

ON THE NUMERICAL APPROXIMATION OF PHASE PORTRAITS NEAR STATIONARY POINTS *

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Abstract. We show that the phase portrait of a dynamical system near a stationary hyperbolic point is reproduced correctly by numerical methods such as one-step methods or multi-step methods satisfying a strong root condition. This means that any continuous trajectory can be approximated by an appropriate discrete trajectory, and vice versa, to the correct order of convergence and uniformly on arbitrarily large time intervals. In particular, the stable and unstable manifolds of the discretization converge to their continuous counterparts.

Key words. numerical methods, dynamical system, phase portrait, stationary point

AMS (MOS) subject classifications. 65L05, 65L20

1. Introduction. We consider an m -dimensional autonomous system

$$(1.1) \quad x'(t) = f(x(t)), \quad t \geq 0, \quad x(t) \in \mathbb{R}^m$$

and compare its trajectories with sequences $x(0), x(h), x(2h), \dots$ generated by a one-step method with uniform step-size h

$$(1.2) \quad x(t+h) = x(t) + hf_h(x(t)), \quad t = 0, h, \dots$$

Our aim is to compare the trajectories of both systems on large time intervals. Classical estimates give error bounds of the form $\exp(Lt)h^r$ where r is the order of the method and L is a Lipschitz constant for f in some domain containing the continuous trajectory. Therefore, the numerical values may completely deviate from the continuous ones after sufficiently long time. Whether this really happens clearly depends on the asymptotic properties of the dynamical system itself.

A simple situation occurs if all trajectories of (1.1) in some bounded domain converge to one and the same stable equilibrium. Then, for sufficiently small h , this property carries over to the discrete system (1.2) and both trajectories stay close for all times (see [13, Chap 3.5] for results of this type).

However, if the system has some kind of sensitive dependence on initial conditions then the discrete and continuous trajectories starting at the same point will go apart after some time even if h is small and if the trajectories of (1.1) stay bounded for all times. The simplest situation of this type occurs in the neighbourhood of unstable stationary points. There the behaviour of the trajectories strongly depends on which side of the stable manifold they start.

This is the situation which we analyze in this paper. We show that in fact any continuous trajectory can be approximated by a discrete trajectory within the order of the method if we allow the discrete initial value to be adjusted. Similarly, any discrete trajectory approximates some continuous trajectory with a suitably chosen starting point. These estimates hold for sufficiently small h and as long as the trajectories stay within some neighbourhood of the stationary point. For initial values on the stable manifold the time interval is in fact infinite. The adapted initial values actually depend on the continuous trajectory which precludes us from using our construction numerically. Rather, our results, in particular the reverse statement, should be taken as an

* Received by the editors September 25, 1985; accepted for publication (in revised form) September 25, 1986.

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indication in which sense numerical computations with (1.2) are still reliable for phase portraits containing unstable modes.

Let us state in more technical terms the approximation problem for the trajectories. For some open set $\Omega \subset \mathbb{R}^m$ we denote by $\bar{x}(t; x_0)$ the solution of (1.1) with $x(0) = x_0$ and maximal interval of existence $J(x_0) = [0, T(x_0))$ in Ω . Similarly, let $x^h(t; y_0) \in \Omega$ be the solution of (1.2) with initial value $y_0 \in \Omega$ and maximal grid of existence $J^h(y_0) = \{0, \dots, Nh\}$, $N \in \mathbb{N} \cup \{\infty\}$. We then ask for conditions on f and Ω such that certain constants $C > 0$, $h_0 > 0$ with the following property can be found. For any $x_0 \in \Omega$ and $h \leq h_0$ there exists $y_0 = y_0(x_0, h) \in \Omega$ satisfying

$$(1.3) \quad \sup \{ \|\bar{x}(t; x_0) - x^h(t; y_0)\| : t \in J(x_0) \cap J^h(y_0) \} \leq Ch^r.$$

Also, to any $y_0 \in \Omega$, $h \leq h_0$ there should exist some $x_0 = x_0(y_0, h) \in \Omega$ which satisfies (1.3). These relations will be obtained for neighbourhoods Ω of hyperbolic points ξ_0 of (1.1), i.e.,

$$(1.4) \quad f(\xi_0) = 0 \text{ and } \operatorname{Re} \lambda \neq 0 \text{ for all eigenvalues } \lambda \text{ of } f'(\xi_0).$$

Our approach will be motivated in § 2 for the constant coefficient case. Again it is crucial that we only consider integration up to a certain finite bound. This is reasonable since in more realistic systems nonlinear effects will usually prevent trajectories from exponential growth to infinity. Sections 3 and 4 contain the main results on one-step and multi-step methods. In addition to (1.3) we show that the mappings from (1.2) have stable and unstable manifolds which converge to their continuous counterparts. For multi-step methods we impose the strong root conditions and use some decoupling techniques as in [5]. Section 5 concludes with some numerical tests of the relation (1.3) in two global cases not directly covered by our results. In particular, we consider a two-dimensional example where Ω contains three stationary points, two stable and one unstable.

Let us finally comment on systems (1.1) with more complicated dynamics where the condition (1.3) seems to be somewhat too restrictive. For instance, for systems with periodic orbits the discrete and continuous trajectories certainly run out of phase after some time. Nevertheless it is possible to get estimates for the Hausdorff distance of the trajectories [1] and to obtain approximating invariant curves [1], [4]. For systems with strange attractors or chaotic behaviour such as the Lorenz system [9], [12] it seems no longer appropriate to compare single trajectories at all. Rather one should compare attracting sets of (1.1) and (1.2) (see the remarkable recent paper [7]) or certain quantities measured from the trajectories such as Lyapunov exponents [8, Chap. 2.9].

Above all, we want to emphasize that our main interest is in the longtime behaviour of (1.2) in the asymptotic case $h \rightarrow 0$. It is well known that, if h is taken too large, the recursion (1.2) may exhibit all kinds of chaotic behaviour [4], [11], [14], whereas (1.1) behaves nicely. In this case, however, (1.2) should rather be considered as a discrete model in its own right than as a numerical method for the system (1.1).

