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Computational Chaos May Be Due to a Single Local Error*

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Nonlinear ordinary differential equations and arbitrary difference methods are considered which satisfy conditions for the convergence of a sequence of true difference solutions. This convergence does not prevent "diversions" of computed difference approximations, a property which is defined here. The occurrence of diversions is demonstrated in examples, namely the *restricted three body problem* and the Lorenz equations. This occurrence is practically unpredictable. In the applied literature, this property has been used to define "(dynamical) chaos." Therefore, observed chaos for solutions of ODEs is not necessarily a consequence of a sensitive dependency on the initial vector but, rather, may be due to a corresponding dependency on computational errors. © 1993 Academic Press, Inc.

1. INTRODUCTION

In this paper, systems of nonlinear ordinary differential equations (ODEs) are considered, namely,

$$\begin{aligned} &y' = f(y) \quad \text{for} \quad t \geqslant 0, \quad f\colon D \to \mathbb{R}^n, \\ &D \subset \mathbb{R}^n, \quad y := (y_1, ..., y_n)^{\mathrm{T}}\colon \mathbb{R} \to \mathbb{R}^n; \end{aligned} \tag{1.1}$$

f is sufficiently smooth; an arbitrary initial vector $y(0) = y_0 \in D$ is admitted. A true solution of the initial value problem (IVP) (1.1) is denoted by $y^* = y^*(t, y_0)$.

A consistent and stable discretization of (1.1) yields a family of finite-dimensional approximations, with the step size h as the family parameter, e.g., [5, 43]. A true (discrete) difference solution of any such system will be denoted by $\tilde{y}_h$ or $\tilde{y}$. Starting from y_0, an approximation $\tilde{y}_h$ deviates from y^* because of the local discretization error. For any fixed $t > 0$, consistency (of order p) and stability imply the pointwise convergence of a sequence $\{\tilde{y}_h\}$ to y^* as $h \to 0$. The global discretization error is a measure for the deviation of $\tilde{y}_h$ from y^*. The usual estimate of this error is

$$\begin{aligned} &\|y^*(t_0, y_0) - \tilde{y}_h|_{t_0}\| \\ &\quad \leqslant c\exp(Mt_0) \quad \text{at any fixed} \quad t_0 > 0, \\ &\quad \text{with} \quad c = O(h^p) \quad \text{as} \quad h \to 0, \end{aligned} \tag{1.2}$$

and M is a Lipschitz constant of the discretization. For any fixed $h > 0$ and as t_0 increases, (1.2) becomes practically useless.

The computer implementation of a discretization involves additional approximations because of local rounding errors and, perhaps, local procedural errors. Concerning any true "difference solution" $\tilde{y}_h$, the corresponding computer-generated "difference approximation" will be denoted by $\tilde{\tilde{y}}_h$ or $\tilde{\tilde{y}}$.

All local errors act as perturbations causing the approximation $\tilde{\tilde{y}}_h|_{t_0}$ to be different from $y^*(t_0, y_0)$ [3]. As will be discussed subsequently, this distance may be large provided the ODEs or their discretization are "perturbation-sensitive." In particular, there may be "perturbation-sensitive neighborhoods" (PSNs) in phase space, see Section 3.

The existence of spurious (or extraneous or ghost) difference solutions $\tilde{y}_{\mathrm{sp},h}$ or, $\tilde{y}_{\mathrm{sp}}$ is well known, e.g., [15, 25, 41, 47, 51]. For arbitrary choices of $y_0 \in D$, these solutions do not approximate any true solution

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$y^* = y^*(t, y_0)$ of (1.1). There are two types of solutions $\tilde{y}_{sp,h}$:

(a) $\tilde{y}_{sp,h}$ is real-valued for all $h \in (0, \bar{h}]$;

(b) as $h \to 0$, a sequence $\{\tilde{y}_h\}$ approaches a true solution $y^* = y^*(t, y_0)$; however, there is an increasing sequence $\{h_\nu\}$ of bifurcation points $h_\nu > 0$ generating a tree of spurious paths $\tilde{y}_{sp,h}$; generally, the qualitative properties of the $\tilde{y}_{sp,h}$ are different from the ones of the true solution y^*.

Remarks: (1) Iserles *et al.* [25] have proved theorems asserting the existence or the non-existence, respectively, of spurious difference solutions for certain classes of discretizations of ODEs.

(2) Stuart [46, 47] has proved the existence of spurious periodic difference solutions for discretizations of a class of nonlinear parabolic initial boundary value problems with PDE $w_t = w_{xx} + \lambda H(w, w_x)$.

(3) For many helpful suggestions, the authors express their appreciation to an unknown referee.

2. DIVERTING DIFFERENCE APPROXIMATIONS

As an introduction to an extension of spurious difference solutions, the following observation is made: for different intervals of time and an arbitrary but fixed $h > 0$, at any given time, a computed approximation $\tilde{\tilde{y}}$ is generally close to different true solutions $y^*_{(1)}, y^*_{(2)}, \ldots$, each belonging to one out of a set of different initial vectors $y_{0(1)}, y_{0(2)}, \ldots$. This is irrelevant if the distance of $y^*_{(i)}$ and $y^*_{(j)}$ with $j \neq i$ is small for all t of interest, which, e.g., may be true in the case that all solutions y^* possess the same monotonicity. The opposite is generally true in the case of a problem in "chaotic dynamics," governed by the ODEs (1.1). As t increases, the "diversion" of $\tilde{\tilde{y}}$ from $y^*_{(1)}$ to $y^*_{(2)}$ at $t \approx t_2$, then to $y^*_{(3)}$ at $t \approx t_3$ etc., may be important if $\|y^*_{(i)}(t) - y^*_{(j)}(t)\|$ is large for at least some $t > \operatorname{Max}\{t_i, t_j\}$. In a situation of this kind, a difference approximation $\tilde{\tilde{y}}$ is said to divert. A diverting difference approximation is spurious in an extended sense since the composition of $y^*_{(1)}, y^*_{(2)}, \ldots$ is not a true solution of (1.1). Generally, spurious difference solutions or diverting difference approximations cannot be detected on the level of the discretization. This detection may be possible if a first integral of the ODEs (1.1) is known. Subsequently, *enclosure methods* for the solutions y^* of (1.1) will be used for this detection, particularly for those dissipative ODEs which do not possess a first integral.

