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Volume-preserving integrators have linear error growth

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Abstract

We present numerical evidence of linear long-term error growth in the calculation of periodic and quasi-periodic orbits of divergence-free ODEs by volume-preserving integration methods. © 1998 Published by Elsevier Science B.V.

1. Introduction

In recent years there has been much interest in structure-preserving integrators [2] for the numerical integration of various special classes of ordinary differential equations (ODEs). These integrators are special-purpose integration methods, designed specifically to preserve certain features of the ODEs *exactly*. Examples are symplectic integrators for Hamiltonian ODEs [1,2], volume-preserving integrators for divergence-free ODEs [3-5], integrators that preserve (linear) symmetries and time-reversing symmetries [6,7], integral-preserving integrators for ODEs possessing first integrals (i.e. constants of the motion) [8-11], Lie group invariant methods [12,13], and integrators preserving the structure of gradient and Lyapunov systems [14,15]. Systematic ways to generate symplectic integrators, momentum-preserving integrators, and even energy-preserving integrators of variational principles are given in Refs. [5,16] [3]. For surveys of this area, see Refs. [14,18,19].

Originally the interest in structure-preserving integrators was caused mainly by their *qualitative* superiority, e.g. the preservation of stabilising KAM tori (in symplectic, volume-preserving, and time-reversal invariant integrators) and the preservation of integral surfaces (by integral-preserving integrators) [4]. More recently it has been realised that structure-preserving integrators are in many cases also *quantitatively* superior. That is to say, it has been found numerically and proved analytically that symplectic [22,23], integral-preserving [24,25], and time-reversal invariant integrators [26-28] exhibit *linear* long-term error growth when applied to calculate *periodic* orbits in the corresponding classes of ODEs. There are also analytic arguments and proofs giving linear long-term error growth for symplectic integrators applied to calculate *quasi-periodic* orbits in Hamiltonian ODEs [29,30]. This behaviour contrasts with the *quadratic* long-term error growth exhibited by standard numerical methods (such as the well-known fourth-order Runge-Kutta method) applied to periodic and quasi-periodic orbits.

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[2] Also called mechanical or geometric integrators.

[3] It should be mentioned that one cannot "have it all". Ge and Marsden [17] have shown that (under some hypotheses) one cannot have integrators that are symplectic, momentum-preserving *and* energy-preserving.

[4] An appealing way to interpret structure-preserving integrators is using backward error analysis [2,20,21].

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In this Letter we extend the above results by presenting numerical evidence of linear long-term error growth for *volume-preserving* integrators applied to both periodic and quasi-periodic orbits in divergence-free ODEs.

2. Linear error growth in periodic orbits

In this section we give two numerical examples in which volume-preserving integrators, when applied to the calculation of *periodic* orbits, exhibit linear long-term error growth.

Our first example is the well-known integrable Kepler two-body problem. Using polar coordinates [2] the system is three-dimensional,

$$\frac{dr}{dt} = p, \quad \frac{dp}{dt} = \frac{\mu^2}{r^3} - \frac{1}{r^2}, \quad \frac{d\theta}{dt} = \frac{\mu}{r^2}, \tag{1}$$

where μ represents the constant angular momentum, and p denotes the (linear) momentum.

Fig. 1a shows the numerical error for the Kepler problem as a function of integration time. The two numerical schemes utilised are the standard fourth-order Runge-Kutta method (top line) and a fourth-order non-symmetric, non-symplectic, volume-preserving method [27] (lower line) designed by McLachlan and Atela [31] to have minimal error for systems that are split into vector fields A and B satisfying $[B,[B,[B,A]]] = 0$ (see Section 4 for more details) [5].

The initial conditions are $r = 1 - e, \theta = 0.0, p = 0.0$ and $\mu = \sqrt{(1+e)(1-e)}$, where the eccentricity is $e = 0.5$. The well-known exact solution for these parameters describes an elliptic orbit with period 2π [32].

Both schemes utilise a time step of $2\pi/500$ (so 500 time steps per orbit) and calculate the error once every period (i.e. once every 500 time steps) for the first 40 periods and then once every tenth period for a total of 40 000 periods.

A least squares fit for the volume-preserving error shows that

$$\log_{10}[\mathrm{error}(T)] = 0.9999592 \log_{10}[T] - 7.513888,$$

which demonstrates its long-term linear error growth.

The Runge-Kutta scheme has an error growth for the orbits between the 200th period and the 1500th period of

$$\log_{10}[\mathrm{error}(T)] = 1.994695 \log_{10}[T] - 7.374104,$$

showing the long-term quadratic behaviour of the error. (Actually, the errors using the standard method comprise both a linear and a quadratic term. For large T the quadratic term dominates.)

