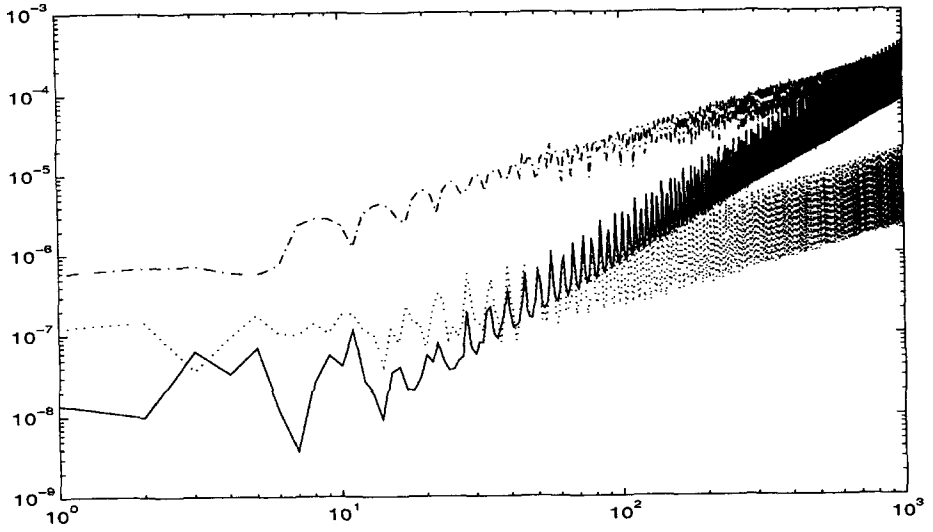

Fig. 1. Error growth of Lobatto IIIA methods, different stepsize strategies.

with eccentricity $e = 0.5$. In Fig. 1 we present the numerical results obtained by applying the five-stage Runge–Kutta method Lobatto IIIA in three different implementations:

(a) constant stepsizes ($h = 0.22$), dashed-dotted line in Fig. 1;

(b) variable stepsizes, classical strategy (see [4, p. 168]) with $Tol = 10^{-7}$, solid line;

(c) variable stepsizes, reversible strategy (see Section 4 below) with $Tol = 10^{-7}$, dotted line.

We observe that the implementation (b) gives rise to a quadratic error growth (in double logarithmic scale this corresponds to a straight line of slope 2) which is in accordance with the above considerations. For the implementations (a) and (c) we see that the error grows only linearly. The aim of the present paper is to give more insight into this phenomenon.

2. Linear error growth—the periodic case

It is somewhat surprising that in some special situations the growth of the global error is only linear in t_n. This has been observed by Stoffer [12] and a rigorous analysis for sympletic integrators applied to the two-body problem has been given in [1]. We shall give here a different explanation of this phenomenon.

Our analysis is based on the fact that the numerical solution of a pth-order method (applied with constant stepsizes) can be formally interpreted as the exact solution of a perturbed differential equation (see [2,3])

$$z' = f(z) + h^p f_p(z) + h^{p+1} f_{p+1}(z) + \cdots . \tag{2.1}$$

Since the series in (2.1) usually diverges, we have to truncate it, say, after the h^P-term. We then have $y_n - z(t_n) = O(h^{P+1})$. Assuming that solutions of (2.1) behave similar to that of (1.1) (i.e., (1.2) is satisfied also for (2.1)) the constant symbolized by the $O(h^{P+1})$-term grows at most quadratically in t_n. Hence, for $P \geqslant 2p$, this error term can be neglected.

Lemma 1. *Assume that the solutions of* (1.1) *and* (2.1) *with initial values* $y(0)=z(0)=y_0$ *are periodic with periods* T *and* $\hat{T}$, *respectively, and that* $T-\hat{T}=\mathrm{O}(\hat{T}h^p)$. *Then we have*

$$\| y(t_n, 0, y_0) - y_n \| \leqslant M t_n h^p \tag{2.2}$$

for $t_n h^p \leqslant C$.

