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Convergence and Stability in the Numerical Approximation of Dynamical Systems

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1 Outline

In this article we give an overview of the application of theories from dynamical systems to the analysis of numerical methods for initial-value problems. We start by describing the classical viewpoints of numerical analysis and of dynamical systems and then indicate how the two viewpoints can be merged to provide a framework for both the interpretation of data obtained from numerical simulations and the design of efficient numerical methods. This is done in Section 2.

In addressing the question of how to interpret data, we will show in Section 3 how the concept of convergence can be generalized to the numerical approximation of dynamical systems. The main theory is developed for one-step methods for ordinary differential equations and extensions to the study of multistep methods, adaptive time-stepping algorithms and partial differential equations are then outlined.

In addressing the question of designing efficient schemes we will show in Section 4 how the concept of stability can be generalized to dynamical systems. Stability theory is developed for both one-step and multistep methods for ordinary differential equations; extensions to adaptive time-stepping and to partial differential equations are also outlined.

A variety of surveys of this field already exist: see [13] for a complete study, see [9] for a discussion of convergence in the dynamical systems context, [12] for a discussion of stability in the dynamical systems context and see [5] for a discussion of both issues in relation to discretization of partial differential equations. Since these surveys contain fairly exhaustive bibliographies we refer to them for detailed references.

The impetus for the work described here is the fact that the classical convergence and stability theories do not apply to many dynamical systems of interest in science and engineering. Whilst the classical theories can be usefully developed at a very general level, new theories of convergence and stability are tied in a very strong way to particular classes of problems. This article concerns equations

arising from physical systems where an energy loss mechanism, or dissipation, is present. For a discussion of similar issues in the context of conservative physical systems see [6].

2 Background

The problem which we wish to solve is

$$\frac{du}{dt} = f(u), \quad u(0) = U. \quad (2.1)$$

Here $f : \mathbb{R}^p \rightarrow \mathbb{R}^p$ satisfies sufficient smoothness and structural assumptions to ensure the existence of a dynamical system on \mathbb{R}^p : that is, a unique solution $u(t) \in C^1([0, \infty), \mathbb{R}^p)$ of Equation 2.1 exists for all $U \in \mathbb{R}^p$. Thus we define the one-parameter semigroup $S(t) : \mathbb{R}^p \mapsto \mathbb{R}^p$ for each $t \in \mathbb{R}^+$ by

$$u(t) = S(t)U.$$

For one-step methods generating a sequence $\{U_n\}_{n=0}^N \approx \{u(n\Delta t)\}_{n=0}^N$ we define, for Δt sufficiently small, $S_{\Delta t}^1 : \mathbb{R}^p \mapsto \mathbb{R}^p$ to be the solution operator for one step of the numerical method. Thus

$$U_{n+1} = S_{\Delta t}^1 U_n, \quad U_0 = U. \quad (2.2)$$

We may then define $S_{\Delta t}^n : \mathbb{R}^p \mapsto \mathbb{R}^p$ by

$$U_n = S_{\Delta t}^n U := S_{\Delta t}^1 \circ \dots \circ S_{\Delta t}^1 U.$$

The primary objectives in solving Equation 2.1 numerically are:

1. to get quantitative and qualitative information about solutions to the equation; and
2. to obtain the information as quickly or cheaply as possible.

The concepts of *convergence* and *stability* have arisen in the theory of numerical analysis to enable these issues to be addressed. See [2,3] for example.

Classical convergence theory in numerical analysis is concerned with the following question. Fix $T > 0$ and $U \in B(0, R)$ and find the maximal real number r such that

$$\limsup_{n\Delta t=T, \Delta t \rightarrow 0} \frac{\|S(n\Delta t)U - S_{\Delta t}^n U\|}{\Delta t^r} \leq C, \quad (2.3)$$

for some constant $C = C(R, T)$. Typically $C \rightarrow \infty$ as $T \rightarrow \infty$. Thus a convergent scheme yields quantitative information about Equation 2.1 on time-intervals sufficiently small that $C\Delta t^r$ is small. Roughly speaking, the important concepts

required to analyse the convergence of numerical methods are those of *truncation error* and *well-posedness*.

Classical (practical) stability theory in numerical analysis is concerned with the following question. Fix $\Delta t > 0$ and $U \in \mathbb{R}^p$ and find conditions which ensure that

$$\lim_{n \rightarrow \infty} S_{\Delta t}^n U = 0, \tag{2.4}$$

for the problems:

$$f(u) = \lambda u, \quad \text{Re}(\lambda) < 0, \tag{2.5}$$

and

$$\exists \mu > 0 : \langle f(u) - f(v), u - v \rangle \leq -\mu \|u - v\|^2, \quad \forall u, v. \tag{2.6}$$

Note that, for Equation 2.6 we may assume without loss of generality that 0 is the unique equilibrium point. A non-autonomous version of Equation 2.5 is also important, namely:

$$f(u) = \lambda(t)u, \quad \text{Re}(\lambda(t)) \leq -\mu < 0 \quad \forall t > 0. \tag{2.7}$$

(Note that, for this class of problems a semigroup does not exist since the equation is not time-translation invariant). For all the problems Equations 2.5–2.7, the true solution converges exponentially to a unique equilibrium point which, without loss of generality, we may assume to be 0. Useful concepts in addressing stability for Equations 2.5–2.7 are *A-stability* (for Equation 2.5 and both Runge-Kutta methods (RKM) and linear multistep methods (LMM)), *AN-stability* (for Equation 2.7 and both Runge-Kutta and multistep methods), *B-stability* (for Runge-Kutta methods applied to Equation 2.6) and *G-stability* (for multistep methods applied to Equation 2.6). See [1,3] for example. These stability theories categorize methods which preserve property Equation 2.4 for all values of $\Delta t > 0$ and all initial data U . It is interesting to note that, roughly speaking, *AN-* and *B-*stability are equivalent for Runge-Kutta methods and that *A-* and *G-*stability are equivalent for multistep methods. Thus, intuition from linear problems is useful in the understanding of nonlinear problems. However, Equations 2.5–2.7 all have the same, essentially trivial, asymptotic behaviour. Nonetheless, the attendant stability concepts developed for them will turn out to be invaluable in many of the more recent stability theories for numerical approximation of dynamical systems with decidedly nontrivial asymptotic behaviour.

In the theory of dynamical systems, interest is focussed on the limit $t \rightarrow \infty$ and on the evolution of sets of initial data. Useful concepts include:

1. Invariant sets I :

$$S(t)I \equiv I \quad \forall t \geq 0.$$

2. Positively invariant sets I :

$$S(t)I \subseteq I \quad \forall t \geq 0.$$

3. ω -limit sets ω : for points $U \in \mathbb{R}^p$,

$$\omega(U) = \{x | \exists t_i \rightarrow \infty : S(t_i)U \rightarrow x\},$$

or, for sets $B \in \mathbb{R}^p$,

$$\omega(B) = \{x | \exists y_i \in B, t_i \rightarrow \infty : S(t_i)y_i \rightarrow x\}.$$

Here $t_i \in \mathbb{R}^+$ for Equation 2.1 or $t_i \in \mathbb{Z}^+$ for Equation 2.2 (with $S(n) = S_{\Delta t}^n$).

4. Basin of attraction \mathcal{B} of I :

$$\mathcal{B} = \{y | \omega(y) \subseteq I\}.$$

5. Attractor \mathcal{A} : a compact invariant set \mathcal{A} whose basin of attraction contains an open neighbourhood of \mathcal{A} itself.
6. Global attractor: an attractor \mathcal{A} for which every bounded set B is in its basin of attraction. Thus for all bounded $B \subset \mathbb{R}^p$:

$$\text{dist}(S(t)B, \mathcal{A}) \rightarrow 0 \quad \text{as } t \rightarrow \infty.$$

Here

$$\text{dist}(A, B) < \epsilon \Leftrightarrow \bar{A} \subseteq \mathcal{N}(\bar{B}, \epsilon),$$

so that

$$\text{dist}(A, B) = 0 \Leftrightarrow \bar{A} \subseteq \bar{B}.$$

To illustrate these concepts we consider some examples. Figure 1 shows the solution of the scalar equation

$$\frac{du}{dt} = u - u^3, \quad u(0) = 10.$$

It is clear that $u \rightarrow 1$ as $t \rightarrow \infty$ and hence that $\omega(10) = 1$. Thus the ω -limit set is the point $u = 1$, representing a steady state.

