

RUNGE–KUTTA METHODS FOR DISSIPATIVE AND GRADIENT DYNAMICAL SYSTEMS*

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Abstract. The numerical approximation of dissipative initial value problems by fixed time-stepping Runge–Kutta methods is considered and the asymptotic features of the numerical and exact solutions are compared. A general class of ordinary differential equations, for which dissipativity is induced through an inner product, is studied throughout. This class arises naturally in many finite dimensional applications (such as the Lorenz equations) and also from the spatial discretization of a variety of partial differential equations arising in applied mathematics.

It is shown that the numerical solution defined by an algebraically stable method has an absorbing set and is hence dissipative for any fixed step-size $h > 0$. The numerical solution is shown to define a dynamical system on the absorbing set if h is sufficiently small and hence a global attractor \mathcal{A}_h exists; upper-semicontinuity of \mathcal{A}_h at $h = 0$ is established, which shows that, for h small, every point on the numerical attractor is close to a point on the true global attractor \mathcal{A} . Under the additional assumption that the problem is globally Lipschitz, it is shown that if h is sufficiently small any method with positive weights defines a dissipative dynamical system on the whole space and upper semicontinuity of \mathcal{A}_h at $h = 0$ is again established.

For gradient systems with globally Lipschitz vector fields it is shown that any Runge–Kutta method preserves the gradient structure for h sufficiently small. For general dissipative gradient systems it is shown that algebraically stable methods preserve the gradient structure within the absorbing set for h sufficiently small. Convergence of the numerical attractor is studied and, for a dissipative gradient system with hyperbolic equilibria, lower semicontinuity at $h = 0$ is established. Thus, for such a system, \mathcal{A}_h converges to \mathcal{A} in the Hausdorff metric as $h \rightarrow 0$.

Key words. Runge–Kutta methods, dynamical systems, dissipativity, gradient systems, attractors

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1. Introduction. Many interesting problems in physics and engineering are modeled by dissipative dynamical systems. These systems are characterized by the property of possessing a bounded *absorbing set* which all trajectories enter in a finite time and thereafter remain inside. In the study of dissipative systems it is often the asymptotic behaviour of the system that is of interest, and so it is highly desirable to have numerical methods that retain the dissipativity of the underlying system.

We consider the numerical approximation by fixed time-stepping Runge–Kutta methods of dynamical systems defined by

$$(1.1) \quad \frac{dy}{dt} = f(y), \quad t \geq 0 \quad \text{and} \quad y(0) = y_0,$$

where $y(t) \in \mathbb{R}^m$ and $f: \mathbb{R}^m \rightarrow \mathbb{R}^m$ is assumed to be locally Lipschitz.

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We make the additional structural assumption on f that

$$(1.2) \quad \langle f(\mathbf{y}), \mathbf{y} \rangle \leq \alpha - \beta \|\mathbf{y}\|^2$$

for some $\alpha \geq 0$ and $\beta > 0$ and some inner product on \mathbb{R}^m . The system (1.1)–(1.2) has an absorbing set B that can be any ball of radius larger than $\sqrt{\alpha/\beta}$. Except where explicitly stated, the norm in this paper is the norm defined by the inner product used in assumption (1.2). Dissipativity is defined precisely in §2, where we show that (1.1)–(1.2) defines a dissipative dynamical system.

Systems of the form (1.1)–(1.2) arise in many applications and indeed the class defined by (1.1)–(1.2) contains many well-known problems. The Cahn–Hilliard equation that models the process of coarsening in solid phase separation, the Navier–Stokes equations in two dimensions, the complex Ginzburg–Landau equation, and the Kuramoto–Sivashinsky equation all satisfy an infinite dimensional analogue of (1.2) [26]. Under suitable spatial discretization they generate systems of the form (1.1)–(1.2). In Appendix A it is shown that the Lorenz equations also define a dissipative system of the form (1.1)–(1.2).

We approximate the solution of (1.1)–(1.2) numerically using a fixed time-stepping Runge–Kutta method. A general s -stage Runge–Kutta method may be written as

$$(1.3) \quad \mathbf{Y}_i = \mathbf{y}_n + h \sum_{j=1}^s a_{i,j} f(\mathbf{Y}_j), \quad i = 1, \dots, s,$$

$$(1.4) \quad \mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^s b_i f(\mathbf{Y}_i).$$

Here \mathbf{y}_n approximates the exact solution at $t = nh$, where $h > 0$ is the fixed step size. The method is often represented using the Butcher Tableau notation

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \end{array} \equiv \begin{array}{c|cccc} c_1 & a_{1,1} & a_{1,2} & \dots & a_{1,s} \\ c_2 & a_{2,1} & a_{2,2} & \dots & a_{2,s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & a_{s,2} & \dots & a_{s,s} \\ \hline & b_1 & b_2 & \dots & b_s \end{array},$$

where $c_j := \sum_{l=1}^s a_{j,l}$, $j = 1, \dots, s$. We will always assume that the method is consistent, which implies that $\sum_{i=1}^s b_i = 1$, and that for an implicit method the defining equations (1.3) are solved exactly.

We will assume throughout that the Runge–Kutta method (1.3)–(1.4) is DJ irreducible.

DEFINITION 1.1. *A Runge–Kutta method is said to be DJ reducible, if for some nonempty index set $T \subset \{1, \dots, s\}$,*

$$b_j = 0 \quad \text{for } j \in T$$

and

$$a_{ij} = 0 \quad \text{for } i \notin T, j \in T,$$

and is said to be DJ irreducible otherwise.

For a DJ-reducible method, the stages for which $j \in T$ do not affect the solution, and so deleting these stages gives an equivalent Runge–Kutta method with fewer

stages. For this reason DJ-reducible methods are not used in practice, and there is no loss of generality in considering only DJ-irreducible methods.

We will require two $s \times s$ matrices B and M associated with the Runge–Kutta method (1.3)–(1.4), defined by

$$(1.5) \quad B = \text{diag}(b_1, b_2, \dots, b_s),$$

$$(1.6) \quad M = BA + A^T B - \mathbf{b}\mathbf{b}^T.$$

We will denote the entries of M by

$$(1.7) \quad m_{ij} = \{M\}_{ij}.$$

Many authors have made systematic studies of the numerical solution of (1.1) under structural assumptions on \mathbf{f} different from (1.2). Dahlquist [6] first studied the linear stability problem

$$(1.8) \quad \frac{dy}{dt} = \lambda y, \quad \text{for } t \geq 0,$$

where $y(t) \in \mathcal{C}$ and $\Re(\lambda) < 0$. A numerical method that satisfies $y_n \rightarrow 0$ as $n \rightarrow \infty$ for any $h > 0$ and any λ such that $\Re(\lambda) < 0$ is said to be *A stable*. The study of A-stable numerical methods provides insight into the behaviour of numerical methods for both the linear problem (1.8) and, in certain cases, the general nonlinear problem (1.1).

Later Dahlquist [7] generalized (1.8), and considered the solution of (1.1) for nonlinear \mathbf{f} satisfying

$$(1.9) \quad \langle \mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle \leq 0.$$

If $\mathbf{u}(t)$ and $\mathbf{v}(t)$ are two solutions of (1.1), (1.9) with different initial conditions then

$$\frac{d}{dt} \|\mathbf{u}(t) - \mathbf{v}(t)\|^2 \leq 0.$$

It is natural to ask which numerical methods retain this contractivity property. Such methods are often referred to as dissipative in the numerical analysis literature, but this conflicts with the dynamical systems terminology and *we will only use the term “dissipative” in its dynamical systems context*, made precise by Definition 2.3.

Dahlquist [7] considered linear multistep methods in their one-leg formulation and defined such a method to be *G stable* if a certain norm associated with the difference of two solution sequences of the method applied to (1.1), (1.9) is nonincreasing. Remarkably Dahlquist [8] proved that for one-leg methods A-stability and G-stability are equivalent.

Butcher [4] first considered the solution of (1.1), (1.9) by Runge–Kutta methods, and Burrage and Butcher [2] introduced the concept of algebraic stability.

DEFINITION 1.2. *A Runge–Kutta method is said to be algebraically stable if the matrices B and M defined by (1.5)–(1.6) are both positive semidefinite.*

Burrage and Butcher showed that if $\{\mathbf{u}_n\}_{n=0}^\infty$ and $\{\mathbf{v}_n\}_{n=0}^\infty$ are two solution sequences of an algebraically stable Runge–Kutta method applied to (1.1), (1.9) then $\|\mathbf{u}_n - \mathbf{v}_n\|$ is nonincreasing. Unlike the analogous situation for one-leg methods, A-stability and algebraic stability are not equivalent for Runge–Kutta methods and nonautonomous problems need to be studied to provide a link [9]. Algebraic stability will play a crucial role in our study of dissipative problems.

Although great insight into the behaviour of numerical methods was gained by studying (1.8) and (1.1), (1.9), it should be emphasised that the practical applications of either class of systems is very limited. The linear system (1.8) clearly has a unique stable fixed point at the origin which attracts all trajectories, whilst for (1.1), (1.9) it is shown in Stuart and Humphries [25] that the fixed points of the system define a convex set and that, if a fixed point is unique, then it is globally attracting. Such a limited range of dynamical behaviour clearly precludes most applications.

One way of broadening the class of problems to which the theory applies is to generalize (1.9) and consider systems of the form (1.1) that satisfy the so-called one-sided Lipschitz condition

$$(1.10) \quad \langle \mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle \leq c \|\mathbf{u} - \mathbf{v}\|^2$$

for some $c > 0$. It is easy to show that for two solutions $\mathbf{u}(t)$ and $\mathbf{v}(t)$ of (1.1), (1.10) with different initial conditions

$$\frac{1}{2} \frac{d}{dt} \|\mathbf{u}(t) - \mathbf{v}(t)\|^2 \leq c \|\mathbf{u}(t) - \mathbf{v}(t)\|^2.$$

Thus the condition (1.10) allows some divergence of solutions to occur. It is a natural condition to apply to stiff systems and the solvability of the Runge–Kutta equations (1.3)–(1.4) and the behaviour of solution sequences has been widely studied in this context; the material is well presented in Dekker and Verwer [9] and Hairer and Wanner [15].

However, *dissipative systems need not satisfy a one-sided Lipschitz condition*, and so we will not assume a condition of the form (1.10) when studying (1.1)–(1.2). To illustrate this we show in Appendix A that after translation of the origin, the Lorenz equations are dissipative in the sense of (1.1)–(1.2), but do not satisfy a one-sided Lipschitz condition (1.10). Nonetheless, the theory of solvability of Runge–Kutta equations developed for (1.1), (1.10) will be of use to us in developing a related theory for (1.1)–(1.2).

We emphasise that problems satisfying (1.1)–(1.2) can exhibit a variety of interesting dynamical features ranging from multiple competing equilibria (the Cahn–Hilliard equation) through periodic and quasi-periodic behaviour (the complex Ginzburg–Landau equations) to chaos (the Lorenz equations and the Kuramoto–Sivashinsky equation). Thus many applications are possible in this context.

In the next section we review the background theory of dissipative dynamical systems required in later sections. We also show that if \mathbf{f} is locally Lipschitz then (1.1)–(1.2) defines a dissipative dynamical system. When considering discretizations of (1.1)–(1.2) we find that the numerical method does not necessarily define a dynamical system, since the solution sequence may not be unique, and so we generalize the concept of dissipativity to deal with this case.

In §3 we consider the numerical approximation of (1.1)–(1.2). We study the solubility of (1.3) and show in particular that for a DJ-irreducible algebraically stable method [15] with invertible A a solution sequence always exists using a combination of techniques from [9], [12], and [13]. To show that solution sequences need not be unique, we construct an example where the backward Euler method has multiple solutions for h arbitrarily small when applied to a problem satisfying (1.2) (see Appendix B).

The existence of an absorbing set often requires step-size bounds that are dependent on initial data; however, Foias et al. [12] have constructed absorbing sets with step-size bounds independent of initial data for certain discretizations of the

Kuramoto–Sivashinsky equations, and Elliott and Stuart [11] have derived similar results for reaction–diffusion equations. The main result in §3 is to employ techniques similar to [11] and [12] to show that DJ-irreducible, algebraically stable methods applied to (1.1)–(1.2) have an absorbing set B for arbitrary initial data and for arbitrarily large step sizes. Thus a DJ-irreducible algebraically stable method is dissipative for any fixed step-size $h > 0$. We then show that if h is sufficiently small the numerical method defines a dynamical system on B . In addition we show that if \mathbf{f} is globally Lipschitz then any Runge–Kutta method with positive weights defines a dissipative dynamical system on \mathbb{R}^m for h sufficiently small. The bound on h is again independent of initial data.

The dissipativity of the map defined by applying the numerical method to (1.1)–(1.2) enables us to prove existence of a global attractor \mathcal{A}_h . The convergence of the numerical attractor \mathcal{A}_h to the attractor \mathcal{A} of (1.1)–(1.2) is also considered in §3 and we show that $\text{dist}(\mathcal{A}_h, \mathcal{A}) \rightarrow 0$ as $h \rightarrow 0$, where $\text{dist}(\bullet, \bullet)$ is defined in Definition 2.5. This is referred to as upper semicontinuity at $h = 0$. A number of results of this nature have already appeared in the literature. Hale [16], [17] and Temam [26] both give upper semicontinuity results for perturbations of an evolution operator on a Banach space and our approach is to follow their method of proof. Kloeden and Lorenz [23] derive related results for one-step discretizations of ordinary differential equations by considering the weaker concept of asymptotically stable sets. Our upper semicontinuity result is closely related to the result of Kloeden and Lorenz; however, we obtain the result without assuming global boundedness of \mathbf{f} and obtain *global* attraction of \mathcal{A}_h by restricting our attention to algebraically stable Runge–Kutta methods and to problems of the form (1.1)–(1.2). This approach provides the kind of global bounds required to apply the results of [23].

In §4 we consider gradient systems. We show that if \mathbf{f} is globally Lipschitz then any Runge–Kutta method preserves the gradient structure for h sufficiently small. This result allows us to show that if (1.1)–(1.2) is in gradient form then for h sufficiently small the numerical solution preserves the gradient structure on any positively invariant set. Under the assumption that the fixed points of the system are all hyperbolic it is proved that $\text{dist}(\mathcal{A}, \mathcal{A}_h) \rightarrow 0$ as $h \rightarrow 0$. Such lower semicontinuity results have been given previously by Hale [16] and Hale and Raugel [18] for perturbations of gradient systems with hyperbolic equilibria on Banach spaces and again we employ their method of proof.

2. Dissipative dynamical systems. In this section we review the concepts and definitions relating to dissipative dynamical systems that we will need in later sections. We conclude the section by generalizing the concept of dissipativity to cover multivalued maps.

Before we can define a dissipative dynamical system, we must define what we mean by a dynamical system and its evolution semigroup.