Proof. Since the difference $y_n - z(t_n)$ can be neglected, it remains to estimate $z(t_n)-y(t_n)$, where $z(t)$ and $y(t)$ are the solutions of (2.1) and (1.1) with initial values $y(0)=z(0)=y_0$. For $t_n = N\hat{T}+\tau$ (with $0 \leqslant \tau < \hat{T}$) we have

$$\begin{aligned} y(t_n)-z(t_n) &= y(N\hat{T}+\tau)-z(N\hat{T}+\tau) \\ &= y\big(N(\hat{T}-T)+\tau\big)-z(\tau) \\ &= y\big(N(\hat{T}-T)+\tau\big)-y(\tau)+y(\tau)-z(\tau). \end{aligned} \tag{2.3}$$

Since the value of τ is restricted to the compact interval $[0, \hat{T}]$ and the defect of $z(t)$ inserted into (1.1) is $\mathrm{O}(h^p)$, it follows from the nonlinear variation of constants formula (see [4, p. 96]) that

$$y(\tau)-z(\tau)=\mathrm{O}(\tau h^p). \tag{2.4}$$

Furthermore, the mean value theorem gives

$$y\big(N(\hat{T}-T)+\tau\big)-y(\tau)=\mathrm{O}\big(N(\hat{T}-T)\big)=\mathrm{O}(N\hat{T}h^p). \tag{2.5}$$

The two estimates (2.4) and (2.5) together with (2.3) yield the statement of the lemma. □

The main difficulty for the application of Lemma 1 is the verification of the periodicity of the numerical solution, i.e., of the solution of the differential equation (2.1). This, however, is possible in several interesting situations.

- For a *Hamiltonian problem* with one degree of freedom the solution lies on a level curve of the Hamiltonian function. If this level curve is bounded and free from stationary points of the problem, the exact solution is periodic. A constant stepsize application of a symplectic numerical integrator (see [11]) to such a problem leads to a perturbed differential equations (2.1) which is again Hamiltonian (see [3]). The numerical solution thus lies on the level curve of the perturbed Hamiltonian function and is periodic, too.
- Consider a two-dimensional system $p'=f(p, q)$, $q'=g(p, q)$ satisfying the *symmetry relations* $f(-p, q)=f(p, q)$ and $g(-p, q)=-g(p, q)$; for example, the pendulum problem where $f(p, q)=-\sin q$ and $g(p, q)=p$. If a solution starting from the q-axis comes back to the q-axis after a finite time σ, its continuation is a reflection at the q-axis and we obtain a 2σ-periodic solution. In this situation we apply a symmetric one-step method (see [4, p. 221]). The perturbed differential equation (2.1) then satisfies the same symmetry relations and the numerical solution is also periodic (this follows from the explicit representation of (2.1) given in [3]).
- The exact solution of the *Volterra–Lotka equation* $p'=p(\alpha-\beta q)$, $q'=q(-\gamma+\delta p)$ lies on the curve $-\gamma \ln p+\delta p-\alpha \ln q+\beta q=Const$ and is therefore periodic. Some special methods (integrator of W. Kahan [10] or the symplectic Euler method, see also [7])

preserve the differential 2-form $(\mathrm{d}p/p) \wedge (\mathrm{d}q/q)$. Hence, the numerical solution lies on a perturbed curve and is periodic, too.

- Application of a symplectic integrator with constant stepsizes to the *Kepler problem* (Hamiltonian problem corresponding to (1.6) with $\varepsilon = 0$) only leads to quasi-periodic solutions, so that the above lemma cannot be applied directly. The linear error growth for this problem has been investigated in detail by [1].

3. Linear error growth—integrable systems

Our next result concerns integrable systems. We shall apply KAM theory (see [8]) which has been developed for the study of perturbations of integrable systems.

Consider Hamiltonian differential equations,

$$q' = \frac{\partial H}{\partial p}(p, q), \qquad p' = -\frac{\partial H}{\partial q}(p, q), \tag{3.1}$$

with n degrees of freedom. The integrability of such a system is characterized by the fact that there exist coordinates $x = (x_1, \ldots, x_n)$, $y = (y_1, \ldots, y_n)$ via a canonical transformation

$$(q, p) = w(x, y) \tag{3.2}$$

such that w has period 2π in the variables $x_1, \ldots, x_n$ and such that the Hamiltonian function in the new variables is independent of x. In these new variables the system has the simple form

$$x' = \frac{\partial H}{\partial y}(y), \qquad y' = 0$$

(we use the same notation in both coordinate systems, i.e., $H(y) = H(w(x, y))$) and can easily be solved to give

$$x(t) = x(0) + \omega(c)t, \qquad y(t) = c, \tag{3.3}$$

where the frequencies of the system are given by $\omega(c) = \partial H/\partial y(c)$.