Figure 2 shows the solution of the pair of coupled equations

$$\begin{aligned} \frac{dx}{dt} &= x + y - x(x^2 + y^2), & x(0) &= 3, \\ \frac{dy}{dt} &= -x + y - y(x^2 + y^2), & y(0) &= -3. \end{aligned}$$

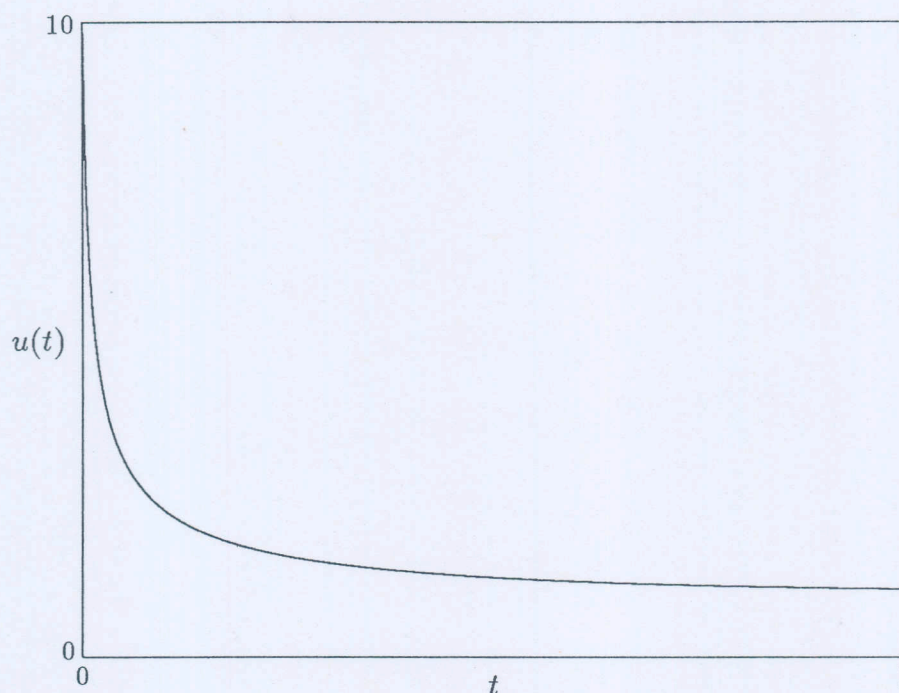


Figure 1. Approach to equilibrium point

In Figure 2 (c) we define $R(t)^2 = x(t)^2 + y(t)^2$. Clearly the solution converges to a limit cycle as $t \rightarrow \infty$. Thus the omega limit set in this case is the set $\{(x, y) : x^2 + y^2 = 1\}$, representing a periodic solution.

To illustrate a more complicated limit set, consider Equation 2.1 in \mathbb{R}^p , $p > 2$, with solution $u(t) = (u_1(t), \dots, u_p(t))^T$. Assume that the first two solution components satisfy

$$u_1(t) = e^{-t} + \sin(t), \quad u_2(t) = e^{-t} + \cos(at),$$

and that the remaining solution components approach 0 as $t \rightarrow \infty$. Then, if a is irrational, as $t \rightarrow \infty$ the limiting solution is known as a *quasi-periodic solution*. Figure 3 (a) illustrates this type of behaviour in the case $a = 10\pi/31$; the notation $x(t) = u_1(t)$, $y(t) = u_2(t)$ is used. The omega limit set here is the set

$$\{u = (u_1, \dots, u_p) \in \mathbb{R}^p : -1 \leq u_i \leq 1, i = 1, 2 \text{ and } u_i = 0, i \geq 2\}.$$

In Figure 3 (b) a similar phenomenon is illustrated: the function $u(t) = e^{-t} + \sin(t) + \cos(\delta t)$ is shown with $\delta = \sqrt{2}$.