3. ON (COMPUTATIONAL) CHAOS

A famous example for case (b), addressed at the end of Section 1, is the relationship between the set of solutions y^* of the Logistic ODE [22]

$$y' = ay(1 - y) \qquad \text{for} \quad t \geq 0 \text{ with } y(0) \in (0, 1) \quad (3.1)$$

and the set of difference solutions $\tilde{\eta}_h$ of its explicit Euler discretization [36]

$$\begin{aligned} \tilde{\eta}_{h,j+1} &= F_h(\tilde{\eta}_{h,j}) \qquad \text{with} \quad \tilde{\eta}_{h,j} := \tilde{\eta}_h(t_j), \\ F_h(\tilde{\eta}_{h,j}) &:= b\tilde{\eta}_{h,j}(1 - \tilde{\eta}_{h,j}), \qquad (3.2) \\ \tilde{\eta}_{h,j} &:= (ha/b)\,\tilde{y}_{h,j}, \qquad b := 1 + ah. \end{aligned}$$

This is a classical paradigm in the theory of dynamical chaos; see, e.g., [4, 17, 28, 48]. In dependency on the parameter b in (3.2), Li and Yorke [32] have postulated that the "onset of chaos" is at a certain b beyond the point of accumulation of the sequence $\{h_\nu\}$ of bifurcation points. This is arbitrary; in fact, there is no mathematical definition of chaos, e.g., [16]. Since this is a global property of a set of solutions, a sufficiently comprehensive definition would be correspondingly difficult. In the mathematical literature on mappings $F: \mathbb{R}^q \to \mathbb{R}^q$ with $q \geq 2$ (e.g., [18, 42]), the existence of a *horseshoe map* [16] is employed as an indication for the presence of chaos in a set of solutions.

For general, sufficiently smooth functions $F_h: D \to \mathbb{R}$ with $D \subset \mathbb{R}$, now approximations $\tilde{\tilde{\eta}}_h$ of true difference solutions $\tilde{\eta}_h$ are considered. It is assumed that there is a $\delta_F \in \mathbb{R}^+$ such that

$$|\tilde{\tilde{\eta}}_{h,j+1} - F_h(\tilde{\tilde{\eta}}_{h,j})| < \delta_F \qquad \text{for} \quad j = O(1)\,N - 1. \quad (3.3)$$

The shadowing theorem by Chow and Palmer ([10]; see also [11]) asserts that

$$|\tilde{\tilde{\eta}}_{h,j} - \tilde{\eta}_{h,j}| \leq \delta_\eta(M, \sigma, \tau) \qquad \text{for} \quad j = 1(1)N \quad \text{provided } M\sigma\tau \leq \tfrac{1}{2}. \quad (3.4)$$

The constants $M, \sigma, \tau \in \mathbb{R}^+$ depend on $\prod_{k=j}^{N} (F'_h(\tilde{\tilde{\eta}}_{h,k}))^{-1}$ and $\sup\{F''_h(\eta) \mid \eta \in [0, 1]\}$. For $j = 1(1)N$, then, there is a true difference solution $\tilde{\eta}_h$ that shadows its computed approximation $\tilde{\tilde{\eta}}_h$; see also [16]. For dissipative maps $F_h: \mathbb{R}^2 \to \mathbb{R}^2$, Hammel *et al.* [19, 20] propose the conjecture that $\delta_\eta \leq \sqrt{\delta_F}$ if $N \leq 1/\sqrt{\delta_F}$. In view of a system (1.1) of ODEs, the shadowing property for its discretizations is almost useless; in fact, the local discretization error then is not known quantitatively; i.e., there is no information on the magnitude of δ_F.

In the theory of dynamical chaos, shadowing theorems are considered to be of pivotal importance since they (seem to) suggest a practical computability of the true solutions y^* in a chaotic set. This property will be denoted by "ODE-chaos." Concerning sets of solutions of ODEs, the existence of a horseshoe map has been verified mathematically for a few special ODEs [18, 42]. The ODE for the periodically excited pendulum is the only one of physical relevance.

In particular, it is not known at present whether there are "chaotic properties" in the sets of true solutions y^* of the following systems of nonlinear ODEs:

• the ones of celestial mechanics, a special case of which is investigated in Section 5 (see also [26]) and

• the Lorenz equations which are discussed in Sections 6 and 7.

The system of ODEs (1.1) is now considered for the special case of $n = 2$. The following situation will be discussed:

• in the phase space $\mathbb{R}^2$, a segment of a straight line is chosen, $A := [y_{(1)}(0), y_{(2)}(0)]$; with n the unit normal vector of A, it is assumed that $n \cdot f(y) \neq 0$ possesses a fixed sign for all $y \in A$;

• for all $t > 0$, then the true solutions $y^*_{(1)} = y^*_{(1)}(t, y_{(1)}(0))$ and $y^*_{(2)} = y^*_{(2)}(t, y_{(2)}(0))$ bound the set of all true solutions starting in the interval A; this defines a "function strip" in $\mathbb{R}^2$;

• consequently, no solution y^* can enter or leave this strip for any $t \geqslant 0$.