DEFINITION 2.1. *The equation (1.1) is said to define a dynamical system on an open set $U \subseteq \mathbb{R}^m$ if for any $\mathbf{y}_0 \in U$ there exists a unique solution of (1.1) with $\mathbf{y}(t) \in U$ for all $t \geq 0$. We define the evolution semigroup $S(t): U \rightarrow U$ for the dynamical system to be the operator such that $\mathbf{y}(t) = S(t)\mathbf{y}(0)$. This operator has the properties that*

- (i) $\mathbf{y}(t + t') = S(t)\mathbf{y}(t') = S(t')\mathbf{y}(t) = S(t + t')\mathbf{y}(0)$ for all $t, t' \geq 0$,
- (ii) $S(0) = I$, the identity operator.

The semigroup $S(t)$ is merely a convenient notation for advancing a solution through t time units. For any set $E \subseteq U$ the action of the evolution semigroup is

defined by

$$S(t)E = \bigcup_{\mathbf{y}_0 \in E} S(t)\mathbf{y}_0.$$

DEFINITION 2.2. A dynamical system is said to be continuous with respect to initial data (or simply referred to as a continuous dynamical system) if given any $\mathbf{y}_0 \in U$, any $T > 0$, and any $\varepsilon > 0$ there exists $\delta = \delta(\mathbf{y}_0, T, \varepsilon)$ with $\|S(t)\mathbf{y}_0 - S(t)\mathbf{y}\| < \varepsilon$ for $0 \leq t \leq T$ and all $\mathbf{y} \in U$ such that $\|\mathbf{y} - \mathbf{y}_0\| < \delta$.

Our assumption that \mathbf{f} is locally Lipschitz ensures that (1.1) is always continuous with respect to initial data. We can now define a dissipative dynamical system; see Hale [16].

DEFINITION 2.3. A dynamical system is dissipative if there is a bounded set B with the property that, for any bounded set $E \subseteq U$, there exists $t^*(E) \geq 0$ such that $S(t)E \subseteq B$ for $t > t^*$. The set B is called an absorbing set.

Remark. Hale [16] notes that for a continuous dynamical system on a locally compact space (like \mathbb{R}^m) to show dissipativity it is sufficient to show that for any initial condition $\mathbf{y}_0 \in U$ there exists $t^*(\mathbf{y}_0) \geq 0$ such that $S(t)\mathbf{y}_0 \in B$ for $t > t^*$.

A dissipative dynamical system possesses a global attractor. To enable us to study attractors we must first define ω -limit sets and a distance function for sets.

DEFINITION 2.4. For any $\mathbf{y}_0 \in U$ the ω -limit set of \mathbf{y}_0 is defined by

$$\omega(\mathbf{y}_0) = \bigcap_{\tau \geq 0} \overline{\bigcup_{t \geq \tau} S(t)\mathbf{y}_0}.$$

For a bounded set $E \subseteq U$ we define the ω -limit set of E by

$$\omega(E) = \bigcap_{\tau \geq 0} \overline{\bigcup_{t \geq \tau} S(t)E}.$$

The sets $\omega(\mathbf{y}_0)$ and $\omega(E)$ are positively invariant under $S(t)$ and are also closed (as an intersection of closed sets). Note that, in general,

$$(2.1) \quad \bigcup_{\mathbf{x} \in E} \omega(\mathbf{x}) \subset \omega(E)$$

with the inclusion being sharp. This is because $\omega(E)$ includes heteroclinic and homoclinic connections between the limit sets of individual trajectories originating in E .

DEFINITION 2.5. Given a set $B \subset \mathbb{R}^m$ and a point $\mathbf{x} \in \mathbb{R}^m$ we define

$$\text{dist}(\mathbf{x}, B) = \inf_{\mathbf{y} \in B} \|\mathbf{x} - \mathbf{y}\|.$$

For two sets $A, B \subset \mathbb{R}^m$ we define

$$\text{dist}(A, B) = \sup_{\mathbf{x} \in A} \text{dist}(\mathbf{x}, B).$$

Given a set A we also define the ε -neighbourhood of A by

$$N(A, \varepsilon) = \{\mathbf{x}: \text{dist}(\mathbf{x}, A) < \varepsilon\}.$$

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Remark. Note that in general $\text{dist}(A, B) \neq \text{dist}(B, A)$. If $\text{dist}(A, B) = 0$ then $A \subseteq \overline{B}$ and if $\text{dist}(A, B) = \text{dist}(B, A) = 0$ then $\overline{A} = \overline{B}$. We now define the global attractor for a continuous dynamical system.

DEFINITION 2.6. For a continuous dynamical system a set A is said to attract a set B under $S(t)$ if for any $\varepsilon > 0$ there exists $t^* = t^*(\varepsilon, A, B)$ such that

$$S(t)B \subseteq N(A, \varepsilon) \quad \forall t > t^*.$$

A is said to be a local attractor if it is a compact invariant set that attracts an open neighbourhood of itself. A is said to be a global attractor if it is a compact invariant set that attracts all bounded subsets of U .

For a dissipative system the global attractor \mathcal{A} can be constructed as

$$\mathcal{A} = \omega(B),$$

where B is any absorbing set of the system and it follows that \mathcal{A} is compact and invariant under $S(t)$. By virtue of (2.1) it is not sufficient to study limit sets of individual trajectories to construct \mathcal{A} . We now show that (1.1)–(1.2) defines a dissipative dynamical system.

THEOREM 2.7. Suppose $\mathbf{y}(t)$ is a solution of (1.1) where \mathbf{f} satisfies (1.2). Then (1.1)–(1.2) defines a dynamical system on \mathbb{R}^m and for any $\varepsilon > 0$ there exists $t = t^*(\mathbf{y}_0, \varepsilon)$ such that for all $t > t^*$

$$(2.2) \quad \|\mathbf{y}(t)\|^2 < \frac{\alpha}{\beta} + \varepsilon.$$

Hence the dynamical system is dissipative, the open ball $B = B(0, \sqrt{\alpha/\beta} + \varepsilon)$ is an absorbing set for any $\varepsilon > 0$, and the system possesses a global attractor \mathcal{A} defined by $\mathcal{A} = \omega(B)$.

Proof. First we establish an a priori bound on the solution $\mathbf{y}(t)$. Note that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|\mathbf{y}\|^2 &= \langle \mathbf{y}, \mathbf{f}(\mathbf{y}) \rangle \\ &\leq \alpha - \beta \|\mathbf{y}\|^2. \end{aligned}$$

Now integration shows that

$$(2.3) \quad \|\mathbf{y}(t)\|^2 \leq \frac{\alpha}{\beta} + e^{-2\beta t} \left[\|\mathbf{y}_0\|^2 - \frac{\alpha}{\beta} \right].$$

Thus it follows that

$$\|\mathbf{y}(t)\| \leq \max \left(\|\mathbf{y}_0\|, \frac{\alpha}{\beta} \right)$$

for $t \geq 0$. Hence the solution of (1.1)–(1.2) cannot blow up and since \mathbf{f} is locally Lipschitz the standard theory of ordinary differential equations implies that (1.1) defines a dynamical system on \mathbb{R}^m .

The bound (2.2) follows from (2.3) and this implies that (1.1)–(1.2) is dissipative, with B an absorbing set and a global attractor \mathcal{A} defined by $\mathcal{A} = \omega(B)$. \square

Next we define a dynamical system for mappings. We suppose that Φ_h defines a family of maps parameterized by h . When we come to consider the numerical

approximation of (1.1)–(1.2) by a Runge–Kutta method (1.3)–(1.4) the parameter h will be the step-size of the method.

DEFINITION 2.8. *If $\Phi_h: U \rightarrow U$ is uniquely defined on $U \subseteq \mathbb{R}^m$ then for any $\mathbf{y}_0 \in U$ the sequence $\{\mathbf{y}_n\}_{n=0}^\infty$ is uniquely defined in U by $\mathbf{y}_{n+1} = \Phi_h(\mathbf{y}_n)$, and Φ_h is said to define a dynamical system on U . The evolution semigroup $S_h^n: U \rightarrow U$ is defined to be the operator such that $\mathbf{y}_n = S_h^n \mathbf{y}_0$.*

Note that, in this definition, $S_h^n \bullet$ is simply an n -fold composition of $\Phi_h(\bullet)$.

We define continuity, dissipativity, ω -limit sets, and attractors for discrete dynamical systems in the natural way by replacing $S(t)$ with S_h^n in Definitions 2.2–2.4 and 2.6 with n playing the role of t for integer n . Whilst continuity with respect to initial data is automatic for (1.1)–(1.2) with Lipschitz \mathbf{f} we need to show continuity for dynamical systems generated by a numerical discretization of (1.1)–(1.2).

When modeling a dissipative problem numerically it is natural in many circumstances to require that the numerical method preserve the dissipativity. In the next section we investigate this issue for the numerical solution of (1.1)–(1.2) using a fixed time-stepping Runge–Kutta method; when it is dissipative we compare the absorbing sets and global attractors of the two systems.

In previous works many authors have assumed that numerical methods define continuously differentiable dynamical systems. However, when implicit methods are applied to (1.1), the numerical method does not even necessarily define a dynamical system since solutions of the Runge–Kutta defining equation (1.3) need not exist or may not be unique for a given $\mathbf{y}_n \in \mathbb{R}^m$ and $h > 0$. Instead of restricting our attention to the case where the numerical method does define a dynamical system, which would exclude the Runge–Kutta methods with the best stability properties, we will define a generalized evolution operator, which allows us to prove results regardless of whether or not the numerical method defines a dynamical system.

For an implicit method rewrite the Runge–Kutta equations (1.3)–(1.4) as

$$(2.4) \quad \begin{cases} \mathbf{Y}_i - \mathbf{y}_n - h \sum_{j=1}^s a_{i,j} \mathbf{f}(\mathbf{Y}_j) = 0, & i = 1, \dots, s \\ \mathbf{y}_{n+1} - \mathbf{y}_n - h \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) = 0 \end{cases}$$

and consider the \mathbf{Y}_i 's to be functions of \mathbf{y}_n . Then we may think of (2.4) as an implicit map

$$(2.5) \quad \Upsilon_h(\mathbf{y}_n, \mathbf{y}_{n+1}) = 0.$$

The generalized evolution map is then defined as follows.

DEFINITION 2.9. *Consider an implicit Runge–Kutta method defined by an implicit map (2.5). The generalized evolution map G_h^n for Υ_h is defined by*

$$\begin{aligned} G_h^1(\mathbf{u}) &= \{\mathbf{v}: \Upsilon_h(\mathbf{u}, \mathbf{v}) = 0\}, \\ G_h^1(E) &= \bigcup_{\mathbf{u} \in E} G_h^1(\mathbf{u}), \end{aligned}$$

and inductively by

$$\begin{aligned} G_h^n(\mathbf{u}) &= G_h^1(G_h^{n-1}(\mathbf{u})), \\ G_h^n(E) &= \bigcup_{\mathbf{u} \in E} G_h^n(\mathbf{u}). \end{aligned}$$

The generalized evolution map G_h^n is the natural extension of the evolution map S_h^n to multivalued maps. If Υ_h defines a dynamical system then S_h^n and G_h^n agree. In general, however, the evolution map $G_h^1(\mathbf{y}_n)$ returns all the possible values of \mathbf{y}_{n+1} for the implicit map and should be thought of as a set-valued function on subsets of \mathbb{R}^m rather than a map from \mathbb{R}^m to itself. Note that if (2.5) is insoluble for some initial condition \mathbf{y}_n then $G_h^1(\mathbf{y}_n) = \emptyset$, and we also define $G_h^1(\emptyset) = \emptyset$.

It should be noted that our definition of the generalized evolution operator is analogous to the usual definition of negative orbits for discrete dynamical systems. Since the map defining a discrete dynamical system need not be one-to-one, negative orbits need not be unique, and it is usual to define the negative orbit of a point to be the union of all possible such orbits (see, for example, Hale [16]).

The generalized evolution map allows us to extend the concept of dissipativity to cover multivalued maps in a natural way by replacing S_h^n by G_h^n in the definition of dissipativity. We will use this generalized concept in the next section, which will allow us to consider the approximation of dissipative systems by both explicit and implicit numerical maps without making any assumption as to whether or not the numerical method defines a unique solution sequence.

3. Runge–Kutta methods for dissipative systems. In this section we will discuss the dynamics of solution sequences of Runge–Kutta methods applied to (1.1)–(1.2). First we will establish that for certain implicit methods a solution sequence always exists.

The use of implicit Runge–Kutta methods was first proposed by Butcher [3], and he proved the following existence and uniqueness result for solutions of the Runge–Kutta equations (1.3)–(1.4) in the case where \mathbf{f} is assumed to be globally Lipschitz.

THEOREM 3.1 [3]. *If \mathbf{f} is globally Lipschitz with Lipschitz constant L and*

$$(3.1) \quad h < \frac{1}{La}$$

where

$$(3.2) \quad a = \max_i \sum_{j=1}^{i-1} |a_{ij}| + \max_i \sum_{j=i}^s |a_{ij}|,$$

then the equations (1.3)–(1.4) are uniquely soluble. Furthermore, this solution can be found by iteration. Set $\mathbf{Y}_i^0 = \mathbf{y}_n$ for all $i = 1, \dots, s$ then iterate

$$(3.3) \quad \mathbf{Y}_i^{N+1} = \mathbf{y}_n + h \sum_{j=1}^{i-1} a_{ij} \mathbf{f}(\mathbf{Y}_j^{N+1}) + h \sum_{j=i}^s a_{ij} \mathbf{f}(\mathbf{Y}_j^N).$$

Then $\mathbf{Y}_i = \lim_{N \rightarrow \infty} \mathbf{Y}_i^N$ exists and defines the solution of (1.3).

We now consider the existence of solutions to (1.3) in the general case where \mathbf{f} is locally Lipschitz and satisfies (1.2). Recall Definition 1.2 from the introduction. We will show that for a DJ-irreducible [15] algebraically stable Runge–Kutta method with A invertible, the defining equations (1.3) are soluble for any $h > 0$ and any value of \mathbf{y}_n , and hence a solution sequence always exists. We will require the function $\Psi_D(A)$, which is defined below as in Dekker and Verwer [9].

DEFINITION 3.2. *Let D be a positive diagonal $s \times s$ matrix, so $d_{ii} > 0$ for all i , and A an arbitrary $s \times s$ matrix. Then the function $\Psi_D(A)$ is defined by*

$$(3.4) \quad \Psi_D(A) = \inf_{\xi \neq 0} \frac{\langle DA\xi, \xi \rangle}{\langle D\xi, \xi \rangle}.$$

Now let \mathcal{D} be the set of positive diagonal $s \times s$ matrices and define $\Psi_0(A)$ by

$$(3.5) \quad \Psi_0(A) = \sup_{D \in \mathcal{D}} \Psi_D(A).$$

The following lemma will be needed in the proof of the existence of solutions to (1.3). To prove the lemma we need the fact that for a DJ-irreducible algebraically stable Runge–Kutta method, $b_i > 0$ for all i , so that B is positive definite (see [9], [15]).