2. The constant coefficient case. Consider the scalar equation

$$(2.1) \quad x' = \lambda x, \quad x(0) = x_0$$

with solution $\bar{x}(t; x_0, \lambda) = x_0 e^{\lambda t}$ and the one-step method

$$(2.2) \quad (x_{j+1} - x_j)h^{-1} = \alpha(\lambda x_{j+1}) + (1 - \alpha)\lambda x_j, \quad j = 0, 1, \dots$$

with solution $x_j = x^h(jh; x_0, \lambda, \alpha) = x_0 g_\alpha(h\lambda)^j$ where $g_\alpha(z) = (1 + (1 - \alpha)z)(1 - \alpha z)^{-1}$, $\alpha \in [0, 1]$. Then, for any sector in the negative half plane

$$S = S(\gamma, \sigma) = \{z \in \mathbb{C} : \operatorname{Re} z \leq 0, |\operatorname{Im} z| \leq \gamma |\operatorname{Re} z|, |z| \leq \sigma\}$$

one easily finds constants $C > 0, h_0 > 0$ such that

$$(2.3) \quad |\bar{x}(jh; x_0, \lambda) - x^h(jh; x_0, \lambda, \alpha)| \leq C(|\lambda| h)^r$$

for all $h \leq h_0, \lambda \in S, \alpha \in [0, 1]$ and $|x_0| \leq 1$. Here, $r = 2$ if $\alpha = \frac{1}{2}$ and $r = 1$, otherwise.

Now we consider the unstable case $\lambda \in -S, \lambda \neq 0$. For $0 < |x_0| \leq 1$ the solution of (2.1) reaches the unit circle at time $T = -\ln |x_0| (\operatorname{Re} \lambda)^{-1}$. We then define

$$(2.4) \quad N = [Th^{-1}], \quad x_f = x_0 \exp(\lambda Nh), \quad y_0 = x_f (g_\alpha(h\lambda))^{-N}.$$

For h sufficiently small, we have $|x_f| \leq 1, |y_0| \leq 1$ and, by a simple calculation, $\bar{x}(jh; x_0, \lambda) = \bar{x}((N-j)h; x_f, -\lambda), x^h(jh; y_0, \lambda, \alpha) = x^h((N-j)h; x_f, -\lambda, 1 - \alpha)$. We may therefore apply (2.3) with x_f in place of x_0 and obtain

$$(2.5) \quad |\bar{x}(jh; x_0, \lambda) - x^h(jh; y_0, \lambda, \alpha)| \leq C(|\lambda| h)^r$$

for all $h \leq h_0, \lambda \in -S, 0 \leq j \leq N, \alpha \in [0, 1]$. This proves our assertion (1.3) with $\Omega = \{z \in \mathbb{C} : |z| \leq 1\}$ for all $\lambda \in S \cup (-S)$.

Notice that y_0 is actually scaled up in case $\lambda > 0, \alpha < \frac{1}{2}$. Moreover, the scaling (2.4) of the initial value x_0 in the unstable case is necessary if we want (1.3) to hold with a constant C independent of x_0 . For example, consider Euler's method for (2.1) with fixed $\lambda > 0$. For $N = [h^{-2}\lambda^{-2} + 1], x_0 = e^{-Nh}$, we have $\bar{x}(Nh; x_0) = 1$ but $x^h(Nh; x_0) = \exp(N(\ln(1 + h\lambda) - h\lambda)) = \exp(N(-\frac{1}{2}h^2\lambda^2 + O((h\lambda)^3))) \leq \exp(-\frac{1}{2} + O(h\lambda))$.

The generalization of the result (1.3) from the scalar equation (2.1) to a system with constant coefficients

$$(2.6) \quad x' = Ax, \quad \operatorname{Re} \lambda \neq 0 \text{ for all eigenvalues } \lambda \text{ of } A$$

proceeds in the standard way. Assume that A can be put into diagonal form so that (2.6) decouples into m scalar equations. Choose an appropriate sector S where $S \cup (-S)$ contains all eigenvalues of A and apply the above result. Transforming back gives the desired result for the α -dependent one-step method applied to (2.6). The general procedure for finding an appropriate y_0 in (1.3) is therefore to keep the stable components of x_0 but to adjust the unstable ones.

3. One-step methods near hyperbolic points. In the neighbourhood of a hyperbolic point the flow of the system (1.1) is dominated by its linear part. All trajectories staying in this neighbourhood for all times form the stable manifold which is tangent to the stable subspace of the linearization (we use [6] as a reference for this classical theory). For initial values x_0 on the stable manifold the supremum in (1.3) will be taken over an infinite set. This suggests as a first step the construction of the stable manifold for the one-step method. In fact, this step is crucial and it turns out that our proof can then be adapted for starting points off the stable manifold.

We start with some notation. For $\varepsilon > 0$ let $K_\varepsilon = \{x \in \mathbb{R}^m : \|x\| \leq \varepsilon\}$ where the norm will be specified later. We assume that 0 is a stationary, hyperbolic point of the system (1.1). The local stable and unstable manifolds at 0 with respect to some $\varepsilon_0 \geq \varepsilon > 0$ are then defined by

$$M_s = \{x \in K_{\varepsilon_0} : \bar{x}(t; x) \in K_{\varepsilon_0} \forall t \geq 0 \text{ and } \bar{x}(t, x) \rightarrow 0 \text{ as } t \rightarrow \infty\},$$

$$M_u = \{x \in K_{\varepsilon_0} : \bar{x}(t; x) \in K_{\varepsilon_0} \forall t \leq 0 \text{ and } \bar{x}(t, x) \rightarrow 0 \text{ as } t \rightarrow -\infty\}.$$

Further, let $X_s, X_u \subset \mathbb{R}^m$ be the stable and unstable subspace for the hyperbolic linear vector field $f'(0)$ ([6, Chap. 4]) such that

$$\mathbb{R}^m = X_s \oplus X_u, \quad (x_s, x_u) = x \in \mathbb{R}^m, \quad \|x\| = \text{Max}(\|x_s\|, \|x_u\|).$$

It is well known that M_s, M_u may be represented as graphs

$$M_s = \{(x_s, p(x_s)): x_s \in K_{\varepsilon,s}\}, \quad M_u = \{(q(x_u), x_u): x_u \in K_{\varepsilon,u}\}$$

where the functions $p: K_{\varepsilon,s} = K_\varepsilon \cap X_s \rightarrow K_{\varepsilon,u} = K_\varepsilon \cap X_u$, and $q: K_{\varepsilon,u} \rightarrow K_{\varepsilon,s}$ are as smooth as f .