This topographically simple structure of the set of solutions in $\mathbb{R}^2$ precludes chaotic properties in this phase space of $y' = f(y)$. According to Ruelle and Takens (see [4]), dimension three at least is necessary (and sufficient) for the existence of chaos. Properties of this kind then may indeed exist in the cases of

(i) any discretization of all these ODEs or

(ii) the additional consideration of a periodic forcing term in these ODEs.

Concerning (i), chaotic properties may be present even in the case of discretizations of scalar ODEs (with $n = 1$).

Concerning (ii), the following periodically excited nonlinear ODEs have been investigated in the physical and the mathematical literature (e.g., [16]), particularly in the context of dynamical chaos:

• the pendulum equation,

• the Duffing equation,

• the Van der Pol equation and the Lorenz equations.

In the recent physical literature, there are numerous references to "computational chaos" (e.g., [21, 35]). This expression refers in particular to a situation where

• there are "chaotic properties" of computed difference approximations $\tilde{\tilde{y}}_h$ serving as approximations of

• qualitatively or quantitatively known true solutions y^* possessing simple topographical structures.

As an example, (1.1) is considered in the cases of $n = 1$ or $n = 2$. Then

(α) the sets of true solutions are topographically simple, however,

(β) sets of difference solutions $\tilde{y}_h$ then may be topographically complicated, and

(γ) the computed difference approximations may appear "chaotic."

The mathematical reasons for (β) are obvious since the discretizations

• depend on artificial parameters not present in the ODEs and

• they are perturbed by the omission of the terms representing the local discretization error.

Concerning the sets of solutions addressed in (α) and (β), this relationship is qualitatively true for all (fixed) dimensions $n \in \mathbb{N}$ in (1.1). In particular, there are the following contributions to computational chaos:

• spurious difference solutions $\tilde{y}_{sp}$ which, if present, are a consequence of the omission of the local discretization errors in the transfer from the ODEs to the discretization or

• computed diverting difference approximations $\tilde{\tilde{y}}_h$ which, if present, may be caused by all kinds of local errors.

In fact, even a single local error may induce a diversion of an individual computed approximation $\tilde{\tilde{y}}_h$, as will be shown in Section 7. Computational chaos is then expected to be present in a phase space, provided sufficiently many individual approximations $\tilde{\tilde{y}}_h$ are affected by this property.

Remark. Concerning the shadowing theorem by Chow and Palmer [10], it is observed that a diversion of $\tilde{\tilde{y}}_h$ from y^* is *not* implied by a violation of the required inequality $M\sigma\tau \leqslant \frac{1}{2}$ as N increases.

(Computational) Chaos is believed to be associated with perturbation-sensitivities such that small causes exert large influences. The *causes* are perturbations due to either

(A) changes of the initial vectors y_0 in phase space or

(B) local numerical errors of any kind.

The corresponding deviations of the solutions or their approximations are the *effects*. A perturbation-sensitivity is to be expected in subdomains of the phase space, where

• the true orbits are (locally) divergent such that

• the Lyapunov exponent [16] is (locally) positive.

This is the situation favoring diversions of computed difference approximations $\tilde{\tilde{y}}$. Concerning the (spatial) relationship of cause and effect, there are the following two possibilities: either

(I) they occur in the same subdomain of the phase space, or

(II) the causes (A) or (B) take place at times before the orbits enter the perturbation-sensitive neighborhood (PSN), where the effect takes place.

Examples for the actual occurrence of (I) and (II) are:

concerning (I), a pole of the ODEs in Section 5 (see also [9]) and

concerning (II), the approach of a saddle point possessing stable and unstable manifolds, see Sections 6 and 7.

4. ON ENCLOSURE METHODS

An enclosure of a true solution y^* of (1.1) consists of a pair of (computed) bounds $\underline{y}$ and $\bar{y}$ such that

$$\underline{y}_i(t, y_0) \leqslant y_i^*(t, y_0) \leqslant \bar{y}_i(t, y_0) \quad \text{for} \quad i = 1(1)n \text{ and } t \in [t_0, t_\infty], \tag{3.1}$$

where $\|\underline{y} - \bar{y}\|_\infty$ is negligibly small for practical purposes, with $\|\cdot\|_\infty$ denoting the supremum norm. For the following reasons, these inequalities are true with respect to all computational errors:

(α) discretization errors can be bracketed by means of Lohner's enclosure algorithms for ODEs ([33]; see also [1]);

(β) rounding errors can be accounted for on the basis of the Kulisch computer arithmetic [30];

(γ) both (α) and (β) can be executed automatically by means of the following products of U. Kulisch and coworkers: the computer languages PASCAL-SC [6] or ACRITH-XSC [24] or PASCAL-XSC [27] or the subroutine library ACRITH [23] supporting FORTRAN.

On the level of (α)–(γ) and for an interval $[t_0, t_\infty]$, a successful completion of an enclosure verifies the existence of the true solution y^*. This follows from the Banach and the Brouwer fixed point theorems, both of which are employed in the execution of (α).

Remark. (1) These *enclosure methods* establish a quantitative relationship between the function space of the true solutions of the ODEs and the Euclidean spaces of their discretizations.

(2) The enclosure is automatically guided by the true solution y^*. Consequently, the local growth of the width of the enclosure is a meaningful quantitative criterion for Rufeger's control of the step size h [37, 38].