Applying a one-step method with constant stepsizes to (3.1) yields a numerical solution which, as in Section 2, can be formally interpreted as the exact solution of a perturbed differential equation (2.1) (truncated series if necessary). The main point is now that for *symplectic* integrators this perturbed equation is again Hamiltonian with

$$\hat{H}(p, q) = H(p, q) + h^p H_p(p, q) + h^{p+1} H_{p+1}(p, q) + \cdots$$

(see [3]). Under the canonical transformation (3.2) we get a system

$$x' = \frac{\partial \hat{H}}{\partial y}(x, y), \qquad y' = -\frac{\partial \hat{H}}{\partial x}(x, y) \tag{3.4}$$

with $\hat{H}(x, y) = H(y) + h^p H_p(x, y) + \cdots$, where $\hat{H}$ has again period 2π in the variables $x_1, \ldots, x_n$ (due to the periodicity of w).

We are now prepared to apply KAM theory. Under the technical assumptions (excluding rationally dependent frequencies) made in Theorem 2.7 of [8] the flow of (3.4) has, for sufficiently small h, an invariant torus

$$\begin{aligned} x &= \theta + h^p u_p(\theta) + h^{p+1} u_{p+1}(\theta) + \cdots, \\ y &= c + h^p v_p(\theta) + h^{p+1} v_{p+1}(\theta) + \cdots \end{aligned} \tag{3.5}$$

(where $u_j(\theta)$ and $v_j(\theta)$ are 2π-periodic in $\theta_1, \ldots, \theta_n$) and the flow on this torus is

$$\theta' = \omega(c), \quad \text{i.e., } \theta(t) = \theta_0 + \omega(c)t.$$

The solution of (3.4) is therefore given by

$$\begin{aligned} x(t) &= \theta_0 + \omega(c)t + h^p u_p(\theta_0 + \omega(c)t) + h^{p+1} u_{p+1}(\theta_0 + \omega(c)t) + \cdots, \\ y(t) &= c + h^p v_p(\theta_0 + \omega(c)t) + h^{p+1} v_{p+1}(\theta_0 + \omega(c)t) + \cdots. \end{aligned} \tag{3.6}$$

For $h = 0$ we recover the solution (3.3) of the unperturbed system corresponding to the initial value

$$(p_0, q_0) = w(\theta_0, c).$$

For $h \neq 0$ we get a solution of the perturbed problem with initial values

$$(\tilde{p}_0, \tilde{q}_0) = w\big(\theta_0 + h^p u_p(\theta_0) + \cdots, c + h^p v_p(\theta_0) + \cdots\big). \tag{3.7}$$

Since the functions $u_j(\theta)$ and $v_j(\theta)$ are 2π-periodic, these two solutions are $O(h^p)$-close, where the constant symbolized by O is independent of t (at least for $th^p \leqslant C$).

We are mainly interested in the difference between the solutions $(p(t), q(t))$ of the unperturbed and $(\hat{p}(t), \hat{q}(t))$ of the perturbed differential equation, both with the same initial value $(p_0, q_0) = w(\theta_0, c)$. Denoting the solution of the perturbed differential equation with initial values (3.7) by $(\tilde{p}(t), \tilde{q}(t))$, we have shown above that $\| p(t) - \tilde{p}(t) \| + \| q(t) - \tilde{q}(t) \| = O(h^p)$. Formula (3.6) implies that perturbations in the initial values are propagated at most linearly so that $\| \hat{p}(t) - \tilde{p}(t) \| + \| \hat{q}(t) - \tilde{q}(t) \| = O(th^p)$. The triangle inequality finally shows the linear error growth.

Conclusion. The global error of a symplectic integration method applied to an integrable Hamiltonian system satisfies in general

$$\| p(t_n) - p_n \| + \| q(t_n) - q_n \| \leqslant M t_n h^p. \tag{3.8}$$

Reversible differential systems

A differential equation

$$p' = f(p, q), \qquad q' = g(p, q) \tag{3.9}$$

is called reversible with respect to the reflection $\rho(p, q) = (-p, q)$ if

$$f(-p, q) = f(p, q), \qquad g(-p, q) = -g(p, q) \tag{3.10}$$

(see [8]). Integrability can be defined as above with the only difference that the transformation (3.2) has to commute with ρ instead of being canonical. If we apply a *symmetric* one-step

method (see [4, p. 221]) to (3.9), the perturbed problem representing the numerical solution is reversible, too. This follows at once from the explicit formula for the perturbed equation given in [3] (observe that for symmetric methods we have $b(t)=0$ for trees t whose number of vertices is odd). In the KAM theory there is an analogue of the above results for reversible systems [8, Theorem 2.9]. Consequently, the global error of a symmetric integration method applied with fixed stepsizes to an integrable ρ-reversible differential equation satisfies also (3.8).