Our consistency assumptions on the one-step method (1.2) are

$$(3.1) \quad f_h \rightarrow f \text{ and } f'_h \rightarrow f' \text{ as } h \rightarrow 0 \text{ uniformly in some } K_\rho, \rho > 0,$$

$$(3.2) \quad \|(\bar{x}(h; x_0) - x_0)h^{-1} - f_h(x_0)\| = O(h^r) \text{ uniformly for } x_0 \in K_\rho.$$

Then it is easy to show (e.g., by Theorem 3.2 below) that (1.2) has a unique fixed point $x_h \in K_{\tilde{\rho}}$ for some $\tilde{\rho} \leq \rho$ and h sufficiently small. Moreover, $x_h = O(h^r)$. However, all commonly used one-step methods even satisfy

$$(3.3) \quad f(x) = 0 \Rightarrow f_h(x) = 0 \text{ for all } h.$$

Therefore, we may assume 0 to be the fixed point of (1.2) for all h , which leads to some technical simplifications. The local stable and unstable manifold of the one-step method are defined by

$$M_s^h = \{x \in K_\varepsilon: x^h(nh; x) \in K_{\varepsilon_0} \forall n \in \mathbb{N}, x^h(nh; x) \rightarrow 0 \text{ as } n \rightarrow \infty\},$$

$$M_u^h = \{x \in K_\varepsilon: x^h(nh; x) \in K_{\varepsilon_0} \forall n \in -\mathbb{N}, x^h(nh; x) \rightarrow 0 \text{ as } n \rightarrow -\infty\}.$$

Our principal result is as follows:

THEOREM 3.1. *Let 0 be a hyperbolic point of (1.1) and let (3.1)–(3.3) hold. Then there exist constants $C^*, \varepsilon, \varepsilon_0, h_0 > 0$ such that M_s^h and M_u^h ($h \leq h_0$) are of the form*

$$(3.4) \quad M_s^h = \{(x_s, p^h(x_s)): x_s \in K_{\varepsilon,s}\}, \quad M_u^h = \{(q^h(x_u), x_u): x_u \in K_{\varepsilon,u}\}$$

where $p^h = p + O(h^r)$ uniformly in $K_{\varepsilon,s}$ and $q^h = q + O(h^r)$ uniformly in $K_{\varepsilon,u}$. Moreover, for any $x_0 \in K_\varepsilon$ and any $h \leq h_0$, there exists a $y_0 = y_0(x_0, h) \in K_{\varepsilon_0}$ satisfying

$$(3.5) \quad \sup \{\|\bar{x}(nh; x_0) - x^h(nh; y_0)\|: \bar{x}(t; x_0) \in K_\varepsilon \text{ for } 0 \leq t \leq nh\} \leq C^* h^r.$$

Correspondingly, for any $y_0 \in K_{\varepsilon_0}$ and any $h \leq h_0$, there exists $x_0 = x_0(y_0, h) \in K_{\varepsilon_0}$ with

$$(3.5) \text{ where the sup is now taken over all } n \text{ satisfying } x^h(jh; y_0) \in K_\varepsilon, j = 0, \dots, n.$$

The proof needs several steps. First, we compare M_s and M_s^h by using the graph mapping technique ([6, Chap. 6]). Let S_0 be the Banach space of sequences $\gamma(n) \in \mathbb{R}^m$ converging to 0 with norm

$$\|\gamma\|_\infty = \sup \{\|\gamma(n)\|: n \in \mathbb{N}\} \text{ and let } S_\varepsilon = \{\gamma \in S_0: \|\gamma\|_\infty \leq \varepsilon\}.$$

We construct M_s^h by solving the equation

$$(3.6) \quad T_h(\gamma) = (x_s, 0), \quad x_s \in K_{\varepsilon,s}$$

where $T_h: S_\rho \rightarrow X_s \times S_0$ is defined by $T_h(\gamma) = (\gamma(0)_s, h^{-1}(\gamma(n+1) - \gamma(n)) - f_h(\gamma(n)), n \geq 0)$. We apply to (3.6) the following Lipschitz inverse mapping theorem ([6, Appendix C11], for the stability inequality see [3], note also that the use of this theorem avoids any manipulation of (3.6) as in [6, (6.7)]).

THEOREM 3.2. *Let $A: X \rightarrow Y$ be a linear homeomorphism between Banach spaces X and Y . Further assume that, for some $x_0 \in X$, $\delta_0 > 0$, the mapping $F: K_{\delta_0}(x_0) \rightarrow Y$ is Lipschitz with constant $\kappa < \sigma \leq \|A^{-1}\|^{-1}$. Then the equation $(A + F)(x) = y$ has a unique solution $x \in K_{\delta_0}(x_0)$ for each $y \in K_\delta(Ax_0 + Fx_0)$, $\delta = \delta_0(\sigma - \kappa)$. Moreover, the following stability inequality holds*

$$(3.7) \quad \|x_1 - x_2\| \leq (\sigma - \kappa)^{-1} \|(A + F)(x_1) - (A + F)(x_2)\| \quad \forall x_1, x_2 \in K_{\delta_0}(x_0).$$

Let us write $T_h = A_h + F_h$ where

$$A_h(\gamma) = (\gamma(0)_s, h^{-1}(\gamma(n+1) - \gamma(n)) - f'(0)\gamma(n), n \geq 0), \text{ and}$$

$$F_h(\gamma) = (0, (f'(0) - f_h)(\gamma(n)), n \geq 0).$$

We estimate $\|A_h^{-1}\|$ uniformly in h by using the following lemmata.