5. DIVERTING DIFFERENCE APPROXIMATIONS IN THE RESTRICTED THREE BODY PROBLEM

The following idealization of celestial mechanics is considered [7, 12]:

(i) the orbits of the earth E and the moon M are confined to a plane in $\mathbb{R}^3$;

(ii) in this plane, there is a suitably rotating Cartesian y_1-y_2-basis whose origin is attached to the center of gravity, C, of E and M; subsequently, E and M are treated as mass points; the points E, C, and M are on the y_1-axis;

(iii) the position of C relative to E and M is determined by the ratio $\mu = 1/82.45$ of the masses of M and E; consequently, $-\mu$ is the location of E and $\lambda := 1 - \mu$ is the one of M, both on the y_1-axis;

(iv) in the y_1-y_2 plane, trajectories of a small satellite S are to be determined;

(v) for these trajectories, the phase space possesses the Cartesian coordinates y_1, y_2, $y_3 := y_1'$ and $y_4 := y_2'$.

For the *restricted three body problem* defined by (i)–(v), the equations of motion are as follows [7, 12] in the employed rotating basis:

$$\begin{aligned} &y_1' = y_3, \qquad y_2' = y_4, \\ &y_3' = y_1 + 2y_4 - \lambda(y_1 + \mu)/r_1^{3/2} - \mu(y_1 - \lambda)/r_2^{3/2}, \\ &y_4' = y_2 - 2y_3 - \lambda y_2/r_1^{3/2} - \mu y_2/r_2^{3/2}, \\ &r_1 := (y_1 + \mu)^2 + y_2^2, \qquad r_2 := (y_1 - \lambda)^2 + y_2^2. \end{aligned} \tag{5.1}$$

For any true solution $y^* = (y_1^*, y_2^*, y_3^*, y_4^*)^{\mathrm{T}}$ of (5.1), the Jacobi integral, J, takes a fixed value:

$$J := \tfrac{1}{2}(y_3^2 + y_4^2 - y_1^2 - y_2^2) - \lambda/r_1^{1/2} - \mu/r_2^{1/2}. \tag{5.2}$$

In agreement with numerous papers in literature (e.g., [7, 45]), the following point is chosen as an initial vector:

$$\tilde{\tilde{y}}_p(0) := (1.2, 0, 0, -1.04935750983)^{\mathrm{T}}. \tag{5.3}$$

With much more than graphical accuracy, numerous applications of "high-precision" difference methods in literature have yielded almost closed orbits $\tilde{\tilde{y}}_p$ whose projections into the y_1-y_2-plane are displayed in Fig. 1. These orbits appear to return to $\tilde{\tilde{y}}_p(0)$ at the time $t = \tilde{\tilde{T}} := 6.192169331396$ [7]. Therefore, $\tilde{\tilde{y}}_p$ is believed to be an approximation of a hypothetical T-periodic solution y_p^* if (5.1) with period $T \approx \tilde{\tilde{T}}$.

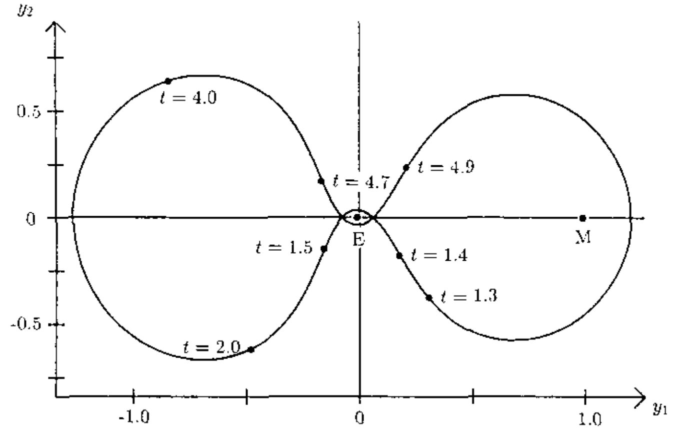

FIG. 1. Projection into y_1-y_2-plane of difference approximation $\tilde{\tilde{y}}_p$ approximating true solution y_p^* (restricted three body problem).

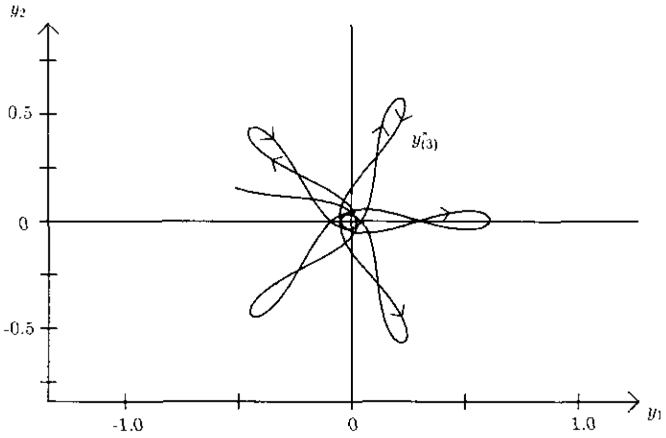

FIG. 3. Enclosure of true solution $y^*_{(3)}$ (restricted three body problem).

By means of a classical Runge–Kutta method [5, 43], Rufeger [37, 38]:

(i) has reproduced published approximations $\tilde{\tilde{y}}_p$ of y_p^*, making use of a step size $h = 10^{-3}$ and

(ii) for $h = 5 \times 10^{-3}$, she has computed the approximation, $\tilde{\tilde{y}}_q$, depicted in Fig. 2.