LEMMA 3.3. *For a DJ-irreducible algebraically stable Runge–Kutta method with invertible A both $\Psi_B(A^{-1}) \geq 0$ and $\Psi_0(A^{-1}) \geq 0$.*

Proof. Observe that

$$\begin{aligned} \langle BA\zeta, \zeta \rangle &= \zeta^T BA\zeta \\ &= \frac{1}{2}\zeta^T (BA + A^T B - \mathbf{b}\mathbf{b}^T)\zeta + \frac{1}{2}\zeta^T \mathbf{b}\mathbf{b}^T \zeta \\ &= \frac{1}{2}\zeta^T M\zeta + \frac{1}{2}(\mathbf{b}^T \zeta)^2 \\ &\geq 0, \end{aligned}$$

since M is positive semidefinite. Now since $\langle B\zeta, \zeta \rangle = \sum_{i=1}^s b_i \zeta_i^2 > 0$ for $\zeta \neq 0$ it follows that $\Psi_B(A) \geq 0$. Dekker and Verwer [9] show that if A is invertible and $\Psi_B(A) \geq 0$ then $\Psi_B(A^{-1}) \geq 0$, and since $\Psi_0(A^{-1}) \geq \Psi_B(A^{-1})$ the result follows. \square

We will require the following notation in our proof of the existence of solutions to (1.3). Define $\mathbf{Y} \in \mathbb{R}^{ms}$ by

$$\mathbf{Y} = [\mathbf{Y}_1^T, \mathbf{Y}_2^T, \dots, \mathbf{Y}_s^T]^T$$

and if D is an $s \times s$ positive definite diagonal matrix define an inner product on \mathbb{R}^{ms} by

$$\langle \mathbf{X}, \mathbf{Y} \rangle_D = \mathbf{X}^T (D \otimes I_m) \mathbf{Y}$$

and the corresponding norm on \mathbb{R}^{ms} by

$$\|\mathbf{Y}\|_D^2 = \langle \mathbf{Y}, \mathbf{Y} \rangle_D = \mathbf{Y}^T (D \otimes I_m) \mathbf{Y} = \sum_{i=1}^s d_i \|\mathbf{Y}_i\|^2,$$

where $(D \otimes I_m)$ denotes the tensor product of D and I_m the m -dimensional unit matrix, and $\|\bullet\|$ denotes the usual norm on \mathbb{R}^m induced by the inner product used in (1.2). Since B is positive definite for a DJ-irreducible algebraically stable Runge–Kutta method, in this case we can define

$$\|\mathbf{Y}\|_B^2 = \sum_{i=1}^s b_i \|\mathbf{Y}_i\|^2.$$

The idea for the proof of the following proposition comes from Foias et al. [12], who used a similar technique to show the existence of solutions to an implicit method for the Kuramoto–Sivashinsky equation; see also French and Jensen [13]. The proof also uses ideas from the study of existence of solutions to (1.3) when \mathbf{f} satisfies a one-sided Lipschitz condition (1.10) (see [9]).

PROPOSITION 3.4. *If \mathbf{f} satisfies (1.2) and A is invertible with*

$$(3.6) \quad \Psi_0(A^{-1}) + h\beta > 0,$$

where $\Psi_0(A)$ is defined by (3.5), then the Runge-Kutta equations (1.3) are soluble.

Proof. Define $\mathbf{y} \in \mathbb{R}^{ms}$ and $\mathbf{F}(\mathbf{Y}) \in \mathbb{R}^{ms}$ by

$$\begin{aligned} \mathbf{y} &= [\mathbf{y}_n^T, \mathbf{y}_n^T, \dots, \mathbf{y}_n^T]^T \\ \mathbf{F}(\mathbf{Y}) &= [\mathbf{f}(\mathbf{Y}_1)^T, \mathbf{f}(\mathbf{Y}_2)^T, \dots, \mathbf{f}(\mathbf{Y}_s)^T]^T \end{aligned}$$

and let

$$(3.7) \quad \Phi(\mathbf{Y}) = (A^{-1} \otimes I_m)(\mathbf{Y} - \mathbf{y} - h(A \otimes I_m)\mathbf{F}(\mathbf{Y}))$$

Equation (3.6) implies that there exists $\varepsilon > 0$ such that

$$\Psi_0(A^{-1}) + h\beta \geq \varepsilon$$

and the definition of $\Psi_0(A^{-1})$ then implies the existence of a positive definite diagonal matrix D such that

$$\Psi_D(A^{-1}) + h\beta > 0.$$

Using this D we have that

$$(3.8) \quad \begin{aligned} \langle \mathbf{Y}, \Phi(\mathbf{Y}) \rangle_D &= \mathbf{Y}^T(DA^{-1} \otimes I_m)\mathbf{Y} - \mathbf{Y}^T(DA^{-1} \otimes I_m)\mathbf{y} \\ &\quad - h\mathbf{Y}^T(D \otimes I_m)\mathbf{F}(\mathbf{Y}). \end{aligned}$$

Consider the terms on the right-hand side of (3.8) individually. For the first term it is known that

$$(3.9) \quad \mathbf{Y}^T(DA^{-1} \otimes I_m)\mathbf{Y} \geq \Psi_D(A^{-1})\|\mathbf{Y}\|_D^2;$$

see for example Dekker and Verwer [9] or Hairer and Wanner [15]. To deal with the second term consider

$$(3.10) \quad \begin{aligned} \mathbf{Y}^T(DA^{-1} \otimes I_m)\mathbf{y} &= \langle \mathbf{Y}, (A^{-1} \otimes I_m)\mathbf{y} \rangle_D \\ &\leq \|\mathbf{Y}\|_D \|(A^{-1} \otimes I_m)\mathbf{y}\|_D. \end{aligned}$$

Finally, we bound the last term by using the dissipativity of the system. By scaling we can assume without loss of generality that $\sum_{i=1}^s d_i = 1$. Then using (1.2) we have

$$\begin{aligned} \mathbf{Y}^T(D \otimes I_m)\mathbf{F}(\mathbf{Y}) &= \langle \mathbf{Y}, \mathbf{F}(\mathbf{Y}) \rangle_D \\ &= \sum_{i=1}^s d_i \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_i) \rangle \\ &\leq \alpha \sum_{i=1}^s d_i - \beta \sum_{i=1}^s d_i \|\mathbf{Y}_i\|^2 \\ &= \alpha - \beta \|\mathbf{Y}\|_D^2. \end{aligned}$$

Substituting all these inequalities into (3.8) implies that

$$\langle \mathbf{Y}, \Phi(\mathbf{Y}) \rangle_D \geq (\Psi_D(A^{-1}) + \beta h)\|\mathbf{Y}\|_D^2 - \|\mathbf{Y}\|_D \|(A^{-1} \otimes I_m)\mathbf{y}\|_D - \alpha h.$$

Now note that by assumption the coefficient of $\|\mathbf{Y}\|_D^2$ is positive so that for R sufficiently large we have that

$$(3.11) \quad \langle \mathbf{Y}, \Phi(\mathbf{Y}) \rangle_D > 0$$

for all $\mathbf{Y} \in \partial B$ where B is the ball of radius R in $(\mathbb{R}^{ms}, \|\cdot\|_D)$. Now from Girault and Raviart [14, p. 279] or Constantin and Foias [5, p. 58] it follows that there exists $\mathbf{Y} \in B$ such that $\Phi(\mathbf{Y}) = 0$. Thus for this value of \mathbf{Y}

$$\mathbf{Y} - \mathbf{y} - h(A \otimes I_m)\mathbf{F}(\mathbf{Y}) = 0,$$

which is equivalent to

$$\mathbf{Y}_i - \mathbf{y}_n - h \sum_{j=1}^s a_{i,j} \mathbf{f}(\mathbf{Y}_j) = 0$$

for all $i = 1, \dots, s$ and hence a solution of (1.3). \square

Remark. Notice that (3.11) holds for $\|\mathbf{Y}\|_D \geq R$. Hence $\Phi(\mathbf{Y}) \neq 0$ for $\|\mathbf{Y}\|_D \geq R$ and any solution of (1.3) must satisfy $\|\mathbf{Y}\|_D < R$.

Recall that by Lemma 3.3 a DJ-irreducible algebraically stable Runge–Kutta method with invertible A satisfies $\Psi_B(A^{-1}) \geq 0$. Hence the following theorem follows trivially from Proposition 3.4.

THEOREM 3.5. *If the Runge–Kutta method (1.3)–(1.4) is DJ-irreducible and algebraically stable with A invertible and \mathbf{f} satisfies (1.2), then the defining equations (1.3) are soluble for any step-size $h > 0$ and any $\mathbf{y}_n \in \mathbb{R}^m$.*

Remark. For a general Runge–Kutta method suppose that A is invertible but that $\Psi_0(A^{-1}) < 0$. In this case Proposition 3.4 implies that if

$$h > -\Psi_0(A^{-1})/\beta$$

then there exists a solution of the Runge–Kutta equations (1.3). The existence of solutions for h sufficiently large is a rather curious result, contrary to intuition. It may be true that under the assumption (1.2) the Runge–Kutta equations (1.3) are soluble for any method with A invertible and any step-size $h > 0$, but our theory is not sufficient to show this.

It should be noted that there exist Runge–Kutta methods of arbitrary high order that satisfy the conditions of Theorem 3.5. The simplest example is the backward Euler scheme. The Butcher Gauss–Legendre methods [3] are DJ-irreducible and algebraically stable with A invertible and have order $2s$ where s is the number of stages. The methods based on Radau quadrature are also DJ irreducible and algebraically stable with A invertible.

Having shown the existence of solutions to the Runge–Kutta equations (1.3) for the dissipative systems defined by (1.1)–(1.2) we would like to also show uniqueness. This is not possible, however, and in Appendix B we give an example of a system of the form (1.1)–(1.2) for which the backward Euler method has multiple solutions with h arbitrarily small. However, it is possible to establish a local uniqueness result for solutions of (1.3); this is done in Proposition 3.9.

We now consider whether the numerical solution defined by a Runge–Kutta method is dissipative. We begin with an example which shows that a numerical discretization of (1.1)–(1.2) need not in general inherit the dissipativity of that system.

Example 3.6. Consider the class of linear scalar systems (1.8) with λ real and negative. Note that this system is dissipative and satisfies (1.2) with $\alpha = 0, \beta = -\lambda$. Solving numerically with the forward Euler method we obtain the numerical solution

$$y_n = (1 + h\lambda)^n y_0,$$

which is dissipative for $h < 2/(-\lambda)$. If $h > 2/(-\lambda)$ the numerical solution will become unbounded. Thus to ensure numerical dissipativity for linear problems we must impose an upper bound on the step size. By generalizing this example to arbitrary linear systems of the form

$$\frac{dy}{dt} = Ay,$$

where $\langle Ay, y \rangle \leq -\|y\|^2$ and A is diagonalizable, it is possible to show that A-stability is a necessary condition for a Runge–Kutta method to be dissipative for all $h > 0$.

For nonlinear problems the situation is worse; consider the numerical solution of

$$(3.12) \quad \frac{dy}{dt} = -y^3, \quad y(0) = y_0$$

using the forward Euler method. Note that $\langle f(y), y \rangle \leq 1 - y^2$ so that (3.12) defines a dissipative system of the form (1.1)–(1.2). The numerical solution has the property that if $|y_0| < \sqrt{2/h}$ then $|y_n| \rightarrow 0$ as $n \rightarrow \infty$, whereas if $|y_0| > \sqrt{2/h}$ then $|y_{n+1}| > |y_n|$ and $|y_n| \rightarrow \infty$. Hence the forward Euler is not dissipative for any $h > 0$.

Thus whenever a non–A-stable method is used to solve (1.1)–(1.2), a restriction must be imposed on the step size used to ensure dissipativity for linear problems. However, for nonlinear problems there is no obvious analogue of λ , and hence no simple bound to apply to the step size. To obtain robust numerical schemes, we must seek methods that are dissipative for any fixed step-size $h > 0$, and Example 3.6 implies that only A-stable methods should be considered. In fact, when seeking a class of methods for which the numerical approximation to the nonlinear problem (1.1)–(1.2) is dissipative, it is natural to restrict attention further and consider numerical approximation by algebraically stable methods, as is desirable for contractive nonlinear problems. This is what we now do. We wish to show that the map defined by the numerical method is dissipative, but as we have seen the numerical method need not define a unique map and (1.3) may have none, one, or many solutions. This forces us to use the generalized concept of dissipativity for multivalued maps from the previous section. Before we state our main result we give a preliminary lemma.

LEMMA 3.7. *Any solution of the Runge–Kutta defining equations (1.3)–(1.4) applied to (1.1) satisfies*

$$(3.13) \quad \|\mathbf{y}_{n+1}\|^2 = \|\mathbf{y}_n\|^2 + 2h \sum_{i=1}^s b_i \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_i) \rangle - h^2 \sum_{i,j=1}^s m_{ij} \langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle.$$

Proof. By (1.4)

$$(3.14) \quad \|\mathbf{y}_{n+1}\|^2 = \|\mathbf{y}_n\|^2 + 2h \sum_{i=1}^s b_i \langle \mathbf{y}_n, \mathbf{f}(\mathbf{Y}_i) \rangle + h^2 \sum_{i,j=1}^s b_i b_j \langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle.$$

Now (1.3) implies

$$\mathbf{y}_n = \mathbf{Y}_i - h \sum_{j=1}^s a_{i,j} \mathbf{f}(\mathbf{Y}_j),$$

hence

$$\langle \mathbf{y}_n, \mathbf{f}(\mathbf{Y}_i) \rangle = \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_i) \rangle - h \sum_{j=1}^s a_{i,j} \langle \mathbf{f}(\mathbf{Y}_j), \mathbf{f}(\mathbf{Y}_i) \rangle,$$

and substituting for $\langle \mathbf{y}_n, \mathbf{f}(\mathbf{Y}_i) \rangle$ in (3.14) implies the required result. \square

We now show that when a DJ-irreducible, algebraically stable Runge–Kutta method is applied to (1.1)–(1.2) the numerical solution retains the dissipativity of the underlying system.