LEMMA 3.3. *Let the $m \times m$ -matrix Q be a hyperbolic automorphism in \mathbb{R}^m with stable and unstable summands X_s, X_u and with skewness $\text{Max}(\|Q_s\|, \|Q_u^{-1}\|) \leq \alpha < 1$ ([6, (4.19)]). Then the linear mapping*

$$B: \begin{cases} S_0 \rightarrow X_s \times S_0, \\ \gamma \rightarrow (\gamma(0)_s, \gamma(n+1) - Q\gamma(n), n \geq 0), \end{cases}$$

is a homeomorphism and satisfies

$$\|B^{-1}(x_s, \eta)\|_\infty \leq \|x_s\| + (1 - \alpha)^{-1} \|\eta\|_\infty \quad \text{for } x_s \in X_s, \eta \in S_0.$$

Proof. A solution γ of $B\gamma = (x_s, \eta)$ is given by

$$\gamma(n)_s = Q_s^n x_s + \sum_{j=0}^{n-1} Q_s^{n-1-j} \eta(j)_s, \quad \gamma(n)_u = - \sum_{j=n}^{\infty} Q_u^{n-1-j} \eta(j)_u.$$

It is readily verified that $\gamma(n) \rightarrow 0$ as $n \rightarrow \infty$ as well as

$$\|\gamma(n)\| = \text{Max}(\|\gamma(n)_s\|, \|\gamma(n)_u\|) \leq \|x_s\| + (1 - \alpha)^{-1} \|\eta\|_\infty.$$

Finally, B is invertible since $B\gamma = (0, 0)$, $\gamma \in S_0$ implies $\gamma(n)_s = 0$ for all $n \in \mathbb{N}$ and $\gamma(0)_u = Q_u^{-n} \gamma(n)_u \rightarrow 0$ as $n \rightarrow \infty$. \square

LEMMA 3.4. *Let Q be a stable $m \times m$ -matrix (i.e., all eigenvalues have negative real part) and let the function $g(z) = 1 + z + O(z^2)$ be real analytic in a neighbourhood of $0 \in \mathbb{C}$. Then there exist constants $h_0 > 0$, $\beta > 0$ and a norm on \mathbb{R}^m such that*

$$(3.8) \quad \|g(hQ)\| \leq 1 - h\beta \quad \text{for all } h \leq h_0.$$

Proof. It is well known [6, (4.37)] that there exists a norm on \mathbb{R}^m and some $\beta > 0$ such that $\|\exp(hQ)\| \leq e^{-h\beta}$ for all $h \geq 0$. Since $g(z) = e^z + O(z^2)$, it is obvious that (3.8) holds with the same norm for sufficiently small h . \square

Applying Lemma 3.4 to $g(z) = 1 + z$, $Q = f'(0)_s$ and $g(z) = (1 - z)^{-1}$, $Q = -f'(0)_u$, we find $h_0, \beta > 0$ and norms on X_s and X_u which are independent of h such that

$$\|I + hf'(0)_s\| \leq 1 - h\beta, \quad \|(I + hf'(0)_u)^{-1}\| \leq 1 - h\beta \quad \text{for } h \leq h_0.$$

Lemma 3.3 then shows that $A_h\gamma = (x_s, \eta) \in X_s \times S_0$ has a unique solution and

$$\|A_h^{-1}(x_s, \eta)\|_\infty \leq \|x_s\| + (1 - (1 - h\beta))^{-1} \|h\eta\|_\infty = \|x_s\| + \beta^{-1} \|\eta\|_\infty.$$

We may therefore take $\sigma = \text{Max}(1, \beta^{-1})$ in Theorem 3.2. Using (3.1) we find $h_0, \delta_0 > 0$ such that F_h is Lipschitz in S_{δ_0} with constant $\kappa = \sigma/2$ for all $h \leq h_0$. Then, with $x_0 = 0$, Theorem 3.2 assures a unique solution $\gamma = \gamma(x_s, h) \in S_{\delta_0}$ of (3.6) for all $x_s \in K_{\delta, s}$, $\delta = \delta_0\sigma/2$. This proves the representation of M_s^h in (3.4) for $p^h(x_s) = [\gamma(x_s, h)(0)]_u$ and with δ, δ_0 in place of $\varepsilon, \varepsilon_0$. Moreover, we have

$$(3.9) \quad \|\gamma_1 - \gamma_2\|_\infty \leq 2\sigma^{-1} \|T_h(\gamma_1) - T_h(\gamma_2)\|_\infty \quad \text{for all } \gamma_1, \gamma_2 \in S_{\delta_0}, h \leq h_0.$$

For any initial value $x_0 = (x_{0s}, p(x_{0s})) \in M_s$, we choose the discrete initial value $y_0 = (x_{0s}, p^h(x_{0s}))$. Setting $\gamma_1(n) = \bar{x}(nh; x_0)$ and $\gamma_2 = \gamma(x_{0s}, h)$ in (3.9) and using (3.2), we have our assertion (3.5). In particular, $\|x_0 - y_0\| = \|p(x_{0s}) - p^h(x_{0s})\| \leq C^* h^r$.

The corresponding result on the unstable manifolds is obtained via the time reversed systems

$$x' = \tilde{f}(x) := -f(x), \quad x(t+h) = x(t) + h\tilde{f}_h(x(t))$$

where $\tilde{f}_h(x) = h^{-1}((I + hf_h)^{-1}(x) - x)$. One verifies that $I + hf_h$ is locally diffeomorphic and that \tilde{f}_h, \tilde{f} satisfy (3.1), (3.2). Then our above result applies.