For each one of the first four loops in Fig. 2, the Jacobi integral, J, has been evaluated by means of $\tilde{\tilde{y}}_q$. For each individual loop, J changes by less than 10^{-5}. Every time $\tilde{\tilde{y}}_q$ comes close to the pole E, J decreases by more than 0.3, thus suggesting a sequence of diversions of $\tilde{\tilde{y}}_q$ close to E, each taking place in approximately four consecutive time steps. Close to E, now four initial vectors $\eta_{(1)}, ..., \eta_{(4)}$ were chosen as follows:

(a) they coincide with computed values of $\tilde{\tilde{y}}_q$ such that

(b) $\tilde{\tilde{y}}_q$ at $\eta_{(i)}$ is beginning to traverse one of the first three loops in Fig. 2. For each fixed $\eta_{(i)}$, the true orbit $y^*_{(i)}$ starting at $\eta_{(i)}$ was enclosed, making use of a step size control developed in [37 or 38]. Figure 3 depicts the enclosure of $y^*_{(3)}$. At $\eta_{(3)}$, the computed approximation $\tilde{\tilde{y}}_q$ diverts from $y^*_{(3)}$ to the continuation of $\tilde{\tilde{y}}_q$ shown in Fig. 2. Consequently, the occurrence of a diversion of the difference solution $\tilde{\tilde{y}}_q$ has been verified and its properties have been demonstrated.

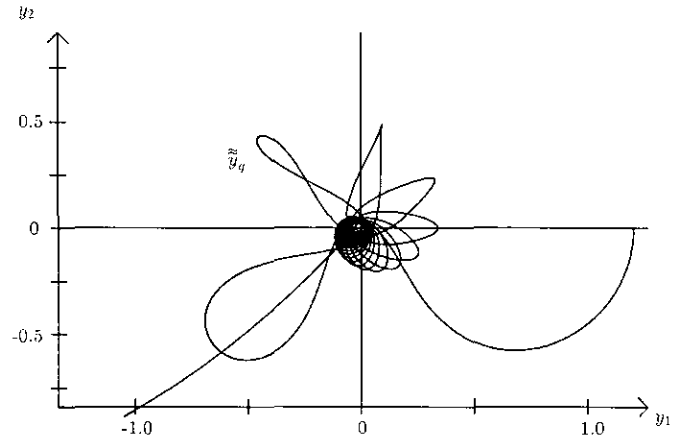

FIG. 2. Projection into y_1-y_2-plane of difference approximation $\tilde{\tilde{y}}_q$ with multiple diversions (restricted three body problem).

The diversions observed here have been obtained by means of the consistent and stable classical Runge–Kutta method with the choice of $h = 5 \times 10^{-3}$. For true orbits with a sufficiently small distance from the pole at E, diverting difference approximations are to be expected even when "high-precision" discretizations are employed. This conjecture on the *unpredictability* of diversions is confirmed by the subsequent discussion of the Lorenz equations.

Remarks. (1) The numerical analysis yielding Fig. 1–3 was executed on a PC "kws" using a PASCAL-SC compiler. For a more detailed presentation of these results see [2, 37, 44].

(2) Swingby maneuvers of space vehicles are (e.g., [14]) executed in near neighborhoods of planets. Because of the proximity of a pole of the ODEs (of celestial mechanics), only the employment of enclosure methods can reliably avoid diversions of computed orbits.

6. THE LORENTZ EQUATIONS, SOLUTIONS, AND APPROXIMATIONS

The Lorenz equations are [40] (see also [31])

$$y' = f(y) \Leftrightarrow \begin{cases} dy_1/dt = \sigma(y_2 - y_1) \\ dy_2/dt = ry_1 - y_2 - y_1 y_3, \\ dy_3/dt = y_1 y_2 - by_3 \end{cases} \qquad (6.1)$$

$$y := \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \qquad y_0 := y(0),$$

where $b, r, \sigma \in \mathbb{R}^+$ are free parameters. There are three real-valued stationary points:

(i) for all $b, r, \sigma \in \mathbb{R}^+$, the origin $(0, 0, 0)^T$ and

(ii) for all $b, r-1, \sigma \in \mathbb{R}^+$, the points C_1 and C_2 with positions $(\xi, \xi, r-1)^T \in \mathbb{R}^3$, where $\xi := \pm\sqrt{b(r-1)}$.

For $r > 1$, the stationary point $(0, 0, 0)^T$ is a saddle point. Consequently and because of the Center Manifold Theorem, i.e., there exist stable and unstable manifolds of this point, both of which consist of true solutions y^* of (6.1).

For special choices of b, r, σ, either

(α) $y^* = y^*(t, b, r, \sigma, y_0)$ can be represented explicitly or

(β) the set of solutions y^* is known to possess simple ("non-chaotic") topographical structures.

For arbitrary $b = 2\sigma \in \mathbb{R}^+$ and $r \in \mathbb{R}^+$, we have found the following equivalent representation of (6.1) (see the Appendix):

$$y_1'' + (\sigma+1)\, y_1' - \sigma((r-1) - ce^{-2\sigma t})\, y_1 + \tfrac{1}{2} y_1^3 = 0, \qquad (6.2)$$

$$y_3(t) - \tfrac{1}{2\sigma}(y_1(t))^2 = ce^{-bt}, \quad \text{with} \quad c := y_3(0) - (\tfrac{1}{2\sigma})(y_1(0))^2, \qquad (6.3)$$

$$y_2' + y_2 = y_1(t)(r - y_3(t)). \qquad (6.4)$$

In the limit as $t \to \infty$, the phase space of (6.2) is two-dimensional. As has been shown in Section 3, this precludes "chaotic" properties of the solutions y_1^* of (6.2) and, therefore, also of the system (6.1) as $t \to \infty$, for any choices of $b = 2\sigma$, $r \in \mathbb{R}^+$. Since (6.2)–(6.4) is a semi-coupled (equivalent) representation of (6.1), the simple properties of the solutions y^* then are inconsistent with the existence of a (chaotic) strange attractor as $t \to \infty$.