THEOREM 3.8. *Suppose (1.1)–(1.2) is approximated numerically using a DJ-irreducible, algebraically stable Runge–Kutta method. Then for any fixed step-size $h > 0$ the map generated by the numerical method is dissipative (in the generalized sense of §2) and the open ball $B(0, R)$ is an absorbing set for any $R > \sqrt{\alpha/\beta} + hC(0, h)$ where C is defined in (3.20).*

Proof. Algebraic stability and (3.13) imply

$$(3.15) \quad \|\mathbf{y}_{n+1}\|^2 \leq \|\mathbf{y}_n\|^2 + 2h \sum_{i=1}^s b_i \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_i) \rangle.$$

Now since (1.2) holds it follows that

$$(3.16) \quad \begin{aligned} \|\mathbf{y}_{n+1}\|^2 &\leq \|\mathbf{y}_n\|^2 + 2h \sum_{i=1}^s b_i [\alpha - \beta \|\mathbf{Y}_i\|^2] \\ &= \|\mathbf{y}_n\|^2 + 2h [\alpha - \beta \|\mathbf{Y}\|_B^2]. \end{aligned}$$

Hence, given any $\varepsilon > 0$ it follows that either

$$(3.17) \quad \|\mathbf{y}_{n+1}\|^2 \leq \|\mathbf{y}_n\|^2 - 2h\beta\varepsilon$$

or, by (3.16),

$$(3.18) \quad \|\mathbf{Y}\|_B^2 \leq \frac{\alpha}{\beta} + \varepsilon.$$

Suppose that (3.18) holds and subtract (1.3) from (1.4) to yield

$$\mathbf{y}_{n+1} = \mathbf{Y}_i + h \sum_{j=1}^s e_{ij} \mathbf{f}(\mathbf{Y}_j),$$

where $e_{ij} = b_j - a_{ij}$, and take norms of both sides to give

$$\|\mathbf{y}_{n+1}\|^2 \leq \|\mathbf{Y}_i\|^2 + 2h \sum_{j=1}^s e_{ij} \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_j) \rangle + h^2 \left\| \sum_{j=1}^s e_{ij} \mathbf{f}(\mathbf{Y}_j) \right\|^2.$$

Recalling that $\sum_{i=1}^s b_i = 1$, multiply both sides by b_i and sum over i to obtain

$$\begin{aligned}
 \|\mathbf{y}_{n+1}\|^2 &\leq \|\mathbf{Y}\|_B^2 + 2h \sum_{i=1}^s \sum_{j=1}^s b_i e_{ij} \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_j) \rangle + h^2 \sum_{i=1}^s b_i \left\| \sum_{j=1}^s e_{ij} \mathbf{f}(\mathbf{Y}_j) \right\|^2 \\
 (3.19) \quad &\leq \frac{\alpha}{\beta} + \varepsilon + 2h \sum_{i=1}^s \sum_{j=1}^s b_i e_{ij} \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_j) \rangle + h^2 \sum_{i=1}^s b_i \left\| \sum_{j=1}^s e_{ij} \mathbf{f}(\mathbf{Y}_j) \right\|^2.
 \end{aligned}$$

Now let E be the $s \times s$ matrix with $\{E\}_{ij} = e_{ij}$ and note that

$$\begin{aligned}
 &2 \sum_{i=1}^s \sum_{j=1}^s b_i e_{ij} \langle \mathbf{Y}_i, \mathbf{f}(\mathbf{Y}_j) \rangle \\
 &+ h \sum_{i=1}^s b_i \left\| \sum_{j=1}^s e_{ij} \mathbf{f}(\mathbf{Y}_j) \right\|^2 = 2\mathbf{Y}^T (BE \otimes I_m) \mathbf{F}(\mathbf{Y}) + h \|(E \otimes I_m) \mathbf{F}(\mathbf{Y})\|_B^2.
 \end{aligned}$$

Define

$$(3.20) \quad C(\varepsilon, h) = \sup_{\|\mathbf{X}\|_B^2 \leq \alpha/\beta + \varepsilon} \left[2\mathbf{X}^T (BE \otimes I_m) \mathbf{F}(\mathbf{X}) + h \|(E \otimes I_m) \mathbf{F}(\mathbf{X})\|_B^2 \right]$$

and note that $C(\varepsilon, h)$ is a nonnegative continuous increasing function in both h and ε . Now (3.19) implies that

$$(3.21) \quad \|\mathbf{y}_{n+1}\|^2 \leq \frac{\alpha}{\beta} + \varepsilon + hC(\varepsilon, h).$$

Hence either (3.17) or (3.21) holds at each step and it follows trivially that the multivalued map generated by the numerical method is dissipative in the generalized sense of the previous section and that $B(0, \sqrt{\alpha/\beta + \varepsilon + hC(\varepsilon, h)})$ is an absorbing set. Since ε is arbitrary the result follows. \square

Remarks. (i) The DJ-irreducibility of the method is used in the definition of C . If $b_i = 0$ for some i then $\|\cdot\|_B$ is a semi-norm and the supremum in (3.20) may be unbounded. However, the solution sequence from a DJ-reducible method is equivalent to that from a DJ-irreducible method and hence all the results in this paper are easily extended to remove the DJ-irreducibility. However, most standard methods are DJ-irreducible and so we have not pursued this further.

(ii) Under the conditions of Theorem 3.8 a solution sequence $\{\mathbf{y}_n\}_{n=0}^\infty$ to (1.3)–(1.4) need not exist, but if such a sequence does exist then for n sufficiently large it enters, and then remains in, the absorbing set. If we assume in addition that A is invertible then Theorem 3.5 ensures that a solution sequence exists. Note also that Proposition 3.4 together with Theorem 3.5 imply an upper bound on $\|\mathbf{Y}\|_B^2$ for the solution of (1.3) at each step. We can also derive a bound on the solution at each step when A is not invertible. Since $\|\mathbf{y}_{n+1}\|^2 \geq 0$, it follows from (3.16) that if a solution to (1.3) exists then that solution satisfies

$$(3.22) \quad \|\mathbf{Y}\|_B^2 \leq \frac{\alpha}{\beta} + \frac{1}{2h\beta} \|\mathbf{y}_n\|^2.$$

(iii) From the proof of Theorem 3.8, by setting $\varepsilon = 0$ we deduce that for any $h > 0$ the ball

$$(3.23) \quad B(0, \sqrt{\alpha/\beta + hC(0, h)}),$$

where C is defined by (3.20), is positively invariant for the numerical method. By this we mean that if $\mathbf{y}_n \in B(0, \sqrt{\alpha/\beta + hC(0, h)})$ then $\mathbf{y}_{n+1} \in B(0, \sqrt{\alpha/\beta + hC(0, h)})$. Note however that the corresponding stage values \mathbf{Y}_i need not be contained in the positively invariant set.

(iv) Notice that $hC(0, h) \rightarrow 0$ as $h \rightarrow 0$, hence given any $\varepsilon > 0$ there exists $H(\varepsilon) > 0$ such that for $h < H(\varepsilon)$ the ball $B(0, \sqrt{\alpha/\beta + \varepsilon})$ is an absorbing set.

Although we cannot derive a global uniqueness result, and to prove global existence we needed to assume that A is invertible, we can prove a local existence and uniqueness result for (1.3) which will enable us to prove that the numerical method defines a dynamical system on the absorbing set.

In the following proposition, reproduced from Humphries [22], $N(B, \varepsilon)$ is the epsilon neighbourhood of B as defined in Definition 2.5.

PROPOSITION 3.9. *Suppose \mathbf{f} is Lipschitz on $N(B, \varepsilon)$ where B is some subset of \mathbb{R}^m and that M is finite where*

$$(3.24) \quad M = \sup_{\mathbf{y} \in N(B, \varepsilon)} \|\mathbf{f}(\mathbf{y})\|.$$

If

$$(3.25) \quad h < \min\left(\frac{\varepsilon}{aM}, \frac{1}{La}\right),$$

where L is the Lipschitz constant and a is as defined by (3.2), then for any $\mathbf{y}_n \in B$ there exists a unique solution of (1.3) such that

$$\|\mathbf{Y}_i - \mathbf{y}_n\| < \varepsilon \quad \forall i,$$

and hence $\mathbf{Y}_i \in B(\mathbf{y}_n, \varepsilon) \subseteq N(B, \varepsilon)$ for all i and the iteration (3.3) converges to this solution.

Remark. Proposition 3.9 is only a local result. For an implicit method it is possible that there exist additional solutions to (1.3) such that $\mathbf{Y}_i \notin N(B, \varepsilon)$ for some or all i .

In Proposition 3.9 no use is made of the dissipativity of \mathbf{f} induced by (1.2). It would be desirable to use (1.2) to show that when B is some appropriate neighbourhood of the absorbing set then there can be no solutions of (1.3) with any $\mathbf{Y}_i \notin N(B, \varepsilon)$. However, the nature of the bound given by (3.22) does not allow us to do this. If we fix $h > 0$ then (3.22) defines a set in which all solutions of (1.3) must lie. To ensure that there is a unique such solution we must also ensure that (3.25) is satisfied, but in general we cannot do this, since reducing h to satisfy (3.25) will enlarge the set defined by (3.22), which will in turn require a smaller h to satisfy (3.25), and so on.

By Theorem 3.8, if (1.1)–(1.2) is approximated numerically using a DJ-irreducible, algebraically stable Runge–Kutta method, then the numerical solution possesses an absorbing set. If we now consider the numerical method within this set, then by applying Proposition 3.9 we can prove that the numerical method defines a dynamical system for h sufficiently small.

THEOREM 3.10. *Suppose (1.1)–(1.2) is approximated numerically using a DJ-irreducible, algebraically stable Runge–Kutta method. Then for any $B = B(0, R)$, where $R > \sqrt{\alpha/\beta}$, and any neighbourhood $N = N(B, \varepsilon)$ of B there exists $H(B, N) > 0$ such that for $h \in (0, H)$, B is an absorbing set for the numerical solution. If the*

solution of (1.3) constructed in Proposition 3.9 is used then the numerical method defines a continuous dynamical system on B so that if $\mathbf{y}_0 \in B$ then $\mathbf{y}_n \in B$ for all $n \geq 0$, and, furthermore, the stage values $\mathbf{Y}_i \in N$ at each step.

Proof. Given a set B as above, then by Theorem 3.8 B is absorbing for $h < H_1(R)$ for some $H_1(R) > 0$. Now, to show that the numerical solution defines a dynamical system on B , first note that by Theorem 3.8, remark (iii), if $\mathbf{y}_n \in B$ then $\mathbf{y}_{n+1} \in B$. Now by Proposition 3.9, there exists $H_2(B, N) > 0$ such that if $h < H_2(B, N)$ and $\mathbf{y}_n \in B$ then (1.3) possesses a unique solution with $\mathbf{Y}_i \in N$ for all i . This defines a unique value of $\mathbf{y}_{n+1} \in B$ and thus the numerical method defines a discrete dynamical system on B .

To establish continuity of this dynamical system on B , let

$$\mathbf{Z}_i = \mathbf{z}_n + h \sum_{j=1}^s a_{ij} \mathbf{f}(\mathbf{Z}_j), \quad i = 1, \dots, s$$

and

$$\mathbf{z}_{n+1} = \mathbf{z}_n + h \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Z}_i).$$

Then

$$\mathbf{Y}_i - \mathbf{Z}_i = (\mathbf{y}_n - \mathbf{z}_n) + h \sum_{j=1}^s a_{ij} [\mathbf{f}(\mathbf{Y}_j) - \mathbf{f}(\mathbf{Z}_j)],$$

and letting

$$M = \max_{1 \leq j \leq s} \|\mathbf{Y}_j - \mathbf{Z}_j\|$$

and

$$(3.26) \quad \mathbb{A} = \max_{i \in \{1, \dots, s\}} \sum_{j=1}^s |a_{ij}|,$$

we obtain

$$(3.27) \quad \begin{aligned} \|\mathbf{Y}_i - \mathbf{Z}_i\| &\leq \|\mathbf{y}_n - \mathbf{z}_n\| + h \mathbb{A} \max_{1 \leq j \leq s} \|\mathbf{f}(\mathbf{Y}_j) - \mathbf{f}(\mathbf{Z}_j)\| \\ &\leq \|\mathbf{y}_n - \mathbf{z}_n\| + L \mathbb{A} h M. \end{aligned}$$

But (3.27) holds for all i and hence if $h < H_3 = 1/L\mathbb{A}$ it follows that

$$\begin{aligned} M &\leq \|\mathbf{y}_n - \mathbf{z}_n\| + L \mathbb{A} h M \\ &\leq \frac{1}{1 - L \mathbb{A} h} \|\mathbf{y}_n - \mathbf{z}_n\|. \end{aligned}$$

Furthermore, letting

$$(3.28) \quad \mathbb{B} = \sum_{i=1}^s |b_i|,$$

it follows that

$$\begin{aligned} \|\mathbf{y}_{n+1} - \mathbf{z}_{n+1}\| &\leq \|\mathbf{y}_n - \mathbf{z}_n\| + h \sum_{j=1}^s |b_j| \|\mathbf{f}(\mathbf{Y}_j) - \mathbf{f}(\mathbf{Z}_j)\| \\ &\leq \|\mathbf{y}_n - \mathbf{z}_n\| + h\mathbb{B}LM \\ &\leq \frac{1 + Lh(\mathbb{B} - \mathbb{A})}{1 - LAh} \|\mathbf{y}_n - \mathbf{z}_n\|, \end{aligned}$$

which proves continuity with respect to initial data. Thus the theorem holds with $H = \min(H_1, H_2, H_3)$. \square

Remark. (i) Since B is bounded the dynamical system defined on B in Theorem 3.10 is trivially dissipative, and its global attractor \mathcal{A}_h is given by $\mathcal{A}_h = \omega(B)$. Since the numerical method is dissipative on \mathbb{R}^m (in the generalized sense of §2) and all trajectories enter B , \mathcal{A}_h is also the global attractor for the numerical method on the full space \mathbb{R}^m .

(ii) If (1.3) is solved using the iteration (3.3) then by Proposition 3.9 this iteration converges to the solution of (1.3) that defines the discrete dynamical system in Theorem 3.10. If a different scheme is used to solve (1.3) then this scheme may converge to a different solution. However, since B is an absorbing set for the method, for n sufficiently large we expect to find a solution of (1.3) with \mathbf{Y}_i in a neighbourhood of B for all i , and we have proved that there exists a unique solution with this property; thus we may consider any other solution of (1.3) to be “wrong.” In practice we expect all sensible schemes for solving (1.3) to converge to the solution defined by (3.3) and thus the conclusions of Theorem 3.10 will hold for any reasonable implementation of (1.3)–(1.4).

We now prove upper semicontinuity of the global attractor for the numerical approximation to the dissipative system (1.1)–(1.2). The basic idea for the proof of Theorem 3.11 can be found in both Hale, Lin, and Raugel [17] and Temam [26]. In both of those works upper semicontinuity was proved for certain perturbations $S_\lambda(t)$ of an infinite dimensional evolution operator $S_{\lambda_0}(t)$. In addition to straightforward perturbations of the infinite dimensional system, the theory in [17], [26] covers the case where $S_\lambda(t)$ represents a finite dimensional spatial discretization of a partial differential equation, under certain conditions. We consider the case where the perturbed systems represent discrete maps generated by temporal discretization of an ordinary differential equation and show that the numerical attractor \mathcal{A}_h of an algebraically stable Runge–Kutta method is upper semicontinuous at $h = 0$. Roughly this says that every point on the numerical attractor is close to a point on the true attractor \mathcal{A} of (1.1)–(1.2). Note that due to the asymmetry of the distance function the converse need not be true, but in the next section we will prove such a converse result for dissipative gradient systems.