4. Variable-stepsize integration

A numerical integrator, which is intended to be efficient for a large class of problems, has to be equipped with the possibility for variable stepsizes. Symplecticness is destroyed by using variable stepsizes (see [1,13]). However, for symmetric methods, new stepsize strategies have been deviced in [6,13] which do not destroy the symmetry. Based on the ideas of [13] we shall develop such strategies for implicit collocation methods.

For the differential equation $y'=f(y)$ we consider implicit Runge–Kutta methods

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j), \qquad y_1 = y_0 + h\sum_{i=1}^{s} b_i f(Y_i), \tag{4.1}$$

where, for given distinct numbers $c_1,\dots,c_s$, the coefficients a_{ij} and b_i are determined by

$$\sum_{j=1}^{s} a_{ij} c_j^{q-1} = \frac{c_i^q}{q}, \quad q=1,\dots,s, \tag{4.2}$$

$$\sum_{i=1}^{s} b_i c_i^{q-1} = \frac{1}{q}, \qquad q=1,\dots,s. \tag{4.3}$$

Such methods are equivalent to collocation methods [4, p. 211] and their order is equal to that of the corresponding quadrature formula.

If the numbers $c_1,\dots,c_s$ are symmetrically distributed on the interval [0,1], i.e.,

$$c_i = 1 - c_{s+1-i} \quad \text{for } i=1,\dots,s, \tag{4.4}$$

then the method (4.1) is symmetric. This means that the numerical result, obtained by applying method (4.1) with stepsize $-h$ to y_1, is exactly the initial value y_0 (see [4, p. 222]).

We now consider the problem (3.9) and we assume that the reversibility property (3.10) is satisfied (for our illustration in Fig. 2 below we shall use the pendulum equations $q'=p$, $p'=-\sin q$). Let (p_1, q_1) be the numerical result obtained by the Runge–Kutta method (4.1) with stepsize h from the initial value (p_0, q_0). Changing the sign in the p-equations of the Runge–Kutta method it follows from (3.10) that $(-p_1, q_1)$ is the numerical result obtained with stepsize $-h$ from $(-p_0, q_0)$. If the considered method is symmetric, this implies that $(-p_0, q_0)$ is the numerical result obtained with stepsize h from $(-p_1, q_1)$. An illustration of this property is given in Fig. 2. If the stepsize is such that the numerical solution hits exactly the q-axis when the solution crosses for the first time this axis, then the numerical solution is symmetric with

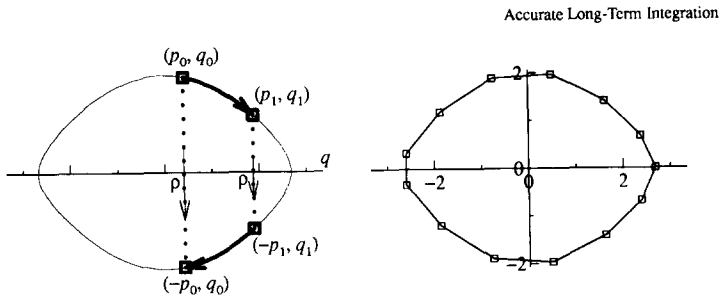

Fig. 2. Reversibility and variable stepsizes.

respect to the q-axis and is thus periodic. This is the reason of the linear error growth of the numerical solution.

Reversible stepsize selection

For the above argument it is not important that the stepsizes are everywhere the same. In order to get a numerical solution which is symmetric with respect to the q-axis and hence periodic, it is sufficient that the stepsize taken from (p_0, q_0) to (p_1, q_1) is the same as that from $(-p_1, q_1)$ to $(-p_0, q_0)$ (see [13] and Fig. 2, right picture). How this can be achieved will be explained in the sequel.

For our stepsize selection we consider an embedded method and use the difference of the numerical solutions, which is of the form

$$D = h \sum_{i=1}^{s} e_i f(Y_i), \tag{4.5}$$

If we choose the coefficients e_i such that

$$\sum_{i=1}^{s} e_i c_i^{q-1} = \begin{cases} 0 & \text{for } q = 1, \ldots, s-1, \\ 1 & \text{for } q = s, \end{cases} \tag{4.6}$$

then the expression (4.5) satisfies $D = \mathrm{O}(h^s)$ because $Y_i = y(t_0 + c_i h) + \mathrm{O}(h^{s+1})$. Usually the stepsize h is chosen such that $\| D \| \leqslant Tol$. Such a choice, however, does not fullfill the above symmetry requirement.