For several other choices of $b, r, \sigma \in \mathbb{R}^+$, a large number of difference approximations $\tilde{\tilde{y}}$ (of solutions y^*) have been determined and published in the literature. In the preface of his monograph [40] on the Lorenz equations (6.1), C. Sparrow points out: "For some parameter values, numerically computed solutions of the equations oscillate, apparently forever, in the pseudo-random way we now call 'chaotic'." Almost generally in the non-mathematical literature, this property is tacitly assumed to hold for the set of true solutions of (6.1). Mathematically, there arises the question whether this pseudo-randomness of difference approximations $\tilde{\tilde{y}}$ represents not only "computational chaos" but also "ODE-chaos" (of the solutions of (6.1)). This issue will be discussed in view of the possibility of diverting difference approximations.

7. DIVERTING DIFFERENCE APPROXIMATIONS OF THE LORENZ EQUATIONS

For the choices $b = \frac{8}{3}$, $r = 28$, and $\sigma = 6$ in (5.1) Kühn [29, 2, 3] has used

(a) several standard numerical methods and

(b) enclosure methods.

Both (a) and (b) were executed by use of C compilers running on an HP-VECTRA. In the case of (b), a C compiler has been used which was developed by Kühn [29]. By means of (b), Kühn has verified the existence of five different periodic solutions, y_p^*, of (6.1). Figure 4 depicts the projection into the y_1-y_2 plane of a T-periodic orbit y_p^*, where [29, 2, 3]: (i) $T \in 2.5942776279^{9}_{0}$ (this denotes an interval), (ii) the following point $(y_1(0), y_2(0), y_3(0))^T$ is on y_p^*:

$$y_1(0) \in 10.952283216^{4}_{0}, \qquad y_2(0) \in 21.716013685^{8}_{5}, \qquad y_3(0) = 20, \qquad (7.1)$$

and (iii) the characteristic factors (Floquet multipliers) are

$$\lambda_1 = 1, \qquad \lambda_2 = 9.14122\cdots, \qquad \lambda_3 = 1.4052\cdots \times 10^{-13}. \qquad (7.2)$$

Consequently, this orbit possesses tangent planes of two-dimensional stable and unstable manifolds. This is also true for the other periodic solutions which have been verified by Kühn.

Figure 5 depicts the projection into the y_1-y_2 plane of an aperiodic solution y^* and its approximation $\tilde{\tilde{y}}$, both starting at a point y_0, close to y_p^* in Fig. 4. In Fig. 5, (A) the enclosed true solution y^* is demarcated symbolically by boxes and (B) the solid line represents a difference approximation $\tilde{\tilde{y}}$ which was determined by use of a classical Runge–Kutta method with a step size $h = h_0 := \frac{1}{128}$. As y^* and $\tilde{\tilde{y}}$ have (almost) reached the stationary point (0, 0, 0), they begin to separate for the remainder of the interval $[0, t_\infty]$ for which they have been determined. This can be explained by the

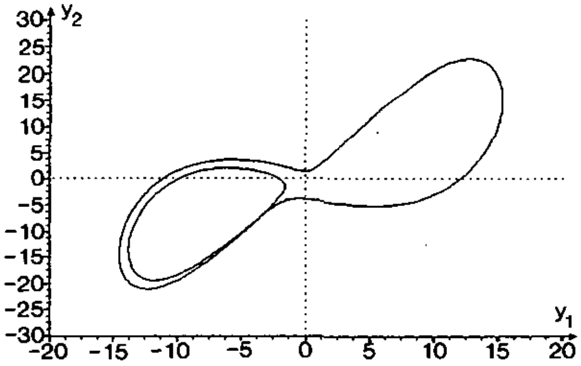

FIG. 4. Projection into y_1-y_2-plane of T-periodic orbit y_p^* (Lorenz equations).

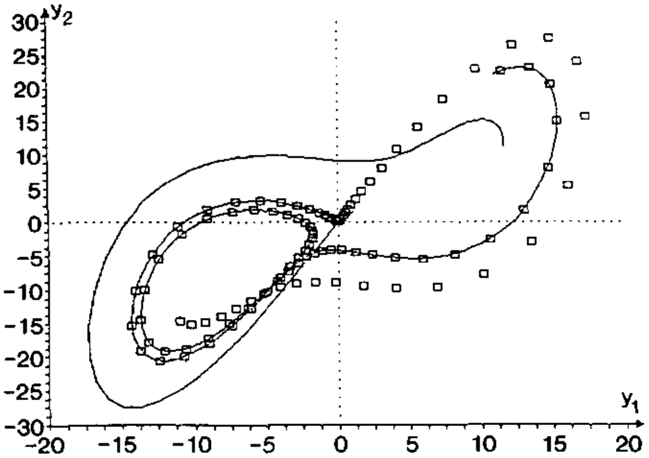

FIG. 5. Projection into y_1-y_2-plane of enclosure of true solution y^* (□ □ □ □) and diverting difference approximation $\tilde{\tilde{y}}$ (———) (Lorenz equations).

conjecture of a diversion of $\tilde{\tilde{y}}$ at the stable manifold of (0, 0, 0), taking place before coming close to this point (0, 0, 0). This diversion occurs presumably as $\tilde{\tilde{y}}$ penetrates the stable manifold in *one time step.* It is remarkable that y^* and $\tilde{\tilde{y}}$ coincide with much more than graphical accuracy for all $t \in [0, t_\infty]$ in the case of the choices $h = \frac{1}{256} < h_0$ *and* $h = \frac{1}{64} > h_0$. This unexpected non-monotonic dependency of $\| y^*(t) - \tilde{\tilde{y}}(t) \|_\infty$ on h is *unpredictable.*

For a starting vector y_0 close to the one in Fig. 4, Kühn found cases where y^* and $\tilde{\tilde{y}}$ are (α) practically coincident for $t \in [0, t_d] \subset [0, t_\infty]$, however, ($\beta$) their Euclidean distance $d = d(t)$ oscillates for $t > t_d$, reaching values comparable with the Euclidean distance of the stationary points C_1 and C_2. Property (β) can presumably be explained by a diversion of $\tilde{\tilde{y}}$, prior to $t \approx t_d$, followed by (i) a certain winding pattern of y^* about C_1 and C_2 and (ii) a corresponding pattern of $\tilde{\tilde{y}}$. The time t_d depends *unpredictably* on the employed numerical method: in the four investigated cases, t_d increased from 13.5 to 28 as the step size h of a classical Runge–Kutta method was reduced or as the value chosen for the precision ε of a Runge–Kutta method with control of h was lowered.