THEOREM 3.11. *Suppose (1.1)–(1.2) is approximated numerically using a DJ-irreducible, algebraically stable Runge–Kutta method. Then there exists $H > 0$ such that for $h < H$ the numerical solution possesses a global attractor \mathcal{A}_h that satisfies*

$$(3.29) \quad \text{dist}(\mathcal{A}_h, \mathcal{A}) \rightarrow 0 \quad \text{as } h \rightarrow 0$$

where \mathcal{A} is the global attractor of (1.1)–(1.2).

Proof. By Theorem 3.10 there exists $H_1 > 0$ such that if $h < H_1$ then $B = B(0, \sqrt{\alpha/\beta} + \varepsilon)$ is absorbing for the numerical method and hence $\mathcal{A}_h = \omega(B)$. Here we also assume that H_1 is sufficiently small so that the numerical method defines a

dynamical system on B . We denote the evolution operator for this dynamical system by S_h^n .

It remains to establish (3.29) only, which we will do by showing that, given any $\varepsilon > 0$, there exists $H(\varepsilon) > 0$ such that if $h \in (0, H(\varepsilon))$ then $\text{dist}(\mathcal{A}_h, \mathcal{A}) \leq \varepsilon$. To do this, note that if $\mathcal{A}_h \subseteq \overline{N}(\mathcal{A}, \varepsilon)$ then $\text{dist}(\mathcal{A}_h, \mathcal{A}) \leq \varepsilon$, and so it is sufficient to show that $\mathcal{A}_h \in \overline{N}(\mathcal{A}, \varepsilon)$ for all h sufficiently small.

Consider the underlying system (1.1)–(1.2). Since \mathcal{A} attracts B under $S(t)$ there exists $t_0 > 0$ such that $S(t)B \subseteq N(\mathcal{A}, \varepsilon/2)$ for all $t \geq t_0$. Also notice that Theorem 2.7 implies that $\mathcal{A} \subseteq B(0, \sqrt{\alpha/\beta})$ and hence it follows that $N(\mathcal{A}, \varepsilon) \subseteq B$.

By the classical convergence theorem for consistent numerical methods, for any $\mathbf{y}_0 \in B$ there exists $H_2(\mathbf{y}_0) > 0$ such that for any $h < H_2(\mathbf{y}_0)$

$$(3.30) \quad \|\mathbf{y}_n - \mathbf{y}(nh)\| \leq \varepsilon/2 \quad \text{if } nh \leq 2t_0.$$

Such an error bound is proved for Lipschitz \mathbf{f} in [21]. Since B is compact and the dynamical system (1.1)–(1.2) is continuous, there exists a uniform bound $H_2 > 0$ such that if $h < H_2$ then (3.30) holds for any $\mathbf{y}_0 \in B$. Hence if $h < \min(H_1, H_2)$ and integer n satisfies $t_0 \leq nh \leq 2t_0$ then for any $\mathbf{y}_0 \in B$

$$\begin{aligned} \text{dist}(\mathbf{y}_n, \mathcal{A}) &= \inf_{x \in \mathcal{A}} \|\mathbf{y}_n - x\| \\ &\leq \|\mathbf{y}_n - \mathbf{y}(nh)\| + \inf_{x \in \mathcal{A}} \|\mathbf{y}(nh) - x\| \\ &\leq \|\mathbf{y}_n - \mathbf{y}(nh)\| + \text{dist}(\mathbf{y}(nh), \mathcal{A}) \\ &< \varepsilon. \end{aligned}$$

Thus $S_h^n B \subseteq N(\mathcal{A}, \varepsilon)$ for all n such that $t_0 \leq nh \leq 2t_0$. We will establish by induction that $S_h^n B \subseteq N(\mathcal{A}, \varepsilon)$ for all integer $n : nh \geq t_0$. Suppose the result holds for integer $n : t_0 \leq nh \leq kt_0$ with $k \geq 2$ and consider integer n such that $kt_0 \leq nh \leq (k+1)t_0$. Choose m and p such that $n = m + p$, $t_0 \leq mh \leq 2t_0$, and p the smallest integer such that $ph \geq (k-1)t_0$; thus $ph \leq kt_0$. Then $S_h^n B = S_h^m S_h^p B$ and by the inductive hypothesis $S_h^p B \subseteq N(\mathcal{A}, \varepsilon) \subseteq B$. Thus $S_h^n B \subseteq S_h^m B$ and since $t_0 \leq mh \leq 2t_0$ it follows that $S_h^n B \subseteq N(\mathcal{A}, \varepsilon)$ and the induction argument is complete.

Finally recall that

$$\mathcal{A}_h = \bigcap_{m \geq 0} \overline{\bigcup_{n \geq m} S_h^n B}.$$

Since $S_h^n B \subseteq N(\mathcal{A}, \varepsilon)$ for all $n \geq n_0$, where n_0 is the smallest integer such that $n_0 h \geq t_0$, it follows that

$$\overline{\bigcup_{n \geq n_0} S_h^n B} \subseteq \overline{N}(\mathcal{A}, \varepsilon),$$

and hence $\mathcal{A}_h \subseteq \overline{N}(\mathcal{A}, \varepsilon)$ as required. \square

Remark. An alternative proof of this result, under the hypothesis that $\mathbf{f} \in C^1(U, \mathbb{R}^m)$, can be obtained by applying the result of Kloeden and Lorenz [23] as follows: they show that, for any uniformly asymptotically stable set (u.a.s.) Λ there is an approximating set Λ_h satisfying

$$\max\left(\text{dist}(\Lambda_h, \Lambda), \text{dist}(\Lambda, \Lambda_h)\right) \rightarrow 0 \quad \text{as } h \rightarrow 0.$$

In our application the global attractor \mathcal{A} is a u.a.s. and so we may take $\Lambda = \mathcal{A}$. The set Λ_h constructed in [23] is locally absorbing and hence for our problem, under the conditions of Theorem 3.11, globally absorbing. Thus $\mathcal{A}_h = \omega(\Lambda_h) \subseteq \Lambda_h$ so that

$$\text{dist}(\mathcal{A}_h, \mathcal{A}) \leq \text{dist}(\Lambda_h, \mathcal{A}) = \text{dist}(\Lambda_h, \Lambda)$$

and upper semicontinuity follows. Note that it is not necessary to assume global boundedness of f and its derivatives as in [23] since the a priori estimate provided by the absorbing set B avoids this.

Finally in this section we consider (1.1)–(1.2) under the additional assumption that f is globally Lipschitz. We can then prove that any Runge–Kutta method with positive weights is dissipative. We state all of the results for f globally Lipschitz in one theorem.

THEOREM 3.12. *If f is globally Lipschitz with Lipschitz constant L and (1.1)–(1.2) is approximated numerically by a Runge–Kutta method with $b_i > 0$ for all i then*

(i) *if*

$$(3.31) \quad h < H_1 = \frac{2\beta}{\rho^2 L^2 \mathbb{M}},$$

where $\rho = \max_i 1/b_i$ and $\mathbb{M} = \sum_{i,j=1}^s |m_{ij}|$, then the numerical solution is dissipative in the generalized sense of §2;

(ii) *if*

$$(3.32) \quad h < H_2 = \frac{1}{La}$$

then the numerical solution defines a dynamical system on \mathbb{R}^m ;

(iii) for $h < \min(H_1, H_2)$ the numerical solution defines a dissipative dynamical system on \mathbb{R}^m and possesses a global attractor \mathcal{A}_h that satisfies

$$\text{dist}(\mathcal{A}_h, \mathcal{A}) \rightarrow 0 \quad \text{as } h \rightarrow 0$$

where \mathcal{A} is the global attractor of (1.1)–(1.2).

Proof. To show dissipativity choose $\varepsilon > 0$ and let $k = 1 + (\varepsilon\beta/2\alpha)$ so that

$$\frac{k\alpha}{\beta} = \frac{\alpha}{\beta} + \frac{\varepsilon}{2}.$$

Recall Lemma 3.7 and apply (1.2) to obtain

$$\begin{aligned} \|\mathbf{y}_{n+1}\|^2 &\leq \|\mathbf{y}_n\|^2 + 2h \sum_{i=1}^s b_i [\alpha - \beta \|\mathbf{Y}_i\|^2] - h^2 \sum_{i,j=1}^s m_{ij} \langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle \\ &\leq \|\mathbf{y}_n\|^2 + 2h \left[\alpha - \beta \|\mathbf{Y}\|_B^2 \right] + h^2 \left\| \sum_{i,j=1}^s m_{ij} \langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle \right\| \\ &= \|\mathbf{y}_n\|^2 + 2h \left[\alpha - \frac{\beta}{k} \|\mathbf{Y}\|_B^2 \right] - 2h\beta \left(1 - \frac{1}{k} \right) \|\mathbf{Y}\|_B^2 \\ (3.33) \quad &+ h^2 \left\| \sum_{i,j=1}^s m_{ij} \langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle \right\|. \end{aligned}$$

The underlying system (1.1)–(1.2) has a fixed point \mathbf{x} such that $\|\mathbf{x}\| \leq \sqrt{\alpha/\beta}$ (see, for example, Constantin and Foias [5, Lem. 7.2]). Thus by Lipschitz continuity $\|\mathbf{f}(\mathbf{0})\| \leq L\sqrt{\alpha/\beta}$, and letting $c = L\sqrt{\alpha/\beta}$ implies

$$\begin{aligned} \|\mathbf{f}(\mathbf{Y}_i)\| &\leq L\|\mathbf{Y}_i\| + c \\ &\leq \rho b_i L\|\mathbf{Y}_i\| + c \\ &\leq \rho L\|\mathbf{Y}\|_B + c. \end{aligned}$$

Thus

$$\begin{aligned} |\langle \mathbf{f}(\mathbf{Y}_i), \mathbf{f}(\mathbf{Y}_j) \rangle| &\leq \|\mathbf{f}(\mathbf{Y}_i)\| \|\mathbf{f}(\mathbf{Y}_j)\| \\ &\leq (\rho L\|\mathbf{Y}\|_B + c)^2, \end{aligned}$$

and (3.33) implies

$$\begin{aligned} (3.34) \quad \|\mathbf{y}_{n+1}\|^2 &\leq \|\mathbf{y}_n\|^2 + 2h \left[\alpha - \frac{\beta}{k} \|\mathbf{Y}\|_B^2 \right] \\ &\quad - 2h\beta \left(1 - \frac{1}{k} \right) \|\mathbf{Y}\|_B^2 + h^2 \mathbb{M} (\rho L\|\mathbf{Y}\|_B + c)^2. \end{aligned}$$

Now assuming $\mathbb{M} \neq 0$ (otherwise the method is irreducible and algebraically stable and the previous theory applies) let

$$H = \min_{\|\mathbf{X}\|_B^2 \geq \alpha/\beta + \varepsilon} \frac{2\beta(1 - \frac{1}{k})\|\mathbf{X}\|_B^2}{\mathbb{M}(\rho L\|\mathbf{X}\|_B + c)^2}$$

and notice that the minimum is achieved with $\|\mathbf{X}\|_B^2 = \alpha/\beta + \varepsilon$ and that H is strictly positive. Suppose $h < H$, then by (3.34) and definition of H either

$$(3.35) \quad \|\mathbf{y}_{n+1}\|^2 \leq \|\mathbf{y}_n\|^2 + 2h \left[\alpha - \frac{\beta}{k} \|\mathbf{Y}\|_B^2 \right]$$

or

$$(3.36) \quad \|\mathbf{Y}\|_B^2 \leq \frac{\alpha}{\beta} + \varepsilon.$$

Suppose (3.35) holds and that

$$\|\mathbf{y}_{n+1}\|^2 \geq \|\mathbf{y}_n\|^2 - h\beta\varepsilon/k,$$

then by (3.35)

$$\begin{aligned} \|\mathbf{Y}\|_B^2 &\leq \frac{k\alpha}{\beta} + \frac{\varepsilon}{2} \\ &= \frac{\alpha}{\beta} + \varepsilon. \end{aligned}$$

Hence we have deduced that for $h < H$ either

$$\|\mathbf{y}_{n+1}\|^2 \leq \|\mathbf{y}_n\|^2 - h\beta\varepsilon/k$$

or (3.36) holds. Now follow the proof of Theorem 3.8 to deduce that (3.36) implies (3.21) holds and hence that the numerical solution is dissipative and that $B(0, \sqrt{\alpha/\beta + \varepsilon + hC(\varepsilon, h)})$ is an absorbing set.

Finally, notice that as $\|\mathbf{X}\|_B \rightarrow \infty$

$$\frac{2\beta(1 - \frac{1}{k})\|\mathbf{X}\|_B^2}{\mathbb{M}(\rho L\|\mathbf{X}\|_B + c)^2} \rightarrow \frac{2\beta(1 - \frac{1}{k})}{\rho^2 L^2 \mathbb{M}},$$

and as $\varepsilon \rightarrow \infty$

$$\frac{2\beta(1 - \frac{1}{k})}{\rho^2 L^2 \mathbb{M}} \rightarrow H_1.$$

Hence, given any $h < H_1$, for ε sufficiently large $h < H$ and the numerical solution is dissipative.

By Theorem 3.1 if (3.32) holds the numerical method defines a dynamical system on \mathbb{R}^m and continuity may be established as in the proof of Theorem 3.10. From (i) and (ii) for $h < \min(H_1, H_2)$ the numerical solution defines a dissipative dynamical system and possesses a global attractor \mathcal{A}_h . Convergence of the attractor follows from the proof of Theorem 3.11. \square

4. Gradient systems. In this section we consider the special case where the dissipative initial value problem (1.1)–(1.2) is in gradient form. We will assume throughout that $\mathbf{f} \in C^1(U, \mathbb{R}^m)$.

DEFINITION 4.1. *If (1.1) defines a dynamical system on $U \subseteq \mathbb{R}^m$ then (1.1) is said to define a gradient system if there exists $F: U \rightarrow \mathbb{R}$ satisfying*

- (i) $F(\mathbf{y}) \geq 0$ for all $\mathbf{y} \in U$,
- (ii) $F(\mathbf{y}) \rightarrow \infty$ as $\|\mathbf{y}\| \rightarrow \infty$,
- (iii) for a solution of (1.1) $F(S(t)\mathbf{y}_0)$ is nonincreasing in t , and
- (iv) if $F(S(t)\mathbf{y}_0) = F(\mathbf{y}_0)$ for $t > 0$ then $\mathbf{y}(0)$ is an equilibrium point.