Our second example of linear error growth in periodic orbits is the non-integrable four-dimensional Hénon-Heiles system [33],

$$\begin{aligned} &\dot{q}_1 = p_1, \quad \dot{q}_2 = p_2, \quad \dot{p}_1 = -q_1 - 2q_1q_2, \\ &\dot{p}_2 = -q_2 - q_1^2 + q_2^2. \end{aligned} \tag{2}$$

Fig. 1b shows the error in a periodic orbit in the Hénon-Heiles system. The two curves shown are for the fourth-order Runge-Kutta scheme (upper curve), and for a fourth-order explicit non-symplectic, non-symmetric volume-preserving scheme (lower curve). Details of this scheme can be found in Section 4.

The initial conditions for the periodic orbit are $p_1 = 0.4205675980631355$, $q_1 = 0.1$, $p_2 = 0.0$ and $q_2 = 0.3026668174699$ which describes an orbit with period 6.07561578.

Both schemes take 500 time steps per period and calculate the error every 10 periods, for a total of 40 000 periods.

A least squares fit on the error for the volume-preserving scheme yields a linear error growth,

$$\log_{10}[\mathrm{error}(T)] = 1.000525 \log_{10}[T] - 8.679995.$$

The Runge-Kutta scheme has quadratic error growth,

$$\log_{10}[\mathrm{error}(T)] = 1.964703 \log_{10}[T] - 11.35003,$$

for the error between period 20 000 and 40 000.

3. Linear error growth in quasi-periodic orbits

In this section we give two numerical examples in which volume-preserving integrators, when applied to calculating *quasi-periodic* orbits, exhibit linear long-term error growth.

[5] Whereas it may be preferable in practice to simultaneously preserve as much mathematical structure as possible, in this Letter we construct integrators that preserve only volume, in order to study whether volume preservation per se yields linear long-term error growth.