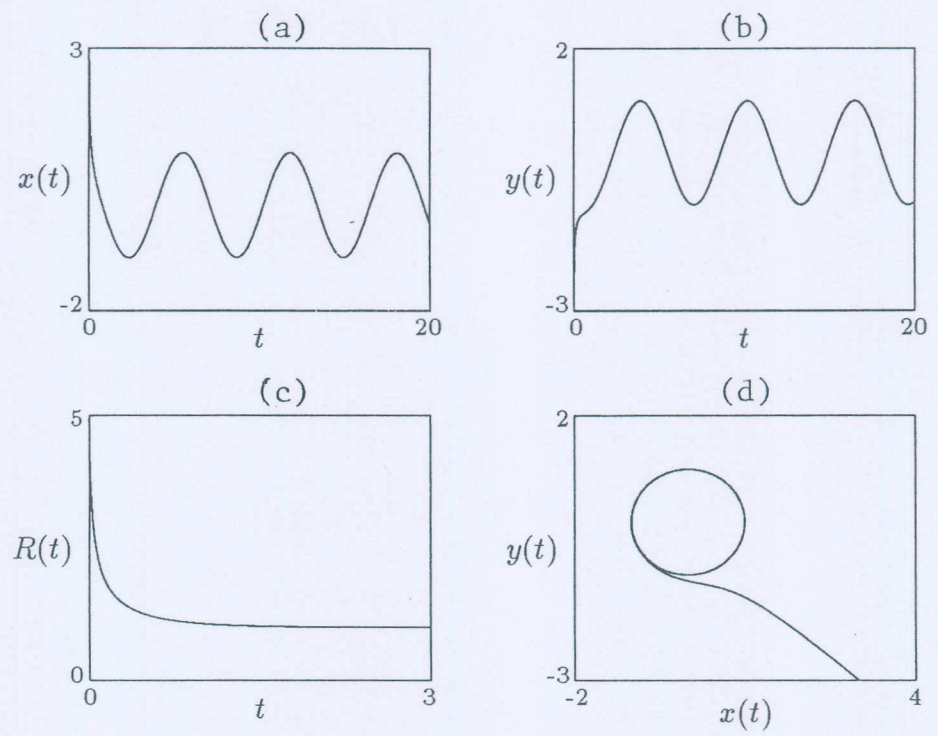


Figure 2. Periodic solution

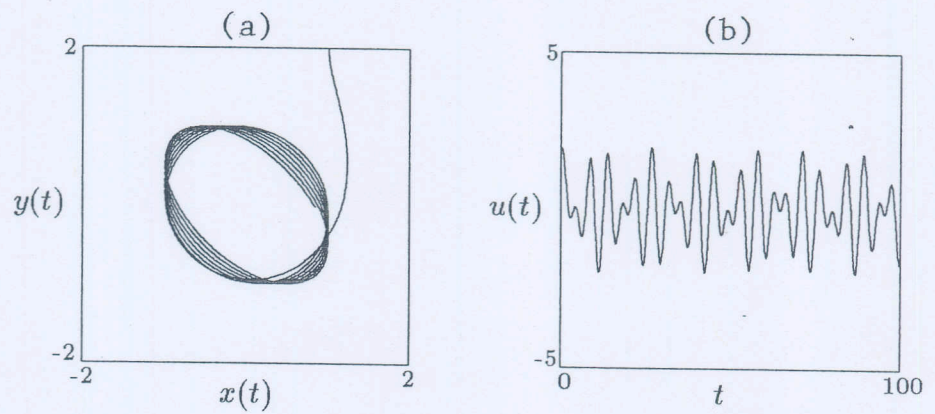


Figure 3. Quasi-periodic behaviour

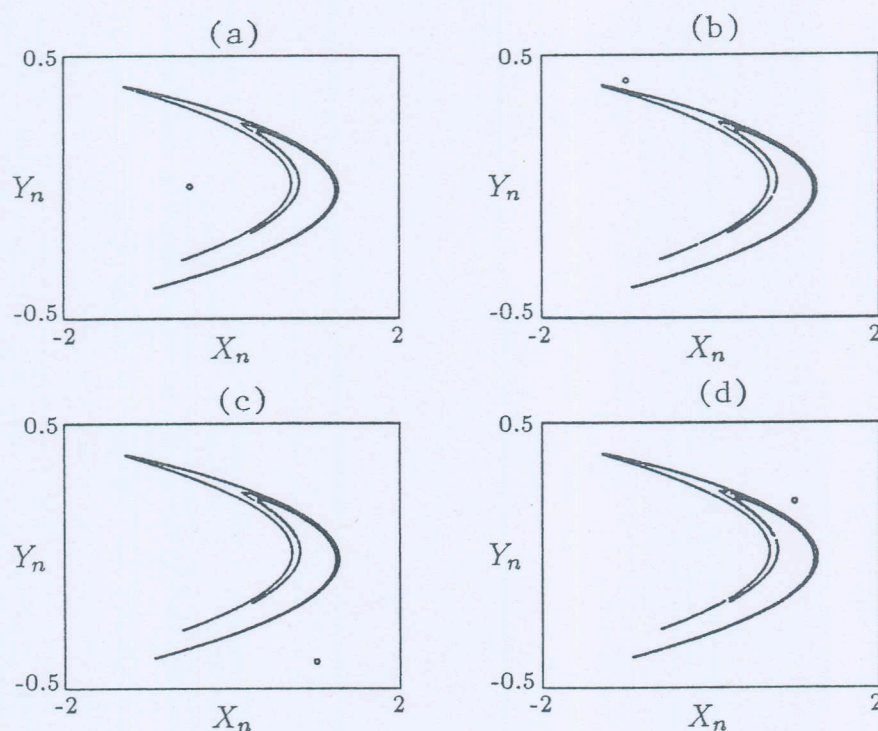


Figure 4. Strange attractor of modified Hénon map. Note that o marks the initial value, (X_0, Y_0)

Figure 4 shows an omega limit set for the modified Hénon map

$$\begin{aligned} X_{n+1} &= 1 + Y_{n+1} - \frac{7}{5}X_n^2, \\ Y_{n+1} &= \frac{3}{10}X_n. \end{aligned}$$

To produce this figure, four different starting points are chosen (marked with circles) and the map iterated. The transients are not shown so that what remains represents the omega-limit set. The important point illustrated by this figure is that the omega-limit set has a very complicated structure which is the same for all four initial conditions. This is an example of a *strange attractor*.

Strange attractors are also found in differential equations. Figure 5 shows various plots of the strange attractor for the *Lorenz equations*

$$\begin{aligned} \frac{dx}{dt} &= 10(y - x), \\ \frac{dy}{dt} &= 28x - y - xz, \\ \frac{dz}{dt} &= xy - 8z/3. \end{aligned}$$

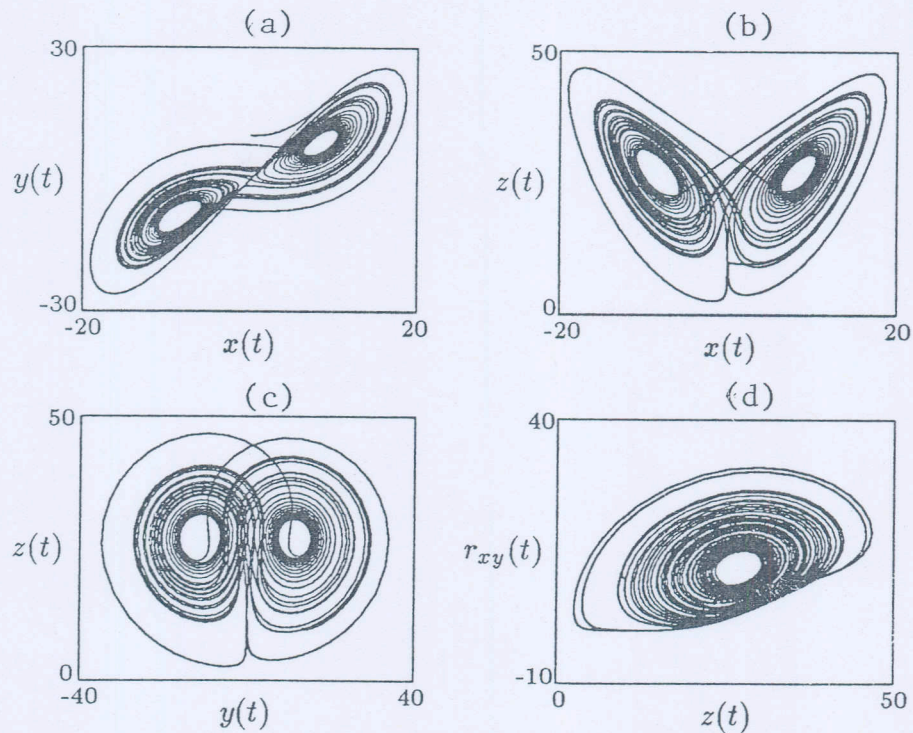


Figure 5. Lorenz attractor

In Figure 5 (d) we have defined $r_{xy}(t)^2 = x^2(t) + y^2(t)$. For these equations the attractor is in fact a global attractor. It is contained inside an ellipsoid which is a positively invariant set for the semigroup and which $S(t)U$ enters at some time $t = T(U)$ for every $U \in \mathbb{R}^p$.

The Figures 1–5 illustrate the wealth of dynamical behaviour that is present in differential equations and mappings when studied over long time intervals. It is clearly desirable that any theory of numerical analysis should encompass this variety. Classical numerical analysis however is somewhat defective in this regard. The focus is on *individual solutions* — $S(t)$ is applied to a single initial data point U . Convergence on finite time intervals is studied and stability theory is developed for problems with trivial asymptotic behaviour — exponential convergence to a unique equilibrium point. In contrast, dynamical systems is focussed on *families* of solutions: $S(t)$ is applied to sets B of initial data points. Much of the interest is in infinite time intervals and non-trivial omega limit sets (as seen in Figures 1–5.) Note that, in many applications of interest, the exact initial condition is not known in practice. In such a situation it is natural to study all possible limit sets and their basins of attraction.

Whilst the classical theories of convergence and stability have been invaluable in the development of accurate and efficient algorithms for initial-value problems, they are far from being the last word in the subject. As an example, consider again the Lorenz equations. These equations have interesting long-time dynamics

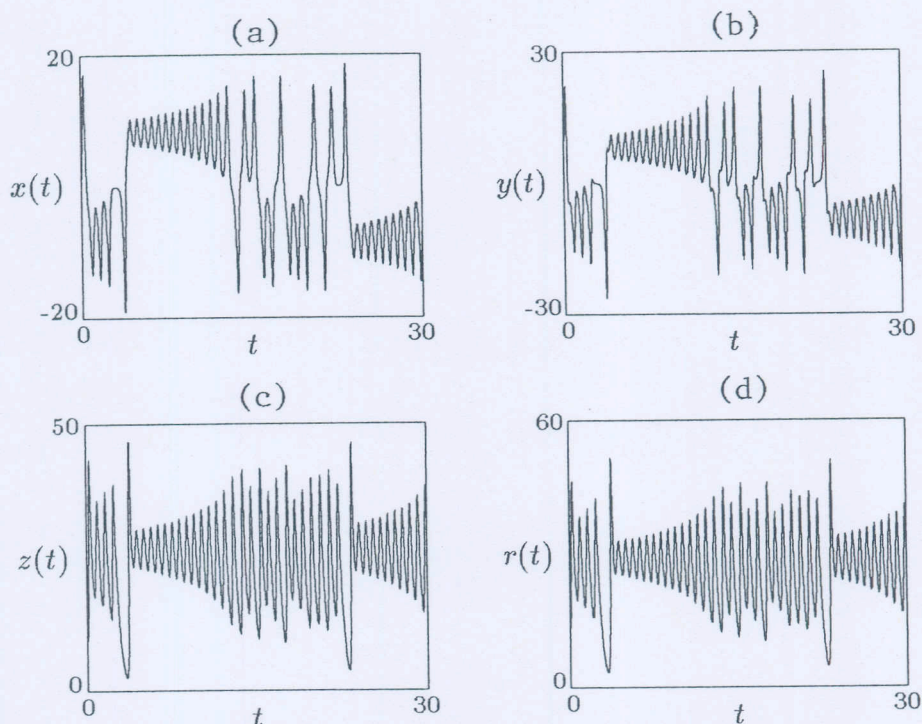


Figure 6. "Unpredictable" nature of the Lorenz equations

(see Figures 5 and 6; in Figure 6 (d) we have defined $r(t)^2 = x(t)^2 + y(t)^2 + z(t)^2$) and, to fully investigate this phenomenon, it is necessary to integrate the equations past the time at which the classical error bound Equation 2.3 is small. (Improved approximate error estimates can be obtained by estimating the constant multiplying Δt^n numerically, rather than majorizing it by an exponential, but nonetheless, the fact remains that for any given Δt there is a time after which the error in the approximation of an individual trajectory will be $\mathcal{O}(1)$). Furthermore, the equations do not satisfy Equation 2.6 and so the stability theories alluded to are of no direct use here — this is manifest in the fact that the asymptotic behaviour is far from trivial.