Remark. For a more detailed presentation of these results see [29, 2, 3].

On the basis of a Taylor-polynomial of (variable) order p, we have developed an explicit one-step method with a near-optimal control of h and p by means of the following conditions: (α) the moduli of each one of the three last terms of the polynomial are required to be smaller than an ε with, e.g., $\varepsilon = 10^{-30}$, and (β) the computational cost is to be as small as possible. The (uncontrolled) local rounding errors are characterized by the fixed double numerical precision, corresponding to 15 decimal mantissa digits of the employed HP-Workstation. In applications concerning (5.1),

(i) we chose y_0 on a Poincaré-map [16] defined by $y_2 - y_1 = 0$, then

(ii) we determined the first intersection, $\tilde{\tilde{y}}_{\text{int}}$, of $\tilde{\tilde{y}}$ with $y_2 - y_1 = 0$, and then

(iii) we returned $\tilde{\tilde{y}}$ from $\tilde{\tilde{y}}_{\text{int}}$ through replacing t by $-t$.

We observed cases where $\| \tilde{\tilde{y}} - y_0 \|_\infty$ reached a minimum less than 10^{-15} for the returning difference approximation $\tilde{\tilde{y}}$ and cases where this distance was large. The latter cases can presumably be explained by diversions of $\tilde{\tilde{y}}$. For a fixed choice of the initial vector and the time t_∞, the observed diversions were absent when a sufficiently extended number format was used. Here, too, the presence or absence of diversions is *unpredictable.*

W. Espe [13] has used a Runge–Kutta–Fehlberg method of order eight with control of h [5, 43] to approximate the periodic orbit y_p^* depicted in Fig. 4. He chose y_0 as the midpoint of the interval in (7.1). For λ_2 as given in (7.2), the difference $\lambda_2 - 1 > 0$ is relatively large, thus indicating a "strong instability." Consequently,

(a) after one revolution past y_p^*, Espe's approximation $\tilde{\tilde{y}}$ did not return to y_0 within graphical accuracy,

(b) a diversion must have occurred in the execution of the second revolution (here $\| y^*(t) - \tilde{\tilde{y}}(t) \|_\infty$ is smaller than in the case depicted in Fig. 5), and

(c) in the execution of the six revolutions depicted in Fig. 6, an aperiodic curve was generated which resembles those proclaimed to indicate "chaos" in the non-mathematical literature, see Fig. 7.

The details of the curve in Figs. 6 and 7 are as *unpredictable* as the strange attractor of the Lorenz equations [40].

The details of the aperiodic orbits computed by us or by W. Espe depend *unpredictably*, on the employed computer, compiler, number format, numerical method, and its artificial parameters.

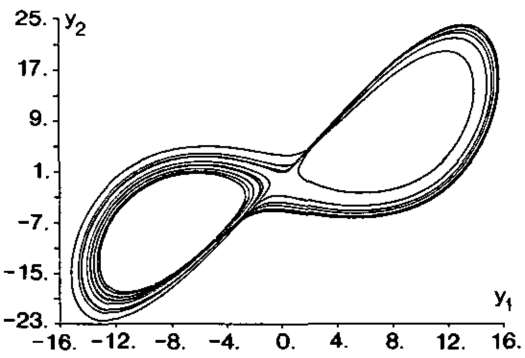

FIG. 6. Projection into y_1-y_2-plane of approximation $\tilde{\tilde{y}}$ of T-periodic orbit y_p^* (see Fig. 4) by use of a Runge–Kutta–Fehlberg method of order eight: the computed difference approximation diverts (Lorenz equations).

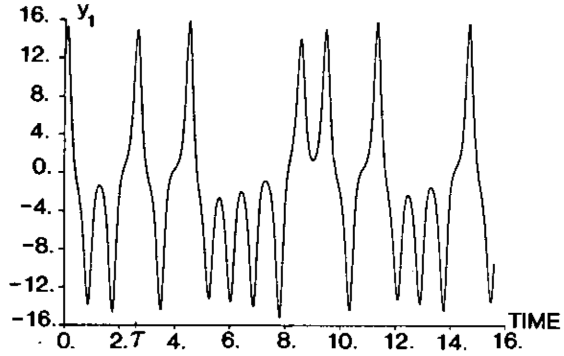

FIG. 7. $\tilde{\bar{y}}_1$ from Fig. 6 as a function of time t.

8. CONCLUDING REMARKS

For the restricted three body problem, the existence of diversions of computed difference approximations has been verified in Section 5, topographical properties favoring the occurrence of diversions are discussed at the end of Section 3, with a distinction of types (I) and (II) of "cause and effect." For the Lorenz equations and their topographically complicated strange attractor, in Section 7 the conjecture is offered that the cause of the observed diversions of type (II) is associated with the stable and the unstable manifolds of the origin. There are the following analogous situations:

(i) stable and unstable manifolds of periodic solutions of ODEs, such as the ones which have been verified by Kühn for the Lorenz equations, see Section 6, and

(ii) stable and unstable point sets of spurious constant difference solutions (stationary points) or spurious periodic difference solutions.