F is called a Lyapunov functional.

This definition can be generalized, in a natural way, to dynamical systems generated by maps of the form

$$(4.1) \quad \mathbf{y}_{n+1} = \Phi_h(\mathbf{y}_n)$$

by replacing $S(t)$ with S_h^n and t with n in Definition 4.1. Throughout we assume that Φ_h is Lipschitz for mappings of the form (4.1).

Henceforth we consider the particular case where \mathbf{f} is a gradient vector field, so that

$$(4.2) \quad \mathbf{f}(\mathbf{y}) = -\nabla F(\mathbf{y}).$$

It is straightforward to show [19] that if (4.2) holds for some F then (iii) and (iv) of Definition 4.1 follow automatically, and hence that if F satisfies (i) and (ii) then (1.1), (4.2) define a gradient system. The following theorem shows that the dynamics of a gradient system must be relatively simple. Let $E = \{\mathbf{y}: \mathbf{f}(\mathbf{y}) = 0\}$. Then we have the following theorem.

THEOREM 4.2 [19]. *If (1.1) is a gradient system then $\omega(\mathbf{y}(0)) \subseteq E$. Furthermore, if the zeros of \mathbf{f} are isolated then $\omega(\mathbf{y}(0)) = x$ for some $x \in E$.*

Let $E_h = \{\mathbf{y}: \Phi_h(\mathbf{y}) = \mathbf{y}\}$. An analogous result to Theorem 4.2 holds for gradient mappings; related results may be found in [10] and [13].

THEOREM 4.3. *If (4.1) defines a gradient system with Φ_h Lipschitz on any bounded subset of U , then $\omega(\mathbf{y}_0) \subseteq E_h$. Furthermore, if the fixed points of Φ_h are isolated then $\omega(\mathbf{y}_0) = \mathbf{x}$ for some $\mathbf{x} \in E_h$.*

Proof. Note that the dynamical system is continuous since Φ_h is a Lipschitz function. Property (iii) in Definition 4.1 implies that $F(\mathbf{y}_n) \leq F(\mathbf{y}_0)$ for all n , and then property (ii) implies that $\bigcup_{n \geq 0} S_h^n \mathbf{y}_0$ is bounded. Thus $\overline{\bigcup_{n \geq 0} S_h^n \mathbf{y}_0}$ is compact and hence, by Lemma 2.1.2 in [16], it follows that $\omega(\mathbf{y}_0)$ is nonempty, compact, and invariant. If $\mathbf{x}_1, \mathbf{x}_2 \in \omega(\mathbf{y}_0)$ then it is clear that $F(\mathbf{x}_1) = F(\mathbf{x}_2)$, otherwise we obtain a contradiction to (iii) of Definition 4.1. Since $\omega(\mathbf{y}_0)$ is invariant it follows that $F(S_h^n \mathbf{x}) = F(\mathbf{x})$ for any $\mathbf{x} \in \omega(\mathbf{y}_0)$. Thus $\mathbf{x} \in E_h$ by Definition 4.1(iv).

Now assume that the fixed points of Φ_h are isolated. Since $\omega(\mathbf{y}_0)$ is compact it follows that $\omega(\mathbf{y}_0)$ contains a finite number of equilibria, say $\mathbf{x}_j, j = 1, \dots, J$. Let $B_j = B(\mathbf{x}_j, \delta), B^+ = \bigcup_{j=1, \dots, J} B_j$, and $B^- = \overline{B} \setminus B^+$ and assume that δ is sufficiently small that $\text{dist}(\mathbf{x}, B_k) \geq \Delta > 0$ for all $\mathbf{x} \in B_j, j \neq k$. Note that $\omega(\mathbf{y}_0)$ is nonempty; assume for the purposes of contradiction that $\mathbf{x}_1 \in \omega(\mathbf{y}_0)$ and that it is not the unique member of $\omega(\mathbf{y}_0)$. Then for all $\delta > 0$ there exists a sequence $n_i \rightarrow \infty$ such that $S_h^{n_i} \mathbf{y}_0 \in B_1$ and $S_h^{n_i} \mathbf{y}_0 \rightarrow \mathbf{x}_1$ as $n_i \rightarrow \infty$. Since \mathbf{x}_1 is not the unique limit point there is an infinite sequence of integers m_j such that $\mathbf{y}_{m_j} \in B_1$ and $\mathbf{y}_{m_j+1} \notin B_1$. Let L be the Lipschitz constant for Φ_h on B_1 , then since \mathbf{x}_1 is a fixed point, we deduce that

$$\|\mathbf{y}_{m_j+1} - \mathbf{x}_1\| = \|\Phi_h(\mathbf{y}_{m_j}) - \Phi_h(\mathbf{x}_1)\| \leq L\|\mathbf{y}_{m_j} - \mathbf{x}_1\| \leq L\delta.$$

Hence, if $L\delta < \Delta$ we deduce that $\mathbf{y}_{m_j+1} \in B^-$ for each j . But B^- is compact and hence the infinite sequence $\{\mathbf{y}_{m_j+1}\}_{j=1}^\infty$ must have a limit point; such a limit point cannot be contained in E_h by definition of B^- and hence we have obtained a contradiction. This completes the proof. \square

Before we consider the dissipative gradient system (1.1)–(1.2), (4.2) we will consider the gradient system (1.1), (4.2) under the assumption that \mathbf{f} is globally Lipschitz. For this system we will be able to show that every Runge–Kutta method preserves the underlying gradient structure for h sufficiently small. Whilst this result is not surprising, it will allow us to show that in the case of a gradient system where (1.2) is also satisfied then a dissipative numerical method preserves the gradient structure on the absorbing set. We can then show that the numerical attractor \mathcal{A}_h is both upper and lower semicontinuous at $h = 0$. We begin with two lemmas needed to prove that the numerical method preserves the gradient structure.

LEMMA 4.4. *Suppose (1.1), (4.2) defines a gradient system on a convex set $U \subseteq \mathbb{R}^m$ and \mathbf{f} is Lipschitz on U with Lipschitz constant L . Then*

$$(4.3) \quad F(\mathbf{u}) - F(\mathbf{v}) \leq \langle \mathbf{f}(\mathbf{v}), \mathbf{v} - \mathbf{u} \rangle + L\|\mathbf{v} - \mathbf{u}\|^2$$

for all $\mathbf{u}, \mathbf{v} \in U$.

Proof. Let $G(x): [0, 1] \rightarrow \mathbb{R}$ be defined by

$$G(x) = F(\mathbf{v} + x[\mathbf{u} - \mathbf{v}]).$$

Then we have

$$\begin{aligned} G'(x) &= \langle \nabla F(\mathbf{v} + x[\mathbf{u} - \mathbf{v}]), \mathbf{u} - \mathbf{v} \rangle \\ &= \langle \mathbf{f}(\mathbf{v} + x[\mathbf{u} - \mathbf{v}]), \mathbf{v} - \mathbf{u} \rangle. \end{aligned}$$

Now by the mean value theorem $G(1) - G(0) = G'(x)$ for some $x \in (0, 1)$. Hence writing $\boldsymbol{\xi} = \mathbf{v} + x[\mathbf{u} - \mathbf{v}]$ implies that

$$F(\mathbf{u}) - F(\mathbf{v}) = \langle \mathbf{f}(\boldsymbol{\xi}), \mathbf{v} - \mathbf{u} \rangle,$$

and since

$$\frac{\mathbf{v} - \mathbf{u}}{\|\mathbf{v} - \mathbf{u}\|} = \frac{\mathbf{v} - \boldsymbol{\xi}}{\|\mathbf{v} - \boldsymbol{\xi}\|},$$

it follows that

$$(4.4) \quad F(\mathbf{u}) - F(\mathbf{v}) = \frac{\|\mathbf{v} - \mathbf{u}\|}{\|\mathbf{v} - \boldsymbol{\xi}\|} \langle \mathbf{f}(\boldsymbol{\xi}), \mathbf{v} - \boldsymbol{\xi} \rangle.$$

Now since \mathbf{f} is globally Lipschitz and $\boldsymbol{\xi} \in U$ by convexity, use of the Cauchy–Schwarz inequality gives

$$\begin{aligned} \langle \mathbf{f}(\boldsymbol{\xi}) - \mathbf{f}(\mathbf{v}), \mathbf{v} - \boldsymbol{\xi} \rangle &\leq \|\mathbf{f}(\boldsymbol{\xi}) - \mathbf{f}(\mathbf{v})\| \cdot \|\mathbf{v} - \boldsymbol{\xi}\| \\ &\leq L\|\boldsymbol{\xi} - \mathbf{v}\|^2, \end{aligned}$$

and hence

$$\langle \mathbf{f}(\boldsymbol{\xi}), \mathbf{v} - \boldsymbol{\xi} \rangle \leq \langle \mathbf{f}(\mathbf{v}), \mathbf{v} - \boldsymbol{\xi} \rangle + L\|\mathbf{v} - \boldsymbol{\xi}\|^2.$$

Now applying this to (4.4) implies

$$\begin{aligned} F(\mathbf{u}) - F(\mathbf{v}) &\leq \frac{\|\mathbf{v} - \mathbf{u}\|}{\|\mathbf{v} - \boldsymbol{\xi}\|} \langle \mathbf{f}(\mathbf{v}), \mathbf{v} - \boldsymbol{\xi} \rangle + L\|\mathbf{v} - \boldsymbol{\xi}\| \cdot \|\mathbf{v} - \mathbf{u}\| \\ &\leq \frac{\|\mathbf{v} - \mathbf{u}\|}{\|\mathbf{v} - \boldsymbol{\xi}\|} \langle \mathbf{f}(\mathbf{v}), \mathbf{v} - \boldsymbol{\xi} \rangle + L\|\mathbf{v} - \mathbf{u}\|^2 \\ &= \langle \mathbf{f}(\mathbf{v}), \mathbf{v} - \mathbf{u} \rangle + L\|\mathbf{v} - \mathbf{u}\|^2, \end{aligned}$$

as required. \square

LEMMA 4.5. *Suppose \mathbf{f} is Lipschitz on $U \subseteq \mathbb{R}^m$ with Lipschitz constant L , $\mathbf{y}_n \in U$, $\mathbf{Y}_i \in U$ for all i and*

$$(4.5) \quad h < H_1 = \frac{1}{L\mathbb{A}(1 + \mathbb{B})}$$

where \mathbb{A} and \mathbb{B} are defined by (3.26) and (3.28), respectively. Then the numerical solution defined by (1.3)–(1.4) satisfies

$$(4.6) \quad \|\mathbf{f}(\mathbf{y}_n) - \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i)\| < \frac{L\mathbb{A}\mathbb{B}}{1 - L\mathbb{A}h(1 + \mathbb{B})} \|\mathbf{y}_{n+1} - \mathbf{y}_n\|.$$

Proof. In Lemma 2.4 of [22] it is shown that under the conditions of Lemma 4.5 the solution of (1.3)–(1.4) satisfies

$$(4.7) \quad \|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)\| < \frac{L\mathbb{A}h}{1 - L\mathbb{A}h} \|\mathbf{f}(\mathbf{y}_n)\| \quad \forall i = 1, \dots, s.$$

Recalling that $\sum_{i=1}^s b_i = 1$ and applying (4.7), we obtain

$$\begin{aligned} \left\| \mathbf{f}(\mathbf{y}_n) - \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) \right\| &= \left\| \sum_{i=1}^s b_i (\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)) \right\| \\ &\leq \mathbb{B} \max_i \|\mathbf{f}(\mathbf{y}_n) - \mathbf{f}(\mathbf{Y}_i)\| \\ &\leq \frac{Lh\mathbb{A}\mathbb{B}}{1 - Lh\mathbb{A}} \|\mathbf{f}(\mathbf{y}_n)\|. \end{aligned} \tag{4.8}$$

Note also that

$$\begin{aligned} \frac{1}{h} \|\mathbf{y}_{n+1} - \mathbf{y}_n\| &= \left\| \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) \right\| \\ &\geq \|\mathbf{f}(\mathbf{y}_n)\| - \left\| \mathbf{f}(\mathbf{y}_n) - \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) \right\|, \end{aligned}$$

and hence by (4.8)

$$(4.9) \quad \frac{1}{h} \|\mathbf{y}_{n+1} - \mathbf{y}_n\| \geq \frac{1 - Lh\mathbb{A}(1 + \mathbb{B})}{1 - Lh\mathbb{A}} \|\mathbf{f}(\mathbf{y}_n)\|.$$

Now the result follows on combining (4.8) and (4.9). \square

THEOREM 4.6. *If \mathbf{f} is globally Lipschitz with Lipschitz constant L and the gradient system (1.1), (4.2) is approximated numerically by an arbitrary Runge–Kutta method (1.3)–(1.4) then there exists $H > 0$ such that for $h < H$ the method defines a discrete gradient dynamical system on \mathbb{R}^m which has the same fixed points and the same Lyapunov functional as (1.1), (4.2).*

Proof. We establish (i)–(iv) of Definition 4.1. For the Lyapunov function we take $F(\bullet)$ and so (i) and (ii) follow automatically from the assumptions about the differential equation. With \mathbb{A} and \mathbb{B} defined by (3.26) and (3.28), suppose that h satisfies (4.5). Note that by consistency $\mathbb{B} \geq 1$ and the bound on the step size given by (4.5) is at least as restrictive as the bound in Theorem 3.1, and hence the numerical solution defines a dynamical system on \mathbb{R}^m if $h < H_1$. Now from (4.3)

$$\begin{aligned} F(\mathbf{y}_{n+1}) - F(\mathbf{y}_n) &\leq \langle \mathbf{f}(\mathbf{y}_n), \mathbf{y}_n - \mathbf{y}_{n+1} \rangle + L \|\mathbf{y}_{n+1} - \mathbf{y}_n\|^2 \\ &= \left(L - \frac{1}{h} \right) \|\mathbf{y}_{n+1} - \mathbf{y}_n\|^2 + \langle \mathbf{f}(\mathbf{y}_n) + \frac{1}{h}(\mathbf{y}_n - \mathbf{y}_{n+1}), \mathbf{y}_n - \mathbf{y}_{n+1} \rangle. \end{aligned}$$

Notice that

$$\begin{aligned} \frac{1}{h}(\mathbf{y}_{n+1} - \mathbf{y}_n) - \mathbf{f}(\mathbf{y}_n) &= \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) - \mathbf{f}(\mathbf{y}_n) \\ &= \sum_{i=1}^s b_i (\mathbf{f}(\mathbf{Y}_i) - \mathbf{f}(\mathbf{y}_n)), \end{aligned}$$

and hence

$$F(\mathbf{y}_{n+1}) - F(\mathbf{y}_n) \leq \left(L - \frac{1}{h} \right) \|\mathbf{y}_{n+1} - \mathbf{y}_n\|^2 + \|\mathbf{y}_{n+1} - \mathbf{y}_n\| \cdot \left\| \mathbf{f}(\mathbf{y}_n) - \sum_{i=1}^s b_i \mathbf{f}(\mathbf{Y}_i) \right\|.$$

Since \mathbf{f} is globally Lipschitz we can apply Lemma 4.5 with $U = \mathbb{R}^m$ and thus (4.6) implies that

$$\begin{aligned} F(\mathbf{y}_{n+1}) - F(\mathbf{y}_n) &\leq \left[L - \frac{1}{h} + \frac{L\mathbb{A}\mathbb{B}}{1 - Lh\mathbb{A}(1 + \mathbb{B})} \right] \|\mathbf{y}_{n+1} - \mathbf{y}_n\|^2 \\ &\leq \left[\frac{-1 + h[1 + L\mathbb{A}(1 + 2\mathbb{B})] - h^2[L\mathbb{A}(1 + \mathbb{B})]}{h - Lh^2\mathbb{A}(1 + \mathbb{B})} \right] \|\mathbf{y}_{n+1} - \mathbf{y}_n\|^2. \end{aligned}$$

Now if $h < H_2 = \gamma$ where γ is the smallest positive root of the quadratic equation $g(x) = 0$ where

$$g(x) = -1 + [1 + LA(1 + 2B)]x - [LA(1 + B)]x^2,$$

then $-1 + h[1 + LA(1 + 2B)] - h^2[LA(1 + B)] < 0$ and noting that (4.5) implies $1 - hLA(1 + B) > 0$, it follows that $F(\mathbf{y}_{n+1}) < F(\mathbf{y}_n)$ unless \mathbf{y}_n is a fixed point of the Runge–Kutta method. This establishes (iii) and (iv), and hence that numerical solution defines a discrete gradient system.