Next we consider initial values $x_0 \notin M_s$. For any $N \in \mathbb{N}$ and $h > 0$, we define $T_{hN} : \mathbb{R}^{m(N+1)} \rightarrow X_s \times \mathbb{R}^{mN} \times X_u$ by

$$(3.10) \quad T_{hN}(\gamma) = (\gamma(0)_s, h^{-1}(\gamma(n+1) - \gamma(n)) - f_h(\gamma(n)) (0 \leq n \leq N-1), \gamma(N)_u).$$

In quite an analogous fashion as above, we then find positive constants δ_0, δ, h_0 such that

$$(3.11) \quad T_{hN}(\gamma) = (x_1, 0, x_2), \quad x_1 \in K_{\delta,s}, \quad x_2 \in K_{\delta,u}$$

has a unique solution in $K_{\delta_0} \subset \mathbb{R}^{m(N+1)}$ for all $h \leq h_0$ and $N \in \mathbb{N}$ (taking suitable minima, we may assume δ_0 and δ to be the same as in the proof for the stable manifold M_s^h). Moreover, T_{hN} satisfies a stability inequality with a stability constant independent of h and N . For $x_0 \in K_\delta \setminus M_s$ the time $\tau = \sup \{t \geq 0 : \bar{x}([0, t]; x_0) \subset K_\delta\}$ is finite (cf. [6, (6.8)]). Let $\tilde{\gamma}$ denote the solution of (3.11) with $N = [\tau h^{-1}]$, $x_1 = x_{0s}$, $x_2 = \bar{x}(Nh; x_0)_u$. Then we set $y_0 = \tilde{\gamma}(0)$ and find the estimate (3.5) from the stability inequality for T_{hN} applied to $\gamma_1 = \tilde{\gamma}$, $\gamma_2(n) = \bar{x}(nh; x_0)$.

Finally, let us start with some discrete initial value $y_0 \in K_\delta$ and some $h \leq h_0$. In case $y_0 = (y_{0s}, p^h(y_{0s})) \in M_s^h$, we use $x_0 = (y_{0s}, p(y_{0s}))$ so that (3.5) has already been proved. For the remaining case, introduce the exact one-step function $\tilde{f}_h(x) = (\bar{x}(h; x) - x)h^{-1}$ and for any $N \in \mathbb{N}$ the operator \tilde{T}_{hN} as in (3.10) with f_h replaced by \tilde{f}_h . Since \tilde{f}_h satisfies (3.1), we obtain the same properties for \tilde{T}_{hN} as for T_{hN} . Then we let $x_0 = \tilde{\gamma}(0)$ where $\tilde{\gamma}$ solves (3.11) with $T_{hN} = \tilde{T}_{hN}$, $x_1 = y_{0s}$, $N = \sup \{n \in \mathbb{N} : x^h(jh; y_0) \in K_\delta \text{ for } j=0, \dots, n\}$ and $x_2 = x^h(Nh; y_0)_u$. From $0 = h^{-1}(\tilde{\gamma}(n+1) - \bar{x}(h; \tilde{\gamma}(n)))$, $0 \leq n \leq N-1$ we find $\tilde{\gamma}(n) = \bar{x}(nh; x_0)$ and then (3.5) by using the stability inequality for \tilde{T}_{hN} with $\gamma_1 = \tilde{\gamma}$, $\gamma_2(n) = x^h(nh; y_0)$. This completes the proof of Theorem 3.1.

Remarks. Theorem 3.1 does not exactly state the relation (1.3) for $\Omega = K_\varepsilon$ because ε_0 may be greater than ε in general. However, this is not very important since $x_0 \in K_\varepsilon$ and $y_0(x_0, h) = x_0 + O(h^r)$. We also note that y_0 is actually determined by a discrete boundary value problem (3.11). The boundary values are given by the continuous solution so that this fact cannot be used numerically. The only exception occurs when 0 is asymptotically stable, in which case we may put $y_0 = x_0$ (cf. [13, Chap. 3.5]).

4. Multi-step methods near hyperbolic points. In this section we generalize our results on the longtime behaviour of one-step methods to multi-step methods of the form

$$(4.1) \quad h^{-1} \sum_{j=0}^k \alpha_j x(t+jh) = f_h(x(t), \dots, x(t+kh)), \quad t=0, h, \dots$$

The solution of this system with starting values x_0, \dots, x_{k-1} will be denoted by $x^h(t; x_0, \dots, x_{k-1})$. As for one-step methods it is crucial to consider first the approximation of the stable manifold. In the present case this amounts to finding all starting values $(x_0, \dots, x_{k-1}) \in \mathbb{R}^{mk}$ which by (4.1) yield a sequence converging to the stationary

point. We will show that these starting values form a manifold in \mathbb{R}^{mk} which is of dimension $m(k-1)+d$ where $d = \dim X_s$. The additional $m(k-1)$ dimensions are caused by the exponentially decaying spurious solutions of the multi-step method. We will also see that a suitable d -dimensional submanifold of this large manifold yields the proper starting values for approximating continuous trajectories within the stable manifold. A similar analysis can then be carried out for trajectories off the stable manifold. Throughout we use the well known technique of rewriting (4.1) as a one-step method in \mathbb{R}^{mk} .

Finally we use our results to deal with the case where (4.1) is completed by a starting procedure (see Theorem 4.3).

Our basic consistency assumptions for the multi-step method are:

- (H1) For some open set $\Omega \subset \mathbb{R}^m$ and some numbers $\beta_j, j = 0, \dots, k, f_h \in C^1(\Omega^{k+1}, \mathbb{R}^m)$, f'_h is equicontinuous on Ω^{k+1} , $f_h(x, \dots, x) \rightarrow f(x)$ and $(\partial f_h / \partial x_j)(x, \dots, x) \rightarrow \beta_j f'(x)$ ($j = 0, \dots, k$) as $h \rightarrow 0$ and uniformly in Ω ,

$$\sum_{j=0}^k \alpha_j = 0, \quad \sum_{j=0}^k j\alpha_j = \sum_{j=0}^k \beta_j = 1, \quad \alpha_k \neq 0.$$

- (H2) There exists a $C > 0$ such that any solution $\bar{x}(t), 0 \leq t \leq T$ of (1.1) in Ω satisfies

$$\sup_{0 \leq t \leq T-hk} \left\| h^{-1} \sum_{j=0}^k \alpha_j \bar{x}(t+jh) - f_h(\bar{x}(t), \dots, \bar{x}(t+kh)) \right\| \leq Ch^r.$$

The stability requirement is the strong root condition which is also used in [5].