For the actual occurrence of diversions in these cases, examples are not known. In case (ii), a diversion would be caused by local rounding errors and, if present, procedural errors. The discussions at the end of Section 7 suggest that diversions may be caused by arbitrarily small (and even single) local numerical errors. This smallness may be achieved by the employment of difference methods with a sufficiently small choice of the step size h or a sufficiently large choice of the order p, provided the numerical precision is chosen accordingly; see examples at the end of Section 7.

Now, evolution problems with nonlinear PDEs are considered. Frequently in engineering or the sciences, a corresponding initial boundary value problem is replaced as follows by an approximating IVP:

(a) the dependency of the true solution on the spatially independent variables is suitably approximated, while

(b) the dependency on time t is retained from the PDEs.

Concerning (a) and (b), in particular, the following methods are customarily used:

(a1) a longitudinal method of lines (e.g., [49]), or

(a2) a method of finite elements (e.g., [4]), or

(a3) a spectral method (e.g., [8]), or

(a4) a Fourier expansion of the dependent variables in the case that the nonlinearities in the PDEs are confined to products of the dependent variables (e.g., [8]).

In each one of these cases, (a1)–(a4) and (b), an IVP is generated, with a system of nonlinear ODEs. A discretization of any such IVP may then lead to diverting difference approximations. In Section 7, this is shown for the Lorenz equations which, by means of (a4), have been derived from the nonlinear PDEs of fluid mechanics [34].

At numerous places in Sections 5 and 7, the observed diversions of difference approximations are characterized as "unpredictable." On first glance, this seems to be a contradiction to the well-known deterministic properties of both hardware and software of any computer. In contrast, the qualitative properties of sets of computed approximations are not known in advance. If they are unexpected, they are unpredictable. Usually it is expected that the distance between the (unknown) true solution y^* and the computed approximation $\tilde{\bar{y}}$ shrinks as either the step size h decreases or the order p increases. Concerning the (time of the) occurrence of a diversion, this expected pattern is not present in the case of discretizations of the Lorenz equations in Section 7.

This is not surprising because of the details of

(α) the cause of a potential diversion and

(β) the subsequent effect, i.e., the actualization of the diversion in a perturbation-sensitive neighborhood.

Concerning (α), it is sufficient to refer to the large number of individual computational operations involved in the execution of an individual time step of a difference method. The (vectorial) superposition of the results of these operations is *practically unpredictable.* Consequently, this is true for the local continuation of the approximation $\tilde{\bar{y}}$ from the execution of one time step to the next.

Concerning (β), it is observed that strange attractors are believed to consist almost everywhere of locally divergent sets of orbits, e.g., [19, 20].

The large number of practically unpredictable contributions suggests a random character of the computed approximations $\tilde{\bar{y}}$. In fact, Sparrow characterizes this situation as follows:

[40, p, 6]: "our approximate solution... to jump randomly from one of these orbits to another",

[40, p. v]: see the quotation at the end of Section 6;

[40, p. 208]: "'chaotic,' 'turbulent,' or 'pseudo random' behaviour which we associate with a 'strange attractor'."

Accordingly, Wedig [50] has carried out stochastic investigations of sets of computed approximations $\tilde{\tilde{y}}$ in strange attractors.

Concerning "chaotic structures" of sets of computed approximations $\tilde{\tilde{y}}$, the examples in Sections 5 and 7 suggest a superposition of the causes (A) and (B) which are introduced at the end of Section 3. *In the context of ODE-Chaos* (A) refers to the sensitive dependency on y_0 of the true solutions $y^* = y^*(t, y_0)$ of the ODEs. *In the context of computational chaos, cause* (B) refers to the influence of all kinds of local numerical errors in the computational determination of the approximations $\tilde{\tilde{y}}$. A knowledge of a set of approximations $\tilde{\tilde{y}}$ does not allow a distinction of the contributions from (A) and (B).

This leads to the following final conclusions:

(I) Concerning a quantitatively reliable information on individual true solutions y^* in a "chaotic set," enclosure methods are the only practically available approach, unless a first integral of the ODEs is known.

(II) An unknown but presumably large portion of the published results on "chaotic sets of solutions of ODEs" is more concerned with computational chaos than with ODE-chaos.

APPENDIX: DERIVATION OF (6.2)–(6.4)

By means of the transformation

$$X := e^{\sigma t} y_1, \qquad Y := e^{t} y_2, \qquad Z := e^{bt} y_3, \tag{A.1}$$

the Lorenz equations (5.1) can be represented as

$$X' = \sigma e^{(\sigma - 1)t} Y, \tag{A2}$$

$$Y' = e^{(1-\sigma)t}(r - e^{-bt}Z)X, \tag{A3}$$

$$Z' = e^{(b - \sigma - 1)t} XY. \tag{A4}$$

If $b = 2\sigma$, then $Z' = XX'/\sigma$; hence,

$$Z = X^2/2\sigma + c \qquad \text{with} \quad c \in \mathbb{R}. \tag{A5}$$

Then, from (A2) and (A3),

$$\begin{aligned} Y' &= (e^{(1-\sigma)t} X'/\sigma)' \\ &= e^{(1-\sigma)t} X \cdot (r - (e^{-bt}/2\sigma) X^2 - e^{-bt}c) \end{aligned} \tag{A6}$$

and, therefore,

$$X'' + (1 - \sigma) X' = \sigma X(r - (e^{-bt}/2\sigma) X^2 - e^{-bt}c). \tag{A7}$$

Going back to the original variables, (A5) yields (6.3) and (A7) yields (6.2). Since all employed transformations are free from any conditions, the systems (6.1) and (6.2)–(6.4) are equivalent, provided $b = 2\sigma$.

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