In this paper we outline some of the theories which help in the design and analysis of appropriate algorithms for equations with complicated long-time dynamics. For instance, the Lorenz equations have unstable periodic solutions and hyperbolic equilibria with stable and unstable manifolds; we will quote theories which show that these periodic solutions persist as unstable invariant curves in any convergent one-step numerical method and that similar results hold for the stable and unstable manifolds. The Lorenz equations have a strange (global) attractor \mathcal{A} ; we quote a theory which indicates that any convergent numerical method also has a local attractor $\mathcal{A}_{\Delta t}$ and that $\text{dist}(\mathcal{A}_{\Delta t}, \mathcal{A}) \rightarrow 0$ as $\Delta t \rightarrow 0$.

Finally we will quote stability theories showing that, for certain particular Runge-Kutta and multistep methods, the numerical attractor is actually a global attractor as for the differential equation.

Taking this discussion of the Lorenz equation as prototypical, we now outline how the theories of convergence and stability might be usefully generalized to dynamical systems.

Note that a solution $\{S(t)U\}_{t \geq 0}$ of Equation 2.1 is a positively invariant set. Thus standard convergence of trajectories corresponds to studying the existence and closeness of a nearby positively invariant set (a single trajectory) for $S_{\Delta t}^n$ as $\Delta t \rightarrow 0$. This suggests that, in the context of dynamical systems, convergence should correspond to studying the existence of nearby (positively) invariant sets of $S_{\Delta t}^n$ as $\Delta t \rightarrow 0$ given the existence of an invariant set for $S(t)$. We pursue this approach in Section 3. (Actually more than this is shown when standard convergence of trajectories is considered, namely that the dynamics on the sets agree; in general it is not possible to extend such results to more complicated invariant sets. For example, phase error prevents this for periodic solutions).

For the problems Equations 2.5–2.7, the global attractor is the origin 0 (without loss of generality). Thus 0 has basin of attraction \mathbb{R}^p . Stability is concerned with finding conditions under which the basin of attraction is preserved for all $\Delta t > 0$, or for Δt independent of stiffness. This suggests that, in the context of dynamical systems, stability might usefully be defined to encompass the study of preservation of basins of attraction of (positively) invariant sets of $S(t)$ under discretization, for all $\Delta t > 0$, or for Δt independent of initial data and/or stiffness. This approach to numerical stability is pursued in Section 4.

3 Convergence

We will make the following basic assumption for all the one-step methods considered in this paper: given any bounded $B \subset \mathbb{R}^p$, there is $\Delta t_c = \Delta t_c(B)$ and $K = K(B)$ such that, for all $(\Delta t, U, V) \in [0, \Delta t_c) \times B \times B$,

$$\begin{aligned} \|S(\Delta t)U - S_{\Delta t}^1 U\| &\leq K(B)\Delta t^{r+1}, \\ \|D_U[S(\Delta t)U - S_{\Delta t}^1 U]\| &\leq K(B)\Delta t^{r+1}, \\ \|S_{\Delta t}^1 U - S_{\Delta t}^1 V\| &\leq [1 + K(B)\Delta t]\|U - V\|, \\ \|D_U[S_{\Delta t}^1 U] - D_V[S_{\Delta t}^1 V]\| &\leq K(B)\Delta t\|U - V\|. \end{aligned}$$

Here D_U denotes the derivative (Jacobian) with respect to U . If this assumption holds we will say that $S(\Delta t)$ and $S_{\Delta t}^1$ are C^1 -close. All Runge-Kutta methods, for example, satisfy this assumption under sufficient smoothness on f .

Using this it is straightforward to prove the following result:

Result 1. There are constants $C_i = C_i(B), i = 1, \dots, 4$ such that, for all $U \in B$ and $\Delta t \in [0, \Delta t_c)$ with $n\Delta t = T$

$$\begin{aligned} \|S(T)U - S_{\Delta t}^n U\| &\leq C_1 e^{C_2 T} \Delta t^r, \\ \|D_U[S(T)U - S_{\Delta t}^n U]\| &\leq C_3 e^{C_4 T} \Delta t^r. \end{aligned}$$

□

Clearly such a result is of no direct use in the dynamical systems context where long time-intervals are considered. Thus we consider instead the effect of numerical approximation on invariant sets. The unifying feature of the convergence theory we describe is that the existence theory for both the invariant sets of Equation 2.1 and of Equation 2.2 is formulated in the same way. To achieve this we need to consider solutions of Equation 2.1 as iterates of a map over a time interval of length Δt .

3.1 The ODE as a map

Near an equilibrium point ($u = 0$ without loss of generality) we may write:

$$\frac{du}{dt} = f(u) := -Au + g(u), \quad u(0) = U.$$

Here $A := D_u f(u)|_{u=0}$ and $g(u)$ is $\mathcal{O}(\|u\|^2)$ as $\|u\| \rightarrow 0$. Then we have the *variation of constants formula*

$$u(t) = e^{-At}U + \int_0^t e^{-A(t-\tau)}g(S(\tau)U)d\tau.$$

If $u_n = u(n\Delta t)$ then

$$u_{n+1} = S(\Delta t)u_n := Lu_n + N(u_n), \tag{3.1}$$

where

$$L = e^{-A\Delta t} \quad \text{and} \quad N(\bullet) = \int_0^{\Delta t} e^{-A(\Delta t-\tau)}g(S(\tau)\bullet)d\tau.$$

We now introduce $N_{\Delta t}(\bullet) : \mathbb{R}^p \mapsto \mathbb{R}^p$ so that the numerical method may be written

$$U_{n+1} = S_{\Delta t}^1 U_n := LU_n + N_{\Delta t}(U_n). \tag{3.2}$$

By C^1 -closeness of $S(\Delta t)$ and $S_{\Delta t}^1$ we have

$$\|N(\bullet) - N_{\Delta t}(\bullet)\|_{C^1} = \mathcal{O}(\Delta t^{r+1}).$$

Hence any results proving the existence of an invariant set for Equation 3.1 (and hence for Equation 2.1) which relies on the smallness of $N(u)$ and $D_u N(u)$ relative to properties of L can also be translated into results for Equation 3.2. (A separate argument is needed to show that the invariant sets of the mapping Equation 3.1 are also invariant under Equation 2.1.) In this manner equilibria, local phase portraits near equilibria and local unstable and stable manifolds of equilibria can all be shown to persist, under numerical approximations satisfying our basic assumptions, provided the equilibrium point is hyperbolic. Similar ideas work in the vicinity of periodic solutions and quasi-periodic solutions. We now outline the general framework in which all these objects may be studied.

3.2 Hyperbolic invariant sets

In this subsection we study equilibria, stable and unstable manifolds, local phase portraits, periodic solutions and quasi-periodic solutions all of which we denote by \mathcal{M} . We will make suitable hyperbolicity assumptions but do not detail these here: see [9] or [12] for details. Roughly speaking it is these conditions which place us in the realm of problems where an energy loss mechanism is present and outside that of the conservative physical systems treated in [6]. In all these cases \mathcal{M} can be constructed as a fixed point of a contraction mapping \mathcal{T} :

$$\mathcal{M}^{k+1} = \mathcal{T}\mathcal{M}^k,$$

in an appropriate closed subset X of a Banach space B . For equilibria the Banach space is the set of points in \mathbb{R}^p ; for unstable and stable manifolds B is a set of Lipschitz graphs $C(P\mathbb{R}^p, (I - P)\mathbb{R}^p)$ where P is an appropriate projection; for construction of the phase portrait B is a set of sequences in \mathbb{R}^p .