- (H3) 1 is a simple root of the characteristic polynomial $p(z) = \sum_{j=0}^k \alpha_j z^j$ and all other roots of p lie inside the unit circle.

For any stationary hyperbolic point $x_0 \in \Omega$ it follows again easily from (H1), (H2) that there exist fixed points $x_h \in \Omega$ of (4.1) (i.e., $f_h(x_h, \dots, x_h) = 0$) for sufficiently small h such that $x_h = x_0 + O(h^r)$. But, since the common multi-step methods satisfy $f(x) = 0 \Rightarrow f_h(x, \dots, x) = 0$, we use the convenient assumption as follows:

- (H0) 0 is a stationary hyperbolic point of (1.1) as well as a fixed point of the multi-step method for all h .

THEOREM 4.1. Assume (H0)-(H3), then there exist constants $\varepsilon, \varepsilon_0, h_0, C^* > 0$ with the following property. For any $x_0 \in K_\varepsilon$ and any $h \leq h_0$ there exist starting values $y_0, \dots, y_{k-1} \in K_{\varepsilon_0}$ satisfying

$$(4.2) \quad \sup \{ \|\bar{x}(nh; x_0) - x^h(nh; y_0, \dots, y_{k-1})\| : \bar{x}([0, nh]; x_0) \subset K_\varepsilon \} \leq C^* h^r.$$

In particular, if x_0 is on the stable manifold of the stationary point 0, then $x^h(nh; y_0, \dots, y_{k-1}) \rightarrow 0$ as $n \rightarrow \infty$.

Proof. Let us rewrite (4.1) as a one-step method $\Phi^h(z(t), z(t+h)) = 0, t = 0, h, \dots$ where $z(t) = (x(t), \dots, x(t+(k-1)h)) \in \mathbb{R}^{mk}$. Furthermore,

$$(4.3) \quad \Phi^h(z, y) = \left(h^{-1}(z_j - y_{j-1}) \cdot (1 \leq j \leq k-1), D_{hk}^{-1} \left[h^{-1}(\alpha_k y_{k-1} + \sum_{j=0}^{k-1} \alpha_j z_j) - f_h(z, y_{k-1}) \right] \right)$$

for $z = (z_0, \dots, z_{k-1}), y = (y_0, \dots, y_{k-1}) \in \Omega^k$ and

$$(4.4) \quad D_{hj} = \alpha_j I - h\beta_j f'(0), \quad j = 0, \dots, k.$$

We want to apply Theorem 3.2 with $X = \{\gamma \in (\mathbb{R}^{mk})^{\mathbb{N}} : \gamma(n) \rightarrow 0 \text{ as } n \rightarrow \infty\}$ and norm $\|\gamma\|_{\infty} = \sup_{n \in \mathbb{N}} \|\gamma(n)\|$. Let $X_s, X_u \subset \mathbb{R}^m$ be as in § 3 and define the $mk \times mk$ matrix Q_h as follows:

$$Q_h = \begin{pmatrix} 0 & I & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & & & & I \\ -D_{hk}^{-1}D_{h0} & \cdots & & & -D_{hk}^{-1}D_{h,k-1} \end{pmatrix}.$$

The stable and unstable summands of Q_h are determined in the following lemma which will be proved at the end of the section.

LEMMA 4.2. *There exist positive constants h_0, μ_1, μ_2 and invertible $mk \times mk$ matrices T_h depending C^{∞} on $h \in [0, h_0]$ such that*

$$(4.5) \quad T_h^{-1}Q_hT_h = \begin{pmatrix} Q_{hu} & 0 \\ 0 & Q_{hs} \end{pmatrix}.$$

Here, Q_{hs} is a square matrix of dimension $m(k-1) + d$, $d = \dim(X_s)$, and for some norm on $\mathbb{R}^{m(k-1)+d}$ which is independent of h we have $\|Q_{hs}\| \leq 1 - \mu_1 h$, $0 \leq h \leq h_0$. Similarly, for some suitable norm on \mathbb{R}^{m-d}

$$\|Q_{hu}\| \leq 1 + \mu_2 h, \quad \|Q_{hu}^{-1}\| \leq 1 - \mu_1 h \quad \text{for } 0 \leq h \leq h_0. \quad \square$$

Following Lemma 4.2, the projectors onto the stable and unstable summands Z_{hs}, Z_{hu} of Q_h are uniformly bounded and given by

$$(4.6) \quad P_{hs} = T_h \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} T_h^{-1}, \quad P_{hu} = I - P_{hs}, \quad \|P_{hu}\|, \|P_{hs}\| \leq \tilde{C}.$$

Now we apply Theorem 3.2 to the equation

$$(4.7) \quad A_h \gamma + F_h(\gamma) = (z, 0) \in Z_{hs} \times X =: Y$$

where $x_0 = 0$ and

$$(4.8) \quad \begin{aligned} A_h \gamma &= (P_{hs} \gamma(0), h^{-1}(\gamma(n+1) - Q_h \gamma(n)), n \geq 0), \\ F_h(\gamma) &= (0, \Phi^h(\gamma(n), \gamma(n+1)) - h^{-1}(\gamma(n+1) - Q_h \gamma(n)), n \geq 0). \end{aligned}$$

Using Lemmata 4.2 and 3.3 as well as the uniform boundedness of $\|T_h\|, \|T_h^{-1}\|$, we obtain an upper bound

$$(4.9) \quad \sigma^{-1} \geq \|A_h^{-1}\| \quad \text{for all } 0 < h \leq h_0.$$