Finally note that by Theorem 2.5 of Humphries [22], if (4.5) holds then \mathbf{y} is a fixed point of the Runge–Kutta method if and only if $\mathbf{f}(\mathbf{y}) = 0$, so \mathbf{y} is also a fixed point of the continuous system. This establishes (iv) and thus the result holds with $H = \min(H_1, H_2)$. \square

Remark. If the weights b_i of the method (1.3)–(1.4) are nonnegative then $B = 1$ and $H_2 = 1/L(1 + A)$. If we also assume that $A \leq 1$ then $H_2 \leq H_1$ and the theorem holds with $H = 1/L(1 + A)$.

Now consider the dissipative gradient system (1.1)–(1.2), (4.2). Since the gradient system is dissipative we can apply Theorem 3.8 to show that for any algebraically stable Runge–Kutta method the numerical solution is dissipative for any $h > 0$. Moreover, we can also apply Theorem 3.10 to show that for h sufficiently small the method defines a discrete dynamical system on the absorbing set B , and the proof of Theorem 4.6 shows that this is in fact a gradient dynamical system with the same Lyapunov functional and fixed points as (1.1)–(1.2), (4.2). Applying Theorem 4.3 we thus obtain the following corollary.

COROLLARY 4.7. *Suppose that (1.1)–(1.2), (4.2) is approximated numerically using a DJ-irreducible, algebraically stable Runge-Kutta method. Then there exists $H > 0$ such that for $h < H$ the fixed points of the numerical method are the same as those of the underlying differential equation and $\omega(\mathbf{y}_0) \subseteq E$ for every $\mathbf{y}_0 \in \mathbb{R}^m$. Furthermore, if each member of E is isolated then $\omega(\mathbf{y}_0) = \mathbf{x}$ for some $\mathbf{x} \in E$.*

By Theorem 3.11 for h sufficiently small the numerical approximation to (1.1)–(1.2), (4.2) possesses a global attractor \mathcal{A}_h and $\text{dist}(\mathcal{A}_h, \mathcal{A}) \rightarrow 0$ as $h \rightarrow 0$. In the case where the fixed points of the gradient system are all hyperbolic we now derive the complimentary lower semicontinuity result; $\text{dist}(\mathcal{A}, \mathcal{A}_h) \rightarrow 0$ as $h \rightarrow 0$. We must first consider the form of the global attractor \mathcal{A} of the gradient system (1.1)–(1.2), (4.2), and to do this we need the concept of unstable manifolds.

DEFINITION 4.8. *If \mathbf{x}_0 is a hyperbolic fixed point of (1.1) then the unstable manifold of \mathbf{x}_0 is defined by*

$$W^u(\mathbf{x}_0) = \{\mathbf{y}: S(t)\mathbf{y} \text{ exists for } t \leq 0 \text{ and } S(t)\mathbf{y} \rightarrow \mathbf{x}_0 \text{ as } t \rightarrow -\infty\}.$$

For some $\delta > 0$ we define the local unstable manifold of \mathbf{x}_0 by

$$W^{u,\delta}(\mathbf{x}_0) = \{\mathbf{y} \in W^u(\mathbf{x}_0): S(t)\mathbf{y} \in \bar{B}(\mathbf{x}_0, \delta) \forall t \leq 0\}.$$

The unstable manifold of a set B is defined naturally by requiring that $\text{dist}(S(t)\mathbf{y}, B) \rightarrow 0$ as $t \rightarrow -\infty$. For a discrete dynamical system parameterized by h similar definitions can be made and we denote the unstable manifold of a fixed point \mathbf{x}_0 by $W_h^u(\mathbf{x}_0)$ and the local unstable manifold by $W_h^{u,\delta}(\mathbf{x}_0)$.

For a dissipative gradient system the global attractor is known (see Hale [16]) to be of the form

$$\mathcal{A} = W^u(E).$$

Since the system is dissipative E is bounded, and so if the fixed points are isolated then E is finite and it follows that

$$(4.10) \quad \mathcal{A} = \bigcup_{x \in E} W^u(x).$$

Beyn [1] considers the numerical approximation of the local stable and unstable manifolds in the neighbourhood of a hyperbolic fixed point. He shows that for both one-step and linear multistep methods, the numerical local stable and unstable manifolds converge to the local stable and unstable manifolds of the underlying system as $h \rightarrow 0$. The following lemma shows that near to the fixed point we can obtain numerical approximations to the unstable manifold of arbitrary accuracy. It is a special case of a result of Beyn, see [1] for the full generality.

LEMMA 4.9 [1]. *If $x \in U$ is a hyperbolic equilibrium of (1.1), where $f \in C^1(U, U)$ and (1.1) defines a dynamical system on U , then for any Runge–Kutta method (1.3)–(1.4), where the solution of (1.3) constructed in Proposition 3.9 is used, there exists $\Delta > 0$ such that for $0 < \delta < \Delta$ and any $\varepsilon > 0$ there exists $H(\delta, \varepsilon) > 0$ such that*

$$(4.11) \quad \text{dist}(W^{u,\delta}(x), W_h^{u,\delta}(x)) < \varepsilon$$

if $h < H$.

We will now prove that the numerical approximation to \mathcal{A} is lower semicontinuous at $h = 0$. The basic idea for the proof comes from Hale [16], [18], where the result is proved for certain perturbations of a gradient system with hyperbolic equilibria on a Banach space. In the sequel we will make use of the following Morse decomposition of \mathcal{A} as in Hale [16]. Let the set of fixed points of the system be $E = \{x_1, \dots, x_M\}$. Let $v_1 > v_2 > \dots > v_N$ be the distinct points of $\{F(x_1), \dots, F(x_M)\}$ and let B be an absorbing set for the gradient system, then define

$$(4.12) \quad E^k = \{x \in E: F(x) = v_k\},$$

$$(4.13) \quad U^k = \{x \in B: F(x) < v_k\},$$

$$(4.14) \quad W^k = \bigcup \{W^u(x): x \in E^k\},$$

$$(4.15) \quad \mathcal{A}^k = \bigcup_{j=k}^N W^j.$$

Notice that $\mathcal{A}^1 = \mathcal{A}$ while $\mathcal{A}^N = E^N$ since the unstable manifold of a point in E^N is the point itself. We will also require the fact that \mathcal{A}^k attracts all compact subsets of U^{k-1} (see Hale [16, Thm. 3.8.7]). Definitions analogous to (4.12)–(4.15) can be made for a dynamical system defined by a mapping provided that it defines a dynamical system on B . For this case we will use the same notation with a subscript h . Notice that since the global attractor must include the union of all unstable manifolds of fixed points, $\mathcal{A}_h^k \in \mathcal{A}_h$ for each k , and this is the only property required of the \mathcal{A}_h^k . We now use the decomposition to prove lower semicontinuity for the numerical method.

THEOREM 4.10. *Suppose the fixed points of the dissipative gradient system (1.1)–(1.2), (4.2) are all hyperbolic and that the system is approximated numerically using a DJ-irreducible algebraically stable Runge–Kutta method. Then there exists $H > 0$ such that for $h < H$ the numerical solution possesses a global attractor \mathcal{A}_h which satisfies*

$$\max(\text{dist}(\mathcal{A}_h, \mathcal{A}), \text{dist}(\mathcal{A}, \mathcal{A}_h)) \rightarrow 0 \quad \text{as } h \rightarrow 0.$$

Proof. By Theorem 3.11 $\text{dist}(\mathcal{A}_h, \mathcal{A}) \rightarrow 0$ as $h \rightarrow 0$ and thus it remains to prove that $\text{dist}(\mathcal{A}, \mathcal{A}_h) \rightarrow 0$ as $h \rightarrow 0$. It is sufficient to prove that given any $\varepsilon > 0$ there exists $H(\varepsilon)$ such that if $h < H(\varepsilon)$ then $\text{dist}(\mathcal{A}, \mathcal{A}_h) \leq \varepsilon$.

First note that hyperbolicity of the fixed points implies that the fixed points are isolated and hence that E is finite, since $E \subseteq B$ and B is bounded. Thus we can find $\delta > 0$ such that $\overline{B}(\mathbf{x}_i, \delta) \cap \overline{B}(\mathbf{x}_j, \delta) = \emptyset$ for $\mathbf{x}_i, \mathbf{x}_j \in E$ with $\mathbf{x}_i \neq \mathbf{x}_j$. Furthermore, by Lemma 4.9, we can pick δ so that given any $\varepsilon > 0$ there exists $H > 0$ such that for $h < H$ the bound (4.11) holds for all $\mathbf{x} \in E$. Choose such a δ and also choose an arbitrary $h_N > 0$.

Recall the notation and decomposition of \mathcal{A} defined before the statement of the theorem and note that $\mathcal{A}^N = E^N = E_h^N = \mathcal{A}_h^N$, since by Corollary 4.7 the numerical method has the same fixed points as the differential equation and since the unstable manifold of $\mathbf{x} \in E_h^N$ reduces to the points of E_h^N itself. Thus it follows that $\text{dist}(\mathcal{A}^N, \mathcal{A}_h^N) = 0$. Now we prove the result by induction. Suppose $\text{dist}(\mathcal{A}^k, \mathcal{A}_h^k) \leq \varepsilon/2^k$ for $h < h_k$. We will show that there exists h_{k-1} such that if $h < h_{k-1}$ then $\text{dist}(\mathcal{A}^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$. Notice that since $\mathcal{A}^{k-1} = W^{k-1} \cup \mathcal{A}^k$ it is sufficient to show that $\text{dist}(W^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$ as $\text{dist}(\mathcal{A}^k, \mathcal{A}_h^{k-1}) \leq \text{dist}(\mathcal{A}^k, \mathcal{A}_h^k) = \varepsilon/2^k$ and $\text{dist}(\mathcal{A}^{k-1}, \mathcal{A}_h^{k-1}) = \max(\text{dist}(W^{k-1}, \mathcal{A}_h^{k-1}), \text{dist}(\mathcal{A}^k, \mathcal{A}_h^{k-1}))$.

Let

$$\Gamma^{k-1} = \bigcup_{\mathbf{x} \in E^{k-1}} (W^{u,\delta}(\mathbf{x}) \cap \partial B(\mathbf{x}, \delta)).$$

Then Γ^{k-1} is compact and

$$W^{k-1} = \bigcup_{\mathbf{x} \in E^{k-1}} \{W^{u,\delta}(\mathbf{x})\} \cup \bigcup_{t \geq 0} S(t)\Gamma^{k-1}.$$

To establish that $\text{dist}(W^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$ we consider three separate cases for different subsets of W^{k-1} .

(a) Since $\Gamma^{k-1} \subset U^{k-1}$ and \mathcal{A}^k attracts all compact subsets of U^{k-1} there exists t_{k-1} such that $\text{dist}(S(t)\Gamma^{k-1}, \mathcal{A}^k) \leq \varepsilon/2^k$ for $t \geq t_{k-1}$. But by the inductive hypothesis $\text{dist}(\mathcal{A}^k, \mathcal{A}_h^k) \leq \varepsilon/2^k$ and hence

$$\begin{aligned} \text{dist}\left(\bigcup_{t \geq t_{k-1}} S(t)\Gamma^{k-1}, \mathcal{A}_h^{k-1}\right) &\leq \text{dist}\left(\bigcup_{t \geq t_{k-1}} S(t)\Gamma^{k-1}, \mathcal{A}_h^k\right) \\ &\leq \text{dist}\left(\bigcup_{t \geq t_{k-1}} S(t)\Gamma^{k-1}, \mathcal{A}^k\right) + \text{dist}(\mathcal{A}^k, \mathcal{A}_h^k) \\ &\leq \frac{\varepsilon}{2^{k-1}}. \end{aligned}$$

(b) Given t_{k-1} and h_k by Lemma 4.9, we may choose $h_{k-1}^{(1)}$ such that for $h < h_{k-1}^{(1)}$

$$(4.16) \quad \text{dist}(W^{u,\delta}(\mathbf{x}), W_h^{u,\delta}(\mathbf{x})) < \frac{\varepsilon}{2^k e^{L(t_{k-1}+h_k)}} < \frac{\varepsilon}{2^{k-1}}$$

for all $\mathbf{x} \in E^{k-1}$, where L is the Lipschitz constant for \mathbf{f} on B . So

$$\text{dist}(W^{u,\delta}(\mathbf{x}), \mathcal{A}_h^{k-1}) < \frac{\varepsilon}{2^{k-1}},$$

since $W_h^{u,\delta}(\mathbf{x}) \subseteq \mathcal{A}_h^{k-1}$.