The mapping \mathcal{T} is constructed from the mapping Equation 3.1. The derivation of \mathcal{T} from Equation 3.1 is different for each of the invariant sets under consideration and will not be elaborated here. The abstract formulation is chosen to show a unifying framework for the analysis. Given \mathcal{T} we may construct a mapping $\mathcal{T}_{\Delta t}$ by following, for each of the invariant sets mentioned, the derivation of \mathcal{T} but using Equation 3.2 instead of Equation 3.1. This leads to the mapping

$$\mathcal{M}_{\Delta t}^{k+1} = \mathcal{T}_{\Delta t}\mathcal{M}_{\Delta t}^k.$$

For all the invariant sets described two important facts follow from C^1 -closeness, namely

$$\sup_{\Phi \in X} \|\mathcal{T}\Phi - \mathcal{T}_{\Delta t}\Phi\|_B = \mathcal{O}(\Delta t^{r+1}), \quad (3.3)$$

$$\text{Lip}\{\mathcal{T}_{\Delta t}\} = \text{Lip}\{\mathcal{T}\} + \mathcal{O}(\Delta t^{r+1}); \quad (3.4)$$

thus \mathcal{T} is $\mathcal{O}(\Delta t^{r+1})$ close to $\mathcal{T}_{\Delta t}$ as an operator from X into X and the Lipschitz constants are similarly close. The following type of result may be proved using this fact:

Result 2. Consider all the invariant sets of Equation 3.1, and hence Equation 2.1, mentioned at the start of this subsection. Under suitable hyperbolicity assumptions on them there exists $\mathcal{M}_{\Delta t}$, invariant for Equation 3.2 and hence Equation 2.2, satisfying

$$\|\mathcal{M}_{\Delta t} - \mathcal{M}\|_B = \mathcal{O}(\Delta t^r).$$

□

Sketch Proof Existence is proved as follows: \mathcal{T} is set up to be a contraction and, because it is constructed from Equation 3.1, it follows that \mathcal{T} approaches the identity as $\Delta t \rightarrow 0$. This is because $L \equiv I$ and $N \equiv 0$ if $\Delta t = 0$. Hence it turns out that

$$\text{Lip}\{\mathcal{T}\} = \lambda = 1 - C\Delta t < 1.$$

By Equation 3.4 we have

$$\text{Lip}\{\mathcal{T}_{\Delta t}\} = \text{Lip}\{\mathcal{T}\} + \mathcal{O}(\Delta t^{r+1}) \leq \lambda_{\Delta t} = 1 - \frac{C\Delta t}{2} < 1,$$

for Δt sufficiently small. Thus by Equation 3.3 we have

$$\begin{aligned} \|\mathcal{M} - \mathcal{M}_{\Delta t}\|_B &= \|\mathcal{T}\mathcal{M} - \mathcal{T}_{\Delta t}\mathcal{M}_{\Delta t}\|_B, \\ &\leq \|\mathcal{T}\mathcal{M} - \mathcal{T}_{\Delta t}\mathcal{M}\|_B + \|\mathcal{T}_{\Delta t}\mathcal{M} - \mathcal{T}_{\Delta t}\mathcal{M}_{\Delta t}\|_B, \\ &\leq K\Delta t^{r+1} + \lambda_{\Delta t}\|\mathcal{M} - \mathcal{M}_{\Delta t}\|_B, \\ &\Rightarrow \|\mathcal{M} - \mathcal{M}_{\Delta t}\|_B \leq \frac{2K\Delta t^r}{C}. \end{aligned}$$

□

Thus we have outlined a very general approach to proving convergence of hyperbolic invariant sets. The general technique shown in the proof is known as the *uniform contraction principle*. See [9] and Chapter 6 of [13], for detailed references to the use of this idea in the context of numerical analysis and dynamical systems. The central individual in the development of the approach outlined is W.-J. Beyn.

3.3 Non-hyperbolic invariant sets: Attractors

For non-hyperbolic objects results as strong as those just quoted for hyperbolic objects do not hold in general. Nonetheless, for attractors it is still possible to say something about the effect of numerical approximation. To illustrate this, consider the *Rossler equations*

$$(3.3) \quad \frac{dx}{dt} = -y - z, \quad x(0) = X,$$

$$(3.4) \quad \frac{dy}{dt} = x + y/5, \quad y(0) = Y,$$

$$\frac{dz}{dt} = 1/5 + z(x - 5), \quad z(0) = Z.$$

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Figure 7 shows numerically computed attractors for this system with initial data $(X, Y, Z) = (-8.0578, 0.6288, 0.0154)$. This point is chosen to be close to the attractor so that transients are not present; the numerical attractors are thus computed simply by running the numerical method from this point over a long time interval and plotting a projection onto the $x - y$ plane. The step size is $\Delta t = 0.00005$ in (a) and is halved successively for each subsequent figure. It is clear that some form of convergence of the attractor is occurring as Δt is refined.

Nonetheless, the trajectories calculated in each figure are not close. This is illustrated in Figure 8 where the solution leading to Figure 7 (d) is taken as "exact" and the errors in trajectories from Figures 7 (a) - (c) calculated. Note that the errors are $\mathcal{O}(1)$ by the end of the interval. Thus Figures 7 and 8 indicate that there is something more to interpreting data from numerical simulations of chaotic systems than simply asking that trajectories remain close. We now try to make this precise.