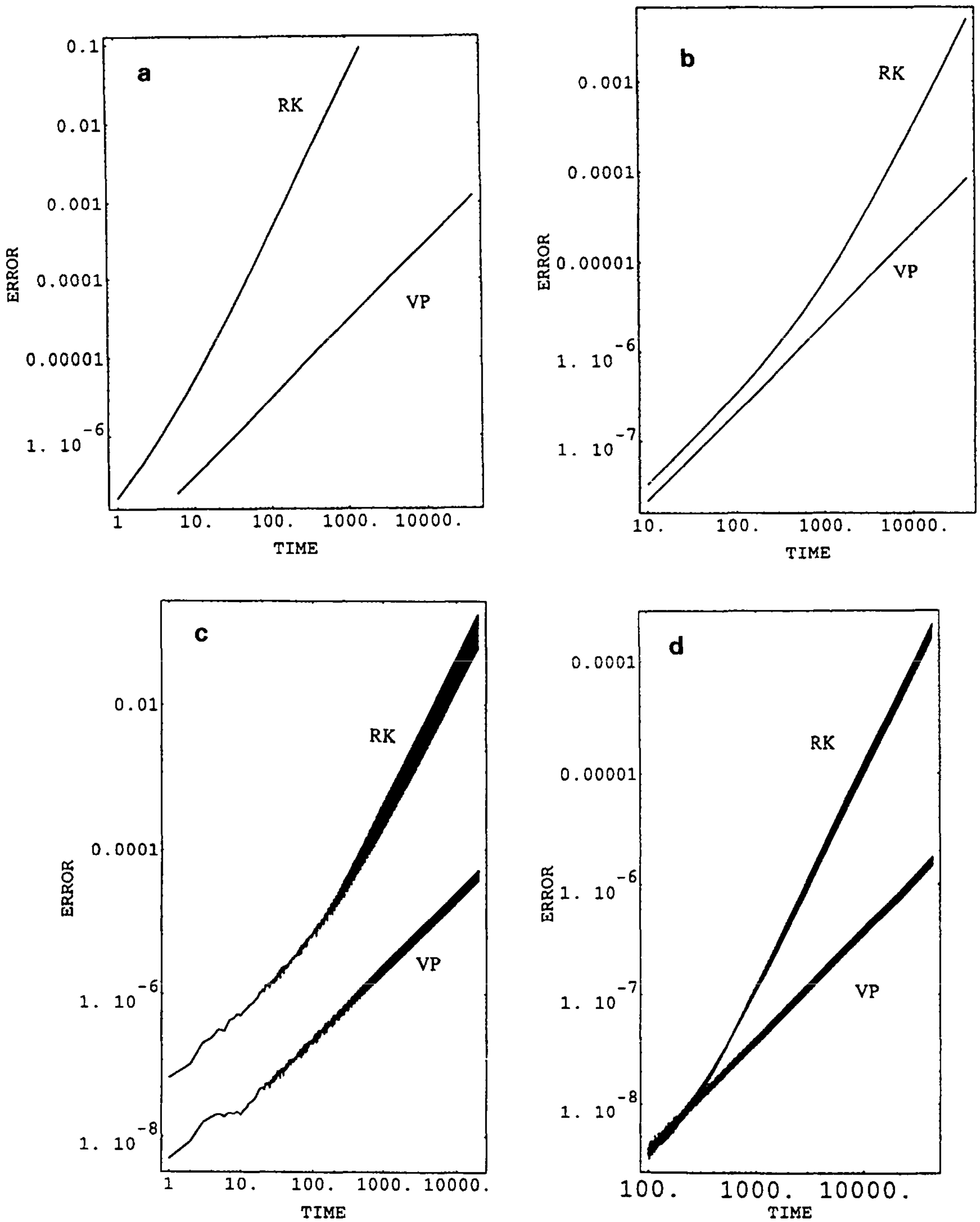

Fig. 1. Numerical error as a function of integration time. In all four graphs, the volume-preserving integrator (VP) exhibits linear long-term error growth; the standard Runge-Kutta method (RK) exhibits quadratic long-term error growth. (a) Numerical error in a periodic orbit in the Kepler problem (Eq. (1)). (b) Numerical error in a periodic orbit in the Hénon-Heiles system (Eq. (2)). (c) Numerical error in a quasi-periodic orbit in the Hénon-Heiles system (Eq. (2)). (d) Numerical error in a quasi-periodic orbit in the ABC flow (Eq. (3)).

Our first example is again the Hénon-Heiles model (Eq. (2)).

Fig. 1c shows the error in a quasi-periodic orbit in the Hénon-Heiles system. The two curves shown are for the fourth-order Runge-Kutta scheme (upper curve), and for a fourth-order explicit non-symplectic, non-symmetric, volume-preserving scheme (lower curve). Details of this scheme can be found in Section 4.

The initial conditions for the calculations are $p_1 = -0.2$, $q_1 = -0.2$, $p_2 = 0.3750555514409394$ and $q_2 = -0.2$.

Both schemes utilise a time step of $\tau = 1/20$ and calculate the error every 20 iterations (i.e. once every time unit) for a total of $T = 20\,000$ time units.

A least squares fit on the error for the volume-preserving scheme yields a linear error growth,

$$\log_{10}[\mathrm{error}(T)] = 0.9975443 \log_{10}[T] - 8.634656,$$

whilst the Runge-Kutta scheme has quadratic error growth,

$$\log_{10}[\mathrm{error}(T)] = 1.966000 \log_{10}[T] - 9.3916218,$$

for the errors between $T = 2\,000$ and $T = 20\,000$.

Our second example of linear error growth in quasi-periodic orbits is the non-integrable three-dimensional ABC flow [34],

$$\frac{dx}{dt} = A\sin(z) + C\cos(y),$$
$$\frac{dy}{dt} = B\sin(x) + A\cos(z),$$
$$\frac{dz}{dt} = C\sin(y) + B\cos(x). \tag{3}$$

Fig. 1d shows the error in a quasi-periodic orbit in the ABC system. The two curves shown are for the fourth-order Runge-Kutta scheme (upper curve), and for a fourth-order explicit non-symplectic, symmetric, volume-preserving scheme (lower curve). Details of this scheme can be found in Section 4.

The initial conditions for the calculations are $x = 1.5\pi$, $y = \pi$, $z = 0.62\pi$.

Both schemes utilise a time step of $\tau = 1/100$ and calculate the error every 100 iterations (i.e. once every time unit) from a time of $T = 100$ time units to $T = 40\,000$ time units.

A least squares fit on the error for the volume-preserving scheme again yields a linear error growth,

$$\log_{10}[\mathrm{error}(T)] = 1.010347 \log_{10}[T] - 10.45465.$$

The Runge-Kutta scheme has quadratic growth

$$\log_{10}[\mathrm{error}(T)] = 1.992870 \log_{10}[T] - 12.90966,$$

for the errors between $T = 1\,000$ and $T = 40\,000$.

4. Numerics

For the Kepler problem we used a composition method due to McLachlan and Atela [31,35]. It uses the volume-preserving splitting

$$A = p\frac{d}{dr}, \quad B = \frac{d}{d\theta} + \left(\frac{\mu^2}{r^3} - \frac{1}{r^2}\right)\frac{d}{dp},$$

for the Kepler vector field. The integrator is then defined as follows,

$$\psi(\tau) = \phi_4(\tau)\phi_3(\tau)\phi_2(\tau)\phi_1(\tau), \tag{4}$$

where the building blocks $\phi_i(\tau)$, $i = 1,\ldots,4$, are given by

$$\phi_i(\tau) = \exp(a_i\tau A)\exp(b_i\tau B), \tag{5}$$

The coefficients a_i and b_i, $i = 1,\ldots,4$, in Eq. (5) are determined by requiring that Eq. (4) be a fourth-order method, and that the error term be minimal. Using the Campbell-Baker-Hausdorff formula and the fact that $[B,[B,[B,A]]] \equiv 0$, the values for a_i and b_i have been calculated numerically and are tabulated in Table 2 of Ref. [31].