(c) Now it remains to show that $\text{dist}(S(t)\Gamma^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$ for $t \in [0, t_{k-1}]$. Notice first that by Lipschitz continuity on any absorbing set B

$$\frac{d}{dt} \| (S(t)\mathbf{x} - S(t)\mathbf{x}') \|^2 \leq 2L \| S(t)\mathbf{x} - S(t)\mathbf{x}' \|^2$$

and hence

$$(4.17) \quad \| S(t)\mathbf{x} - S(t)\mathbf{x}' \| \leq e^{Lt} \| \mathbf{x} - \mathbf{x}' \|.$$

We can also choose $h_{k-1}^{(2)} > 0$ such that for $h < h_{k-1}^{(2)}$ and any $\mathbf{y}_0 \in B$

$$(4.18) \quad \| S_h^n \mathbf{y}_0 - S(nh)\mathbf{y}_0 \| \leq \frac{\varepsilon}{2^k} \quad \text{for } nh \leq t_{k-1} + h_k.$$

Let $h_{k-1} = \min(h_{k-1}^{(1)}, h_{k-1}^{(2)}, h_k)$. Suppose $h < h_{k-1}$ and that $\mathbf{x} \in S(t)\Gamma^{k-1}$ for $t \in [0, t_{k-1}]$. Then there exists $\mathbf{y}_0 \in \overline{B}(\mathbf{x}^*, \delta) \cap W^u(\mathbf{x}^*)$ for some $\mathbf{x}^* \in E^{k-1}$ such that $S(nh)\mathbf{y}_0 = \mathbf{x}$ and $nh \in [0, t_{k-1} + h_k]$. By (4.16) there exists $\mathbf{y}_0^* \in W_h^u(\mathbf{x}^*)$ such that

$$(4.19) \quad \| \mathbf{y}_0 - \mathbf{y}_0^* \| \leq \frac{\varepsilon}{2^k e^{L(t_{k-1} + h_k)}}.$$

Now

$$\begin{aligned} \| \mathbf{x} - S_h^n \mathbf{y}_0^* \| &= \| S(nh)\mathbf{y}_0 - S_h^n \mathbf{y}_0^* \| \\ &\leq \| S(nh)\mathbf{y}_0 - S(nh)\mathbf{y}_0^* \| + \| S(nh)\mathbf{y}_0^* - S_h^n \mathbf{y}_0^* \|. \end{aligned}$$

Applying (4.17) and (4.19) to the first term on the right-hand side and (4.18) to the second term implies

$$\| \mathbf{x} - S_h^n \mathbf{y}_0^* \| \leq \frac{\varepsilon}{2^{k-1}},$$

and thus since $S_h^n \mathbf{y}_0^* \in \mathcal{A}_h^{k-1}$ it follows that $\text{dist}(\mathbf{x}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$. But \mathbf{x} is an arbitrary point in $\bigcup_{t \in [0, t_{k-1}]} S(t)\Gamma^{k-1}$, hence

$$\text{dist} \left(\bigcup_{t \in [0, t_{k-1}]} S(t)\Gamma^{k-1}, \mathcal{A}_h^{k-1} \right) \leq \frac{\varepsilon}{2^{k-1}}.$$

Facts (a), (b), and (c) establish that $\text{dist}(W^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$ and complete the proof of the inductive step. Hence, if $\text{dist}(\mathcal{A}^k, \mathcal{A}_h^k) \leq \varepsilon/2^k$ for $h < h_k$ then there exists h_{k-1} such that if $h < h_{k-1}$ then $\text{dist}(\mathcal{A}^{k-1}, \mathcal{A}_h^{k-1}) \leq \varepsilon/2^{k-1}$. Since the result is true for $k = N$ the induction holds and setting $k = 1$ we deduce that

$$\text{dist}(\mathcal{A}^1, \mathcal{A}_h^1) \leq \varepsilon \quad \text{for } h \leq h_1.$$

Since $\mathcal{A} \equiv \mathcal{A}^1$ and $\mathcal{A}_h^1 \subseteq \mathcal{A}_h$ we have shown that, given any $\varepsilon > 0$, $\text{dist}(\mathcal{A}, \mathcal{A}_h) \leq \varepsilon$ for h sufficiently small, as required. \square

Remark. The assumption that the system is in gradient form is *not* necessary to the proof that $\text{dist}(\mathcal{A}, \mathcal{A}_h) \rightarrow 0$ as $h \rightarrow 0$. The proof of Theorem 4.10 explicitly uses the Morse decomposition of \mathcal{A} induced by the gradient structure. However, a new method of proof of lower semicontinuity is presented in [20], which does not require that the system is in gradient form, but for which it is sufficient for the attractor to have the form

$$\mathcal{A} = \overline{\bigcup_{\mathbf{x} \in E} W^u(\mathbf{x})},$$

where E is the set of hyperbolic equilibria of the system.

Appendix A. Consider the well known Lorenz system of ordinary differential equations in \mathbb{R}^3 defined by

$$(A.1) \quad \begin{cases} \dot{x} &= \sigma(y - x), \\ \dot{y} &= rx - y - xz, \\ \dot{z} &= xy - bz, \end{cases}$$

where $x(t)$, $y(t)$, and $z(t)$ are to be found for $t \geq 0$ and σ , r , and b are positive parameters. This system was first introduced by Lorenz [24] and arises as a finite-dimensional spectral truncation of equations governing Rayleigh–Bénard convection.

If we write $\mathbf{y} = (x, y, z)^T$ and $\mathbf{f}(\mathbf{y}) = (\sigma(y - x), rx - y - xz, xy - bz)^T$ then we see that this system is of the form (1.1) with $\mathbf{f} \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ and hence locally Lipschitz. To show that the Lorenz equations define a dissipative system we translate the origin by $z \mapsto z - r - \sigma$, obtaining

$$(A.2) \quad \begin{cases} \dot{x} &= \sigma(y - x), \\ \dot{y} &= -\sigma x - y - xz, \\ \dot{z} &= xy - bz - b(r + \sigma). \end{cases}$$

Now defining \mathbf{y} as above and \mathbf{f} by $\mathbf{f}(\mathbf{y}) = (\sigma(y - x), -\sigma x - y - xz, xy - bz - b(r + \sigma))^T$ and using the Euclidean inner product we obtain

$$(A.3) \quad \langle \mathbf{f}(\mathbf{y}), \mathbf{y} \rangle = -\sigma x^2 - y^2 - bz^2 - bz(r + \sigma).$$

Temam [26] shows that if $b > 1$ then (A.3) implies that

$$(A.4) \quad \langle \mathbf{f}(\mathbf{y}), \mathbf{y} \rangle \leq -\sigma x^2 - y^2 - z^2 + \frac{b^2(r + \sigma)^2}{4(b - 1)}$$

and hence

$$(A.5) \quad \langle \mathbf{f}(\mathbf{y}), \mathbf{y} \rangle \leq \alpha - \beta \|\mathbf{y}\|^2,$$

where

$$(A.6) \quad \alpha = \frac{b^2(r + \sigma)^2}{4(b - 1)},$$

$$(A.7) \quad \beta = \min(1, \sigma).$$

Hence the translated Lorenz equations (A.2) define a system of the form (1.1)–(1.2).

Next we show that the Lorenz equations do not satisfy a one-sided Lipschitz condition (1.10) for any c , and hence that the existence and uniqueness theory developed for Runge–Kutta methods applied to (1.1), (1.10) cannot be applied when solving the Lorenz equations numerically.

THEOREM A.1. *The Lorenz equations (A.1) do not satisfy (1.10) for any $c > 0$ for the Euclidean inner product on \mathbb{R}^3 .*

Proof. Let $\mathbf{u} = (x, y, z)^T$ and $\mathbf{v} = (x', y', z')^T$. Then

$$\mathbf{f}(\mathbf{u}) = \begin{bmatrix} \sigma(y - x) \\ rx - y - xz \\ xy - bz \end{bmatrix}$$

and $\mathbf{f}(\mathbf{v})$ is defined similarly. Now

$$\begin{aligned} \langle \mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle &= \sigma(x - x') \left[(y - x) - (y' - x') \right] + (z - z') \left[b(z' - z) + xy - x'y' \right] \\ &\quad + (y - y') \left[r(x - x') + (y' - y) + (x'z' - xz) \right] \\ &= -\sigma(x - x')^2 - (y - y')^2 - b(z - z')^2 \\ &\quad + (x - x') \left[(y'z - z'y) + (r + \sigma)(y - y') \right]. \end{aligned}$$

Now suppose that (1.10) holds. Let

$$\mathbf{u} = [\beta, \alpha, \beta]^T, \quad \mathbf{v} = [\alpha, \beta, \alpha]^T,$$

where we will specify the constants α and β below in order to obtain a contradiction. Notice that

$$\|\mathbf{u} - \mathbf{v}\|^2 = 3(\beta - \alpha)^2$$

and observe that

$$\begin{aligned} \langle \mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle &= -(\sigma + 1 + b)(\beta - \alpha)^2 + (\beta - \alpha) \left[(\beta^2 - \alpha^2) + (r + \sigma)(\alpha - \beta) \right] \\ &= \left[(\beta + \alpha) - (r + 2\sigma + 1 + b) \right] (\beta - \alpha)^2 \\ &= \frac{1}{3} \left[(\beta + \alpha) - (r + 2\sigma + 1 + b) \right] \|\mathbf{u} - \mathbf{v}\|^2. \end{aligned}$$

Now choose α and β such that $\beta + \alpha > 3c + r + 2\sigma + 1 + b$ to contradict (1.10). \square

It is easy to show that a translation of (1.1) satisfies a one-sided Lipschitz condition if and only if (1.1) satisfies a one-sided Lipschitz condition, and hence it follows that no translation of the Lorenz equations satisfies a one-sided Lipschitz condition.

In [21] general inner products on \mathbb{R}^3 are considered and an extension of the proof of Theorem A.1 is used to show that the Lorenz equations (A.1) do not satisfy a one-sided Lipschitz condition (1.10) for any inner product on \mathbb{R}^3 .

Appendix B. We will show that there is no general global uniqueness result for the solution of (1.3) by an algebraically stable method when \mathbf{f} satisfies (1.2). To do this we will consider the backward Euler method in one dimension and will exhibit an f which satisfies (1.2) but for which the backward Euler method can have multiple solutions for h arbitrarily small. In one dimension the backward Euler method is defined by

$$(B.1) \quad y_{n+1} = y_n + hf(y_{n+1}).$$

For a given y_n if $h = 0$ then it is trivial that (B.1) is uniquely soluble with $y_{n+1} = y_n$. We can use the implicit function theorem to continue this solution for $h > 0$. Define

$$(B.2) \quad G(y, h) = y - hf(y) - y_n,$$

then $y_{n+1} = y$ is a solution of (B.1) if and only if $G(y, h) = 0$. We know $G(y_n, 0) = 0$ and by the implicit function theorem we can continue this solution in h provided $\partial G / \partial y \neq 0$. Now since

$$\frac{\partial G}{\partial y} = 1 - h \frac{df}{dy(y)}$$

we can extend the solution branch provided $h(df/dy) \neq 1$. If we were to suppose a global bound on df/dy , say

$$(B.3) \quad \frac{df}{dy}(y) \leq c,$$

for all $y \in \mathbb{R}$ then the implicit function theorem gives the existence of a locally unique solution for $h < 1/c$. In fact the solution branch thus defined must be globally unique since two such branches would have to coincide at $h = 0$, contradicting the local uniqueness.

When restricted to one dimension the one-sided Lipschitz condition (1.10) is equivalent to (B.3) and so existence and uniqueness of solutions for the backward Euler method follow in this case.

Equation (1.2) does not imply an upper bound on df/dy , however, and this allows us to construct an example of a system of the form (1.1)–(1.2) for which the backward Euler method admits multiple solutions for any $h > 0$. Suppose

$$(B.4) \quad f(y) = -2y + 2 \sin(y^2),$$

then

$$\begin{aligned} \langle y, f(y) \rangle &= -2y^2 + 2y \sin(y^2) \\ &\leq -2y^2 + y^2 + \sin(y^2) \\ &\leq 1 - y^2, \end{aligned}$$

so f defined by (B.4) satisfies (1.2). We will show the existence of multiple solutions of the backward Euler method for arbitrarily small h for this f . Note that

$$(B.5) \quad \frac{df}{dy}(y) = 4y \cos(y^2) - 2.$$

Let $y = \sqrt{2k\pi}$ for $k = 1, 2, 3, \dots$. Then

$$\frac{df}{dy}(\sqrt{2k\pi}) = 4\sqrt{2k\pi} - 2$$

and since $4\sqrt{2k\pi} - 2 \rightarrow \infty$ as $k \rightarrow \infty$ there is no upper bound on df/dy . We construct multiple solutions graphically. Define $g(y)$ by

$$(B.6) \quad g(y) = f(\sqrt{2k\pi}) + m(y - \sqrt{2k\pi})$$

for $m > 0$ and some positive integer k . Plot $f(y)$ and $g(y)$ against y . In Fig. 1 this is done for $k = 2$. By construction the two lines intersect at $(\sqrt{2k\pi}, f(\sqrt{2k\pi}))$. If we also assume that

$$m < \frac{df}{dy}(\sqrt{2k\pi})$$

then the two lines must also intersect at two other points. Now define y_n by $g(y_n) = 0$ and let $h = 1/m$. Then (B.6) can be rewritten as

$$g(y) = \frac{1}{h}(y - y_n)$$

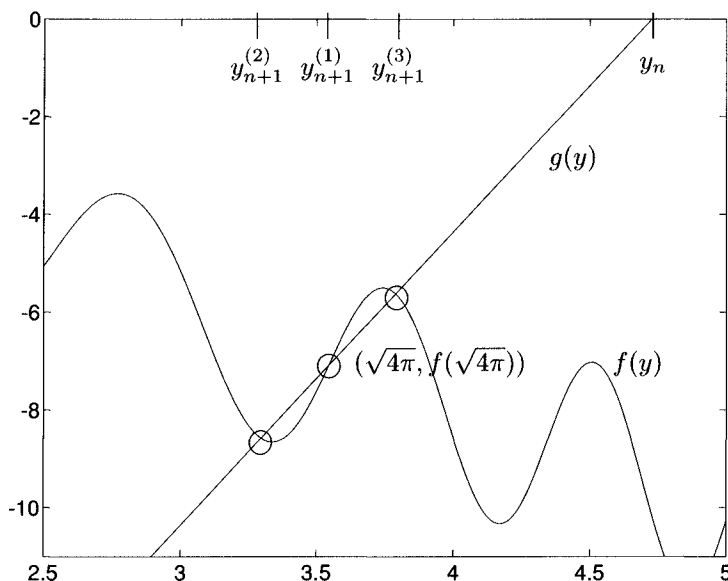


FIG. 1. Graph of $f(y)$ and $g(y)$ against y with multiple solutions indicated.

or

$$y = y_n + hg(y).$$

Hence the three intersections of this line with the graph of $f(y)$ define three solutions of the backward Euler method for this h and this y_n . Since $h = 1/m$ we can do this for

$$h \frac{df}{dy}(\sqrt{2k\pi}) > 1,$$

which implies

$$h > \frac{1}{4\sqrt{2k\pi} - 2}.$$

Since k is an arbitrary positive integer, given any $h > 0$ we can construct multiple solutions for this step size by choosing k sufficiently large; however, note that the y_n resulting in multiple solutions satisfy $|y_n| \rightarrow \infty$ as $h \rightarrow 0$.

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