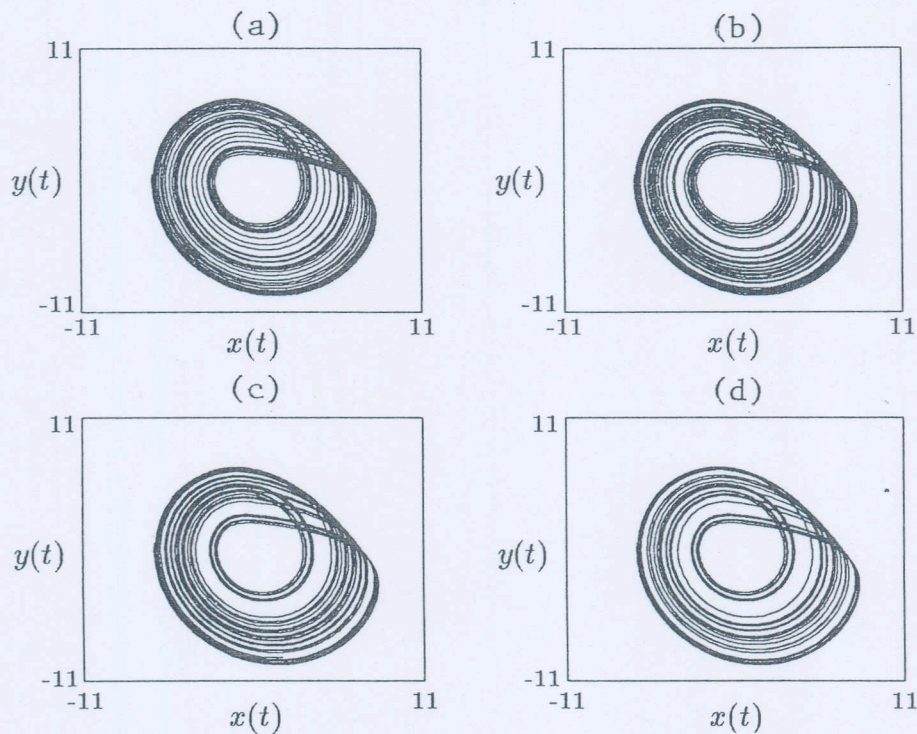


Figure 7. The Rossler attractor with four different Δt

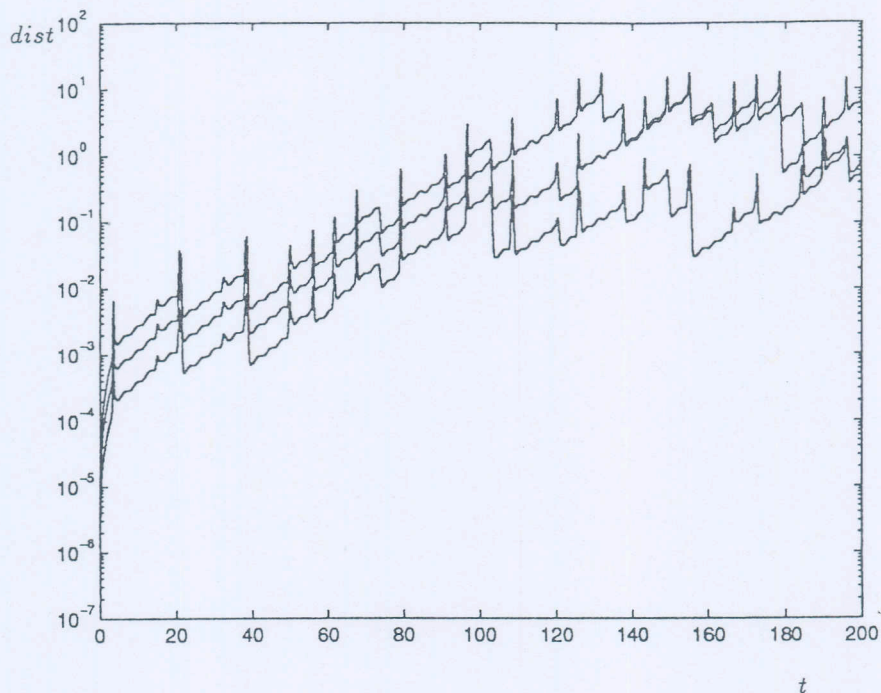


Figure 8. Errors in trajectories for the Rossler system

Result 3. Let Equation 2.1 have an attractor \mathcal{A} . For any ϵ there is $\Delta t_c(\epsilon)$ such that Equation 2.2 has an attractor $\mathcal{A}_{\Delta t}$ and

$$\mathcal{A}_{\Delta t} \subseteq \mathcal{N}(\mathcal{A}, \epsilon) \quad \forall \Delta t \leq \Delta t_c.$$

Thus

$$\text{dist}(\mathcal{A}_{\Delta t}, \mathcal{A}) \rightarrow 0 \quad \text{as} \quad \Delta t \rightarrow 0.$$

□

This shows that every computed point on the numerical attractor is close to a point on the true attractor, for Δt sufficiently small. However \mathcal{A} is not contained in $\mathcal{N}(\mathcal{A}_{\Delta t}, \epsilon)$ in general — it is necessary to make further assumptions about the dynamics on \mathcal{A} to obtain this implication. The most general of these is contained in the following result, where $W^u(\bullet)$ denotes the unstable manifold of an equilibrium point.

Result 4. Let Equation 2.1 have an attractor \mathcal{A} and assume that

$$\mathcal{A} = Cl\left\{\bigcup_{v \in \mathcal{E}} W^u(v)\right\},$$

where \mathcal{E} is a set of hyperbolic equilibria. For any ϵ there is $\Delta t_c(\epsilon)$ such that Equation 2.2 has an attractor $\mathcal{A}_{\Delta t}$ and

$$\mathcal{A} \subseteq \mathcal{N}(\mathcal{A}_{\Delta t}, \epsilon) \quad \forall \Delta t \leq \Delta t_c.$$

Thus

$$\text{dist}(\mathcal{A}, \mathcal{A}_{\Delta t}) \rightarrow 0 \quad \text{as} \quad \Delta t \rightarrow 0.$$

See [9] and Chapter 7 of [13] for further elaboration of these results and for a complete bibliography. The study of attractors under numerical perturbation has been led by P.E. Kloeden and J. Lorenz and by J.K. Hale and co-worker. Important further developments along the lines of Result 4 have been made by A.R. Humphries and I. Kostin.

3.4 Multistep methods as one-step methods

Multistep methods generate a dynamical system on \mathbb{R}^{kp} where k is the number of steps of the method. One way of doing this is as follows: define

$$\tilde{U}_n = (U_n^T, \dots, U_{n+k-1}^T)^T.$$

Then, for Δt sufficiently small, we may define $\tilde{S}_{\Delta t}^1 : \mathbb{R}^{kp} \mapsto \mathbb{R}^{kp}$ by

$$\tilde{U}_{n+1} = \tilde{S}_{\Delta t}^1 \tilde{U}_n, \quad \tilde{U}_0 = \tilde{U}. \quad (3.5)$$

Composing this map over several steps yields

$$\tilde{U}_n = \tilde{S}_{\Delta t}^n \tilde{U} := \tilde{S}_{\Delta t}^1 \circ \dots \circ \tilde{S}_{\Delta t}^1 \tilde{U}.$$

To apply the ideas we have developed for one-step methods we need to extract a map on \mathbb{R}^p . For *strictly stable* multistep methods this can be done, using invariant manifold theory.

We illustrate this by considering the second order backward differentiation formula (BDF):

$$U_{n+2} - \frac{4}{3}U_{n+1} + \frac{1}{3}U_n = \frac{2\Delta t f(U_{n+2})}{3}.$$

We can write this as a one-step method as just described. However, an alternative choice of variables for the one-step formulation is particularly helpful here: we introduce the new variables W_n and V_n by

$$\frac{2}{3}W_n = U_{n+1} - \frac{1}{3}U_n, \quad V_n = U_{n+1} - U_n.$$

Then a short calculation reveals that

$$\left. \begin{aligned} V_{n+1} &= \frac{1}{3}V_n + \frac{2}{3}\Delta t f(W_{n+1} - \frac{1}{2}V_{n+1}) \\ W_{n+1} &= W_n + \Delta t f(W_{n+1} - \frac{1}{2}V_{n+1}). \end{aligned} \right\}$$

The existence of an exponentially attractive invariant manifold, which is representable as a graph $h : \mathbb{R}^p \mapsto \mathbb{R}^p$ on which $v = \Delta t h(w)$, may be proved. To be precise, if f is sufficiently smooth and with compact support then there is a function $h : \mathbb{R}^p \mapsto \mathbb{R}^p$ such that

$$V_{n+1} = \Delta t h(W_{n+1}) \Leftrightarrow V_n = \Delta t h(W_n),$$

$$\|V_n - \Delta t h(W_n)\| \leq C(V_0, W_0)(1/6)^n.$$

On the manifold we have

$$W_{n+1} = W_n + \Delta t f(W_{n+1} - \frac{\Delta t}{2} h(W_{n+1}))$$

and so we have defined a one-step method on \mathbb{R}^p , namely:

$$W_{n+1} = S_{\Delta t}^1 W_n.$$

The map $S_{\Delta t}^1$ on \mathbb{R}^p is C^1 close to $S(\Delta t)$. Hence the foregoing one-step theories can be applied to the multistep method. (Note that, provided we are considering compact invariant sets, smooth modification of f outside a bounded set can always be made to yield a function with compact support; in this way the invariant manifold ideas can be used).

The ideas we have outlined were first introduced by U. Kirchgraber. They may be generalized to all strictly stable multistep methods and to an appropriate class of general linear methods. See Chapter 4 of [13] for further details and for references to the literature.

3.5 Sectorial evolution equations

We now indicate how the foregoing theories can be adapted to partial differential equations. We consider the equation

$$\frac{du}{dt} + Au = F(u), \quad u(0) = U,$$

where A is a *sectorial operator* in a Hilbert space H — the precise definition is given in [10] as are many references to appropriate literature. For the purposes of this survey it is sufficient to think of the example where A is $-\Delta$ with Dirichlet boundary conditions so that $D(A) = H^2(\Omega) \cap H_0^1(\Omega)$. We equip H with the inner-product $\langle \bullet, \bullet \rangle$ and induced norm $|\bullet|$. If we assume, for some $\gamma \in (0, 1)$,

$$|F(u) - F(v)| \leq K(R)|A^\gamma(u - v)| \quad \forall u, v \in B_{A^\gamma}(0, R),$$

then local existence and uniqueness follow for $U \in D(A^\gamma)$. For our illustrative example of A we have $D(A^{1/2}) = H_0^1(\Omega)$.