Furthermore, (4.4) and (4.8) imply

$$\begin{aligned} \|F_h(\gamma) - F_h(\eta)\|_{\infty} &= \sup_{n \geq 0} \left\| D_{hk}^{-1} \left[f_h(\eta(n), \eta_{k-1}(n+1)) - f_h(\gamma(n), \gamma_{k-1}(n+1)) \right. \right. \\ &\quad \left. \left. + f'(0) \left(\beta_k(\gamma_{k-1}(n+1) - \eta_{k-1}(n+1)) \right. \right. \right. \\ &\quad \left. \left. \left. + \sum_{j=0}^{k-1} \beta_j(\gamma_j(n) - \eta_j(n)) \right) \right] \right\| \end{aligned}$$

$$\begin{aligned} &\leq C \sup_{n \geq 0} \left\| \sum_{j=0}^{k-1} \int_0^1 \left(\frac{\partial f_h^{(t)}}{\partial x_j} - \beta_j f'(0) \right) dt (\eta_j(n) - \gamma_j(n)) \right. \\ &\quad \left. + \int_0^1 \left(\frac{\partial f_h^{(t)}}{\partial x_k} - \beta_k f'(0) \right) dt (\eta_{k-1}(n+1) - \gamma_{k-1}(n+1)) \right\|. \end{aligned}$$

Here, the upper index t indicates the argument

$$(\gamma(n), \gamma_{k-1}(n+1)) + t[(\eta(n), \eta_{k-1}(n+1)) - (\gamma(n), \gamma_{k-1}(n+1))].$$

Then, by (H1) we find $\delta_0, h_0 > 0$ such that

$$\|F_h(\gamma) - F_h(\eta)\|_\infty \leq \frac{\sigma}{2} \|\gamma - \eta\|_\infty \quad \text{for } \|\gamma\|_\infty, \|\eta\|_\infty \leq \delta_0 \text{ and } h \leq h_0.$$

Thus (4.7) has a unique solution $\gamma(z) \in K_{\delta_0} \subset X$ whenever $z \in K_{\delta_1} \subset Z_{hs}$, $\delta_1 = \delta_0(\sigma/2)$. Moreover, for all $h \leq h_0$, the following stability inequality holds:

$$(4.10) \quad \|\gamma - \eta\|_\infty \leq 2\sigma^{-1} \|(A_h + F_h)(\gamma) - (A_h + F_h)(\eta)\| \quad \text{for } \gamma, \eta \in K_{\delta_0}.$$

If we define the local stable manifold of the multi-step method (4.1) to be

$$M_s^h = \{z \in \mathbb{R}^{mk} : x^h(nh; z) \in K_{\delta_0} \text{ for all } n \geq 0, \|P_{hs}z\| \leq \delta_1, x^h(nh; z) \rightarrow 0 \text{ as } n \rightarrow \infty\}$$

then we have shown the representation

$$(4.11) \quad M_s^h = \{z + q_h(z) : z \in K_{\delta_1} \subset Z_{hs}\} \quad \text{where } q_h(z) = P_{hu}(\gamma(z)(0)).$$

M_s^h is as smooth as f_h and has dimension $m(k-1) + d$. By (4.6) we may choose $\delta > 0, h_0 > 0$ such that $\delta \leq \delta_1$ and

$$z_h(x_0) := P_{hs}(\bar{x}(0; x_0), \dots, \bar{x}((k-1)h; x_0)) \in K_{\delta_1} \quad \text{for all } x_0 \in K_\delta, h \leq h_0.$$

For initial values x_0 on the stable manifold

$$M_s = \{x \in K_\delta : \bar{x}(t; x) \in K_{\delta_0} \text{ for } t \geq 0 \text{ and } \bar{x}(t; x) \rightarrow 0 \text{ as } t \rightarrow \infty\}$$

we select the discrete starting values $y = (y_0, \dots, y_{k-1}) = z_h(x_0) + q_h(z_h(x_0)) \in M_s^h$. Then we apply (4.10) to $\gamma(n) = (\bar{x}(nh; x_0), \dots, \bar{x}((n+k-1)h; x_0))$,

$$\eta(n) = (x^h(nh; y), \dots, x^h((n+k-1)h; y))$$

and obtain by (H2)

$$(4.12) \quad \sup_{n \geq 0} \|\bar{x}(nh; x_0) - x^h(nh; y)\| = O(h^r).$$

It remains to prove (4.2) for points $x_0 \notin M_s$. Analogous to (3.10) we apply Theorem 3.2 with $X = \mathbb{R}^{mk(N+1)}, Y = Z_{hs} \times \mathbb{R}^{mkN} \times Z_{hu}, T_{hN}(\gamma) = (P_{hs}\gamma(0), \Phi^h(\gamma(n), \gamma(n+1)) (0 \leq n \leq N-1), P_{hu}\gamma(N)) = (A_{hN} + F_{hN})(\gamma)$. A_{hN} and F_{hN} are defined analogously to (4.8). It turns out that, for some $\delta_1, \delta_0, h_0 > 0$, the equations

$$(4.13) \quad T_{hN}(\gamma) = (z_1, 0, z_2), \quad z_1 \in K_{\delta_1} \subset Z_{hs}, \quad z_2 \in K_{\delta_1} \subset Z_{hu}, \quad h \leq h_0$$

have unique solutions $\gamma_{hN}(z_1, z_2) \in K_{\delta_0}$. We then choose $\delta > 0$ such that $P_{hs}(\bar{x}(0; x_0), \dots, \bar{x}((k-1)h; x_0)), P_{hu}(\bar{x}(0; x_0), \dots, \bar{x}((k-1)h; x_0)) \in K_{\delta_1}$ holds for all $x_0 \in K_\delta$. For any $x_0 \in K_\delta \setminus M_s$ we solve (4.13) with $N = [\sup\{t \geq 0; \bar{x}([0, t]; x_0) \subset K_\delta\}] - k + 1, z_1 = P_{hs}(\bar{x}(0; x_0), \dots, \bar{x}((k-1)h; x_0)), z_2 = P_{hu}(\bar{x}(Nh; x_0), \dots, \bar{x}((N+k-1)h; x_0))$. The starting values $(y_0, \dots, y_{k-1}) = \gamma_{hN}(z_1, z_2)(0)$ then have the desired properties and this finishes the proof of Theorem 4.1.

We note that we do not have any suitable converse of Theorem 4.1 as for one-step methods in Theorem 3.1, i.e., we do not know how to characterize those discrete starting values (y_0, \dots, y_{k-1}) for which an appropriate initial value of the system (1.1) may be found.