Due to the symmetry assumption (4.4) the solution e_i of (4.6) satisfies

$$e_{s+1-i} = \begin{cases} e_i, & \text{if } s \text{ is odd}, \\ -e_i, & \text{if } s \text{ is even}. \end{cases} \tag{4.7}$$

Denoting by $Y_i = (P_i, Q_i)$ the internal stage-values of the step from (p_0, q_0) to (p_1, q_1), it follows from the above considerations that $(-P_i, Q_i)$ are the internal stage-values for the step from $(-p_0, q_0)$ to $(-p_1, q_1)$ (with stepsize $-h$). As a consequence of the symmetry of the method, the internal stage-values of the step from $(-p_1, q_1)$ to $(-p_0, q_0)$ with stepsize h are given by $\bar{Y}_i = (-P_{s+1-i}, Q_{s+1-i}) =: \rho Y_{s+1-i}$. The reversibility condition (3.10) (which is equivalent to $\rho f(y) = -f(\rho y)$) together with (4.7) imply that the expression $\| D \|$ is the same for both steps. Consequently the condition

$$\| D \| = Tol \tag{4.8}$$

(an idea of [13]) determines a stepsize which is the same for the step from (p_0, q_0) to (p_1, q_1) and for the reflected one.

Implementation

Since the expression D of Eq. (4.5) depends nonlinearly on h, the condition (4.8) is a nonlinear equation which has to be solved by iteration techniques. In connection with explicit Nyström methods the secant method has been proposed in [13]. Here the situation is different, because the numerical solution y_1 of (4.1) itself is determined implicitly. It is natural to solve (4.1) and (4.8) simultaneously. This can be performed with help of the following algorithm: suppose that approximations $Y_i^{(k)}$ to Y_i and $h^{(k)}$ to h are given, then we compute $Y_i^{(k+1)}$ and $h^{(k+1)}$ as follows:

- apply a fixed-point iteration to (4.1) to obtain

$$\hat{Y}_i := y_0 + h^{(k)} \sum_{j=1}^{s} a_{ij} f\left(Y_j^{(k)}\right),$$

- compute

$$\hat{D} := h^{(k)} \sum_{i=1}^{s} e_i f\left(\hat{Y}_i\right) \quad \text{and} \quad h^{(k+1)} := h^{(k)} \sqrt[s]{Tol / \| \hat{D} \|},$$

- put $Y_i^{(k+1)} := u(t_0 + c_i h^{(k+1)})$ where $u(t)$ is the collocation polynomial, determined by the method (for methods with $c_1 = 0$ it is given by $u(t_0) = y_0$, $u'(t_0) = f(y_0)$ and $u(t_0 + c_i h^{(k)}) = \hat{Y}_i$ for $i = 2, \ldots, s$).

Observe that for methods with $c_s = 1$ it holds $y_1 = Y_s$ so that no further function evaluation is necessary to obtain y_1.

Numerical experiments with an implementation of the Lobatto IIIA methods have shown that the convergence of this iteration is as fast as fixed-point iteration with a constant stepsize. Therefore, in connection with implicit collocation methods, the reversible-stepsize strategy is not more expensive than a constant-stepsize implementation. This is a considerable advantage of these methods compared to explicit integrators. Fig. 1 demonstrates that the reversible-stepsize strategy does not distroy the linear error growth, even for problems whose solution is not periodic.

If the Lobatto IIIA methods are taken as basic method, then the achieved accuracy will usually be much higher than *Tol*. This is due to the fact that the local truncation error of these methods is $O(h^{2s-1})$ whereas $D = O(h^s)$. We therefore propose to replace Eq. (4.8) by $\| D \| = Tol^{\alpha}$ with $\alpha = s/(2s-1)$. This modification has been considered for all computations of this article, in particular also for the computations of Fig. 1.

Remark. We have to take care of the fact that the computation of h from Eq. (4.8) is ill-conditioned. Due to roundoff errors during the computation of $f(Y_i)$ the expression D of Eq. (4.5) is affected by a relative error of size $\epsilon h \| f(y_0) \| / \| D \|$, where ϵ is the unit roundoff. Assuming that $\| D \| \approx Ch^s$, this implies that

$$\frac{\Delta h}{h} \approx \frac{1}{s} \frac{\Delta \| D \|}{\| D \|} \approx \epsilon \frac{h \| f(y_0) \|}{s \cdot Tol}, \tag{4.9}$$

because $\| D \|$ is close to *Tol* (see Eq. (4.8)). Difficulties may thus arise for stringent tolerances.