A dissipativity condition, such as

$$-|A^{1/2}u|^2 + \langle F(u), u \rangle \leq \alpha^2 - \beta^2|u|^2, \tag{3.6}$$

will ensure global existence. In this case we define the semigroup $S(t) : D(A^\gamma) \mapsto D(A^\gamma)$ so that

$$u(t) = S(t)U,$$

and consider perturbations to the problem (numerical or otherwise) yielding an approximate semigroup $S^h(t) : D(A^\gamma) \mapsto D(A^\gamma)$. If the discretization is in space only then $t \in \mathbb{R}^+$ whilst if the discretization is in time alone or in space and time then $t \in \Delta t \mathbb{Z}^+$. We let \mathcal{S} denote \mathbb{R}^+ or $\Delta t \mathbb{Z}^+$ as appropriate.

There is no concept of truncation error in this abstract setting since the space on which $S(t)$ yields a dynamical system may not possess sufficient smoothness. Hence the approach to hyperbolic invariant sets outlined before cannot be used without modification. However, one typically has finite-time error estimates of the form

$$\begin{aligned} |A^\gamma(S(t)U - S^h(t)U)| &\leq \frac{C(T, R)h}{t^\alpha}, \\ |A^\gamma(D_U[S(t)U - S^h(t)U])| &\leq \frac{C(T, R)\kappa(h)}{t^\alpha}, \\ \forall(t, U) &\in (0, T] \cap \mathcal{S} \times B_{A^\gamma}(0, R). \end{aligned}$$

Here $\kappa(h) \rightarrow 0$ as $h \rightarrow 0$.

For hyperbolic objects contraction arguments can still be set up for the semigroups over fixed time-intervals $[0, T]$ rather than $[0, \Delta t]$. Again it is necessary to use a variation of constants formula to write

$$u(t) = e^{-At}U + \int_0^t e^{-A(t-\tau)}F(S(\tau)U)d\tau$$

and hence to formulate a map on $D(A^\gamma)$ for $u_n = u(nT)$. In fact

$$u_{n+1} = Lu_n + N(u_n)$$

with

$$L = e^{-AT} \quad \text{and} \quad N(\bullet) = \int_0^T e^{-A(T-\tau)}F(S(\tau)\bullet)d\tau.$$

The perturbed problem generates a map which is $\mathcal{O}(h)$ close to $L\bullet + N(\bullet)$ in $C^0(D(A^\gamma), D(A^\gamma))$ with the sup-norm topology and $\mathcal{O}(\kappa(h))$ close in $C^1(D(A^\gamma), D(A^\gamma))$ with the induced sup-norm topology. For fixed T the time singularity integrates out of the error estimates between the two maps.

The basic method for studying hyperbolic invariant sets is similar to those used before but with fixed $T > 0$. Now, since T is fixed independent of the discretization constants, the contraction constant is $\mathcal{O}(1)$. Similar arguments to those used for ODEs, employing the uniform contraction principle and now using the finite time C^1 error estimates instead of truncation error bounds, yield convergence of hyperbolic invariant sets. To conclude the proofs it is simply necessary to establish that the invariant sets of $L\bullet + N(\bullet)$ are also invariant

under $S(t)$, and similarly for $S^h(t)$, for $t \neq T$. For attractors the same proofs may be used as in finite dimensions.

References to the literature concerning perturbation of sectorial evolution equations may be found in [10]. Central in the development of this subject area has been the work of S. Larsson and co-workers.

3.6 Adaptive time-stepping algorithms

In real software codes the time-step is varied adaptively as part of the integration procedure. Such methods, when based on one-step integration schemes, can often be formulated as mappings on $\mathbb{R}^p \times \mathbb{R}^+$ of the form

$$U_{n+1} = S^1(U_n, \Delta t_n), \quad U_0 = U,$$

$$\Delta t_{n+1} = \Gamma(U_n, \Delta t_n; \tau), \quad \Delta t_0 = \Delta t_{init}.$$

Here τ is a parameter, input by the user, which controls estimates of the local error committed at each step. The function $S^1(U, t) = S_t^1 U$ defined before. We will not go into the details of realistic models for Γ here. It suffices to say that Γ is chosen to ensure that an estimate of the local error committed at each step is $\mathcal{O}(\tau \Delta t_n)$. Note that in practice Γ is discontinuous due to step-rejections. Further non-smoothness in derivatives of Γ is introduced by maximum step-size and step-size ratio bounds.

If $t_n = \sum_{j=0}^{n-1} \Delta t_j$ then the heuristics underlying the algorithm are such that U_n should approximate $u(t_n)$ to $\mathcal{O}(\tau)$. However, for a fairly realistic model Γ of what is used in practice, the best available result concerning the convergence of such schemes is probabilistic in nature:

Result 5. [11] Let f satisfy certain genericity and smoothness conditions, assume that it has compact support and consider a certain choice of Γ which incorporates step-rejection, maximum step-size ratio and maximum step-size. If U is chosen at random uniformly in $B(0, R)$ with respect to Lebesgue measure then, with probability one, there is Δt_c sufficiently small such that, for all $\Delta t_{init} \in (0, \Delta t_c)$,

$$\|U_n - u(t_n)\| \leq C(T, U, R)\tau, \quad 0 \leq t_n \leq T.$$

□

Thus there are initial data (of zero measure) in $B(0, R)$ for which convergence may not occur. These are initial data points for which the time-step may become large, because the local error estimate is small, even when the true local error is not small. Furthermore, the error constant $C(T, U, R)$ is not uniform across the bounded set $B(0, R)$ — compare this with the classical case of Equation 2.3. Hence it is not at all clear how to progress further with analysis of this problem to encompass dynamical systems and long time intervals where sets of initial

data must be considered, possibly including points for which no error bound exists.

A variety of other authors have considered finite-time convergence and dynamical systems analysis for adaptive time-stepping algorithms prior to Result 5. Stetter [7] avoided the problems leading to the probabilistic nature of Result 5 simply by assuming that f and/or U are chosen so that the undesirable initial data points are avoided. This implies that, for some constant $K = K(U_n, \Delta t_n)$,

$$\Delta t_{n+1}^r \leq K\tau. \quad (3.7)$$

Stoffer and Nipp in [8] avoided the issue by modifying Γ to enforce Equation 3.7; they were then able to prove some very strong results about the effect of adaptive time-stepping algorithms on periodic solutions. The assumption Equation 3.7 implies that, for some constant $C = C(U_{n+1})$,

$$\|S(U_{n+1}, \Delta t_{n+1}) - S^1(U_{n+1}, \Delta t_{n+1})\| \leq C\tau\Delta t_{n+1}. \quad (3.8)$$

In [4] the assumption Equation 3.8 was made and the effect of discretization studied on the long-time behaviour of dissipative and contractive dynamical systems.

In summary the situation is this: for realistic models of Γ only very weak probabilistic finite-time convergence results exist. If certain assumptions (such as Equations 3.7 and 3.8) are made then stronger results can be proved. However it is unclear how to justify these assumptions in general. Thus a coherent analysis of variable time-stepping has yet to emerge.

4 Stability

We discuss three classes of nonlinear problem, starting with the classical theory of contractive systems which is surveyed in [1] and progressing to the dissipative and gradient theories which are surveyed in [12] and Chapter 5 of [13]. The results concerning contractive problems are straightforward modifications of the work of G. Dahlquist and of K. Burrage and J. Butcher from the 1970's. The results concerning dissipative and gradient systems may be found in the work of C.M. Elliott, of A.T. Hill, and of A.R. Humphries and A.M. Stuart. It is often desirable that numerical methods mimic the gross asymptotic features of Equation 2.1 (for example, ultimate boundedness) for intervals $\Delta t \in [0, \Delta t_c]$ with Δt_c independent of initial data. The fact that this does not occur for most methods may be understood by studying *spurious solutions*; see Chapter 5 of [13]. Active research into spurious solutions has died down, but the existing body of papers provides important motivation for the construction of methods, such as those detailed in Results 7,8,10,11,13 and 14, which avoid spurious behaviour.

The results now stated are all followed by the expression (ODE), (RKM) or (LMM) depending upon whether they apply to the original problem Equation 2.1, its Runge-Kutta approximation or its linear multistep approximation.

4.1 Contractive problems

Let Equation 2.6 hold:

$$\exists \mu > 0 : \langle f(u) - f(v), u - v \rangle \leq -\mu \|u - v\|^2, \quad \forall u, v \in \mathbb{R}^p.$$

Without loss of generality we assume that the unique equilibrium point of f is 0.