For both the periodic and quasi-periodic orbits of the Hénon-Heiles system, the following scheme is used. The vector field is split into two volume-preserving (but non-symplectic) vector fields. These are

$$A = p_1\frac{d}{dq_1} + (q_2^2 - q_2 - q_1^2)\frac{d}{dp_2},$$
$$B = p_2\frac{d}{dq_2} - (q_1 + 2q_1q_2)\frac{d}{dp_1}.$$

A second-order symmetric scheme $\phi(\tau)$ is then constructed from A and B,

$$\phi(\tau) = \exp(\tfrac{1}{2}\tau A)\exp(\tau B)\exp(\tfrac{1}{2}\tau A),$$

which is then raised to a fourth-order method $\psi(\tau)$ via

$$\psi(\tau) = \phi(\alpha\tau)\phi(\beta\tau)\phi(\alpha\tau), \qquad (6)$$

where consistency imposes $\beta = 1 - 2\alpha$, and the order condition gives $\alpha = 1/(2-2^{1/3})$ [1] [6]. The symmetry in the method is then destroyed by

$$\Phi(\tau) = \psi(0.33\tau)\psi(0.35\tau)\psi(0.32\tau).$$

Whilst this scheme is a little expensive due to the multiple levels of the integration, it does show that the linear error growth of the scheme is due to its volume-preserving qualities and not because it preserves symplecticness or reversibility.

The final scheme utilised is a symmetric volume-preserving method for the ABC flow. The three components of the flow are solved individually such that

$$f_1(\tau): x = x + \tau(A\sin(z) + C\cos(y)),$$

$$f_2(\tau): y = y + \tau(B\sin(x) + A\cos(z)),$$

$$f_3(\tau): z = z + \tau(C\sin(y) + B\cos(x));$$

a symmetric second-order scheme is then created via

$$\phi(\tau) = f_3(\tau/2)f_1(\tau/2)f_2(\tau)f_1(\tau/2)f_3(\tau/2).$$

From this ϕ, a fourth-order integrator ψ is constructed using Eq. (4). A non-symmetric, volume-preserving Φ is then obtained by

$$\Phi(\tau) = \psi(0.3\tau)\psi(0.1\tau)\psi(0.6\tau).$$

For comparison, in all the numerical calculations presented here, we have utilised the standard fourth-order explicit Runge–Kutta scheme given by the Butcher Tableau [37]. We have

$$\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ - & - & - & - \\ 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

In all the calculations, the error is the Euclidean distance in phase space between the exact solution [7] and the calculated solution at that time. All numerical computations were performed on a Silicon Graphics Indy, using double-precision Fortran 77.

5. Concluding remarks

In this Letter we have presented clear numerical evidence of linear error growth occurring when volume-preserving integrators are applied to the calculation of periodic and quasi-periodic orbits in volume-preserving flows.

This generalises the previously found linear error growth of symplectic integrators applied to Hamiltonian flows. The significance of our result is that it generalises both the class of systems exhibiting linear error growth (from Hamiltonian to volume-preserving) and the class of integrators exhibiting linear error growth. Thus, if one wants to numerically integrate a Hamiltonian system, one would not necessarily use a symplectic integrator to obtain linear error growth. A volume-preserving integrator would be sufficient.

We do not claim, of course, that volume-preserving integrators would have linear error growth for *all* divergence-free problems. In fact, the main remaining open question is: "What are the conditions under which linear error growth using volume-preserving integrators occurs?" The answer to this question can be sought using two complementary approaches.

First of all, it would be interesting to extend the above *numerical* results to systems of ODEs with dimension greater than 4.

Secondly, it would be nice to have an *analytic* proof of linear error growth in the volume-preserving case [8] (analogous to the proofs in the Hamiltonian, reversible and integral-preserving cases [22–25,27,28,30]. We hope to pursue these questions in future publications.

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[6] This actually follows from the condition for third-order accuracy, $2\alpha^3 + \beta^3 = 0$. Fourth-order accuracy then follows using the time symmetry of Eq. (4) [36].

[7] For the quasi-periodic orbits a very accurate numerical solution is used as the "exact" reference solution.

[8] Even if the proof can only be obtained assuming more restrictive conditions.

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