Computations for the outer solar system

Let us investigate the applicability of implicit Runge–Kutta methods to a practical problem. We consider the integration of the so-called outer solar system (Sun, Jupiter, Saturn, Uranus, Neptune and Pluto; the inner planets being considered part of the sun). Working with heliocentric coordinates the equations of motion lead to a system of 30 first-order differential equations (3 position and 3 velocity coordinates for each planet). They are given as problem C5 in [5]. We have taken a corrected value for the mass of Pluto ($m_5 = 1/130\,000\,000$) and initial values corresponding to September 5, 1994. Preliminary computations revealed that a variable-stepsize integration is not important for this problem (for $s = 8$ and $Tol = 10^{-9}$ the stepsizes varied between $h = 820$ and $h = 1105$ days). We therefore decided to apply our Runge–Kutta code with constant stepsizes. For problems with larger eccentricity, however, the use of variable stepsizes will be essential.

We have applied the Lobatto IIIA method with $s = 8$ stages and stepsize $h = 800$ (days). Fig. 3 shows the error as a function of time (upper curve). For $t \leqslant 10^4$ the error varies stronger than in the rest of the considered interval. This is due to the fact that the output points $a_j = 10^{3+j/50}$ are not all multiples of the stepsize and that we have used the collocation polynomial for "dense output". The solution between two grid points is less precise. However, as soon as the global error dominates the local error of the collocation polynomial (i.e., for about $t \geqslant 10^4$), we can nicely observe the linear error growth of the method.

The lower curve in Fig. 3 shows the roundoff (and iteration) errors for our computation in double precision ($\epsilon \approx 10^{-16}$). It has been obtained by a comparison with a computation in quadruple precision and a more stringent error criterion for the fixed-point iterations. We can observe that this error grows like $C\epsilon t_n^{3/2}$.

Remarks. Due to roundoff errors it is impossible to get accurate approximations of the solution over an arbitrarily long time interval. If we require a precision of at least 10^{-2}, then (in double

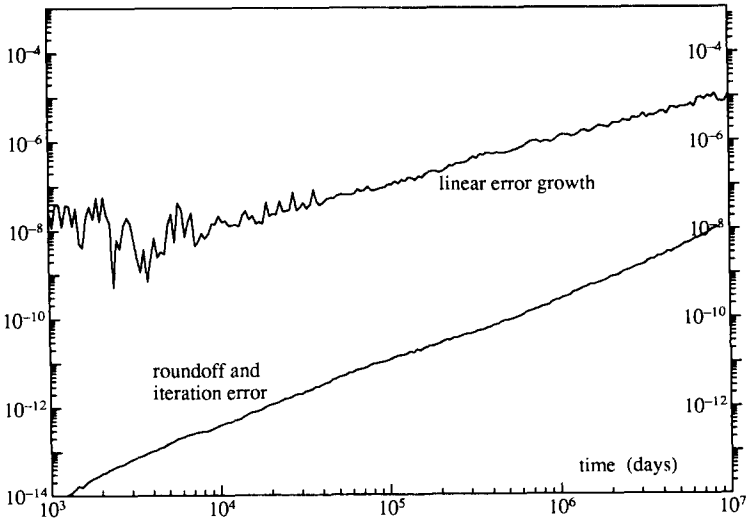

Fig. 3. Numerical experiment with the Lobatto IIIA method ($s = 8$, $h = 800$) at the outer solar problem.

precision, $\epsilon \approx 10^{-16}$) the largest reachable t_n is about 10^{10} (days). Computations beyond this value need a higher precision. The stepsize $h = 800$ (see Fig. 3) has been chosen in order to meet the above accuracy requirement for $t \leqslant 10^{10}$. The computing time on a Sun SPARC station 20 is about 1 second for an interval of 43 years.

An advantage of methods with linear error growth over conventional methods is that larger steps can be taken to advance the integration. In order to get comparable results, conventional methods need stepsizes such that the local truncation error is smaller than the roundoff error.

It is worth mentioning that fixed-point iteration for implicit Runge–Kutta methods is ideal for a parallel computation. If s (number of stages) processors are available, then all function evaluations per iteration can be performed in parallel and a considerable speedup can be expected. Such a gain is not possible with explicit methods which require a serial evaluation of the right-hand side of the differential equation.

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