Result 6. (ODE) $\omega(U) = \{0\}$ for all $U \in \mathbb{R}^p$.

□

Result 7. (RKM) If the method is B -stable then, for any $\Delta t > 0$, $\omega(U) = \{0\}$ for all $U \in \mathbb{R}^p$.

□

Result 8. (LMM) If the method is A -stable then, for any $\Delta t > 0$, $\omega(\tilde{U}) = \{0\}$ for all $\tilde{U} \in \mathbb{R}^{kp}$.

□

Note that B -stability is essentially equivalent to AN -stability (for non-confluent methods) [1] and thus that the preceding three results show the remarkable fact that linear stability theories give a satisfactory understanding of a certain class of contractive nonlinear problems.

However, class Equation 2.6 admits only trivial limiting behaviour in Equation 2.1. To generalize Equation 2.6 it is natural to consider:

$$\exists c > 0 : \langle f(u) - f(v), u - v \rangle \leq c \|u - v\|^2, \quad \forall u, v \in \mathbb{R}^p. \quad (4.1)$$

But this alone is too broad a class to work in — exponentially growing solutions with unbounded limiting behaviour are admitted. Hence we consider other possibilities.

4.2 Dissipative problems

The first such possibility is to consider dissipative problems where

$$\exists \alpha, \beta > 0 : \langle f(u), u \rangle \leq \alpha^2 - \beta^2 \|u\|^2, \quad \forall u \in \mathbb{R}^p. \quad (4.2)$$

The Lorenz equations satisfy this condition showing that complicated limiting behaviour is certainly present within this class — see Figures 5 and 6. The Navier-Stokes equations also satisfy an infinite-dimensional analogue of this condition. The following result holds for Equation 2.1 under Equation 4.2.

Result 9. (ODE) The set $\mathcal{B} := B(0; \frac{\alpha}{\beta} + \epsilon)$ is positively invariant and has basin of attraction \mathbb{R}^p . Hence $\omega(\mathcal{B})$ is a global attractor.

□

Remarkably, the numerical stability theories appropriate for contractive nonlinear problems also turn out to be appropriate for this class of dissipative problems.

Result 10. (RKM) If the method is B -stable then there is a constant $C > 0$ such that, for any $\Delta t > 0$, the set $\mathcal{B}_{\Delta t} := B(0; \frac{\alpha}{\beta} + C\Delta t)$ is positively invariant and has basin of attraction \mathbb{R}^p . Thus $\omega(\mathcal{B}_{\Delta t})$ is a global attractor.

□

Result 11. (LMM) If the method is A -stable then there are constants $C, K > 0$ such that, for any $\Delta t > 0$, the set $\mathcal{B}_{\Delta t, k} := B(0; K\frac{\alpha}{\beta} + C\Delta t)$ is positively invariant and has basin of attraction \mathbb{R}^{kp} . Thus $\omega(\mathcal{B}_{\Delta t, k})$ is a global attractor.

□

4.3 Gradient problems

Another important class of nonlinear problems are gradient systems. These arise in many physical processes where dynamic energy minimization is present and are also important in the theory of dynamical systems. We consider gradient systems under the condition that all equilibria are hyperbolic and under the well-posedness assumption Equation 4.1. Specifically let the following conditions hold:

$$\left\{ \begin{array}{l} \exists F \in C^1(\mathbb{R}^p, \mathbb{R}) \text{ with } F(u) \geq 0, \\ \lim_{\|u\| \rightarrow \infty} F(u) = +\infty \text{ and } f(u) = -\nabla F(u) \\ \text{The set } \mathcal{E} \text{ of equilibria is hyperbolic} \\ \text{Equation 4.1 holds} \end{array} \right\}. \quad (4.3)$$

Note that, under Equation 4.3,

$$\frac{d}{dt} F(u(t)) = -\|f(u(t))\|^2.$$

Using this fact, the following result follows:

Result 12. (ODE) For any $U \in \mathbb{R}^p$ there is $v \in \mathcal{E}$ such that $\omega(U) = \{v\}$.

The stability theory for gradient systems is not as well-developed as for dissipative problems. We consider only the one and two stage *theta* methods (which are A -stable for $\theta \in [1/2, 1]$) and the BDF methods of order ≤ 3 (which are $A(\alpha)$ -stable).

Result 13. (RKM) If the one or two-stage method has $\theta \in [1/2, 1]$ (A -stable) then, for $\Delta t \in (0, \frac{1}{c})$ and for any $U \in \mathbb{R}^p$, there is $v \in \mathcal{E}$ such that $\omega(U) = \{v\}$.

Result 14. (LMM) If the BDF methods of order ≤ 3 are used ($A(\alpha)$ -stable) then for $\Delta t \in (0, \frac{1}{c})$ and for any $\tilde{U} \in \mathbb{R}^{kp}$, there is $v \in \mathcal{E}$ such that $\omega(\tilde{U}) = \{v \otimes e\}$, where e is the unit vector in \mathbb{R}^k .

Once again the preceding results show important connections with the linear theory. Note that gradient systems necessarily have symmetric linearization so that it is not entirely surprising that $A(\alpha)$ stability plays an important role. Further work to generalize Results 13 and 14 to other schemes would be interesting.

4.4 Sectorial evolution equations

For dissipative PDEs such as the Kuramoto-Sivashinsky equation, the Navier-Stokes equation, various reaction-diffusion equations and the Cahn-Hilliard equation, the effect of a variety of space and time discretizations on dissipativity have been investigated. For gradient PDEs such as the Cahn-Hilliard equation and Allen-Cahn equation, the effect of space and time discretization on the gradient structure have been investigated. Much of these investigations have centred around the work of C. Foias, R. Temam and co-workers and C.M. Elliott and co-workers.

4.5 Adaptive time-stepping algorithms

An appropriate generalization of stability in this context is to seek numerical methods which replicate basins of attraction for Equation 2.1 under Equation 2.6, Equation 4.2 or Equation 4.3 for an interval of the tolerance τ which is independent of initial data and/or stiffness. Thus τ plays the role of Δt in the fixed time-step theories.

Such stability results do exist for some simple adaptive time-stepping schemes although a complete theory has not emerged. It is an interesting fact that for contractive, dissipative and gradient problems some schemes are stable in adaptive implementations which are not stable in fixed-step mode. See [12] and [14].

5 Summary

In summary, we have highlighted the differences in philosophy between the classical theories of numerical analysis and theories of dynamical systems. We have shown that natural generalizations of the classical theories of numerical analysis can be made to encompass the dynamical systems context, especially for equations with an energy loss mechanism. These generalizations build heavily on the classical theories, especially in the case of stability. A very general approach to perturbation theory for hyperbolic invariant sets and for attractors exists. This theory applies to one-step and multistep methods for ordinary differential equations and has been extended to a broad class of partial differential equations.

The primary limitation of the convergence theory is for non-hyperbolic attractors. However, this limitation exists even in the context of differential equations where the effect of smooth perturbation to the vector field f is not completely understood. The stability theory is fairly complete for most of the systems mentioned, with the exception of gradient systems where much remains to be done.

A major hole in the theory of numerical analysis for dynamical systems is for adaptive time-stepping algorithms, both for convergence and stability. Some isolated papers exist in this area but a coherent and general view has yet to emerge. This area certainly presents hard mathematical challenges; it might potentially influence software development, but this is difficult to predict.

Another area where interesting questions concerning the dynamics of numerical methods remains is that of conservative and Hamiltonian systems where, typically, hyperbolicity does not hold for invariant sets. No satisfactory and complete theory exists which enables us to interpret data from long-time simulations of these problems. In contrast to the convergence theory outlined in this paper for dynamical systems of energy-loss type, that for conservative and Hamiltonian systems will necessarily involve an interaction between structural properties of the method — such as conservation of energy or symplectic two-form — and its long-time dynamics.

A final area where further active or important research may be anticipated is that of *backward error analysis* and *shadowing*. A variety of scattered, but important, results already exist in this field — see [6] and [13] for further references — but a wider range of results, and consequently a more complete picture, is likely to emerge over the next few years.

Thus the formulation, and study, of new and interesting questions concerning numerical approximation of initial-value problems has been an active research area over the last decade and it seems likely that there are sufficient open, in-

teresting and important questions that it will continue to be an active field over the next decade.

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