Let us finally consider the case in which (4.1) is completed by a starting procedure

$$(4.14) \quad \begin{aligned} x(0) &= x_0, \\ h^{-1} \sum_{i=0}^j \alpha_{ij} x(ih) &= f_{hj}(x(0), \dots, x(jh)), \quad j=1, \dots, k-1. \end{aligned}$$

We need the additional consistency assumptions

$$(H4) \quad \sum_{i=0}^j \alpha_{ij} = 0, \quad \alpha_{ij} \neq 0 \text{ for } j=1, \dots, k-1;$$

$$f_{hj} \in C^1(\Omega^{j+1}, \mathbb{R}^m), \quad f'_{hj} \text{ is equicontinuous on } \Omega^{j+1};$$

$$f_{hj}(x, \dots, x) \rightarrow f(x) \text{ and } \sum_{i=0}^j (\partial f_{hj} / \partial x_i)(x, \dots, x) \rightarrow f'(x) \text{ as } h \rightarrow 0 \text{ uniformly in } x \in \Omega.$$

(H5) There exists a constant C such that

$$\max_{j=0, \dots, k-1} \|h^{-1} \sum_{i=0}^j \alpha_{ij} \bar{x}(ih) - f_{hj}(\bar{x}(0), \dots, \bar{x}(jh))\| \leq Ch^r$$

holds for all solutions $\bar{x}(t)$ of (1.1) with $\bar{x}([0, (k-1)h]) \subset \Omega$.

Moreover, in view of (H0) we assume that

(H6) $f_{hj}(0, \dots, 0) = 0$ for $j=1, \dots, k-1$ and for all h .

THEOREM 4.3. *Let (H0)–(H6) be satisfied and let $x^h(t; x_0)$ denote the solution of the complete multi-step method (4.1), (4.14). Then there are constants $\varepsilon, \varepsilon_0, h_0, C^* > 0$ such that, to any $x_0 \in K_\varepsilon, h \leq h_0$, a suitable $y_0 = y_0(x_0, h) \in K_{\varepsilon_0}$ exists which satisfies (3.5).*

The proof of this theorem makes intricate use of the techniques necessary for Theorem 4.1. It will therefore be given subsequent to the proof of Lemma 4.2.

Proof of Lemma 4.2. We make successive use of the blocking lemma below which is a quantitative version of some well-known decoupling techniques (cf., [5], [10]). Let $n_1, n_2 \in \mathbb{N}$ as well as norms on $\mathbb{R}^{n_1}, \mathbb{R}^{n_2}$ be given. For vectors $x = (x_1, x_2) \in \mathbb{R}^n$, where $x_1 \in \mathbb{R}^{n_1}, x_2 \in \mathbb{R}^{n_2}, n = n_1 + n_2$ we use the norm $\|x\| = \text{Max}(\|x_1\|, \|x_2\|)$. All matrices in the following lemma will have a compatible partitioning.

LEMMA 4.4. *Let $0 \leq r < 1$ be given. Then, for any $n \times n$ blockdiagonal matrix*

$$A = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$$

satisfying $\|A_{22}\| \leq r, \|A_{11}^{-1}\| \leq 1$ and any $n \times n$ matrix

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

satisfying $\|A - B\| \leq (1-r)/8$ there exist uniquely determined matrices V, W, B_1, B_2 such that

$$(4.15) \quad B \begin{pmatrix} I & W \\ V & I \end{pmatrix} = \begin{pmatrix} I & W \\ V & I \end{pmatrix} \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}, \quad \|V\| \leq 1, \quad \|W\| \leq 1.$$

For fixed A , the matrices V, W, B_1, B_2 depend C^∞ on B and satisfy

$$\|V\|, \|W\| \leq \frac{2}{1-r} \|A - B\|; \quad \|B_1 - A_{11}\|, \|B_2 - A_{22}\| \leq \frac{5}{4} \|A - B\|,$$

$$\|B_{11} - B_1\|, \|B_{22} - B_2\| \leq \frac{2}{1-r} \|A - B\|^2, \quad \|B_1^{-1}\| \leq \frac{2}{r+1}.$$

Proof. By our assumption and the Banach Lemma we have

$$\|A_{11} - B_{11}\|, \|A_{22} - B_{22}\|, \|B_{12}\|, \|B_{21}\| \leq \|A - B\| \leq \frac{1-r}{8},$$

$$\|B_{11}^{-1}\| \leq \|A_{11}^{-1}\| (1 - \|A_{11}^{-1}\| \|A_{11} - B_{11}\|)^{-1} \leq \frac{8}{r+7}.$$

It suffices to consider W, B_2 in (4.15) since V, B_1 can be found analogously.

By (4.15) the conditions on W, B_2 are

$$(4.16) \quad B_{11}W + B_{12} - WB_{22} - WB_{21}W = 0,$$

$$(4.17) \quad B_2 = B_{22} + B_{21}W.$$

Let us solve the Riccati equation (4.16) by an application of Theorem 3.2. with $A = B_{11}$, $F(W) = B_{12} - WB_{22} - WB_{21}W$, $x_0 = 0$, $\sigma = (r+7)/8$, $\delta_0 = 1$. F is Lipschitz on K_{δ_0} with constant $(5r+3)/8 < \sigma$ and $\|F(0)\| \leq (1-r)/8 \leq \sigma - (5r+3)/8$. For any two $n_1 \times n_2$ matrices W_1, W_2 with $\|W_1\|, \|W_2\| \leq 1$, we obtain

$$(4.18) \quad \|W_1 - W_2\| \leq \frac{2}{1-r} \|B_{11}(W_1 - W_2) + F(W_1) - F(W_2)\|.$$

The unique solution $W = W(B)$ of (4.16) depends smoothly on B as may be seen from the Lipschitz inverse mapping theorem with parameters [5, Appendix C7]. Setting $W_1 = 0$, $W_2 = W(B)$ in (4.18), we find $\|W(B)\| \leq 2/(1-r) \|B_{12}\| \leq (2/(1-r)) \|A - B\|$. B_2 is uniquely determined by (4.17) and satisfies $\|B_2 - B_{22}\| \leq \|B_{21}\| \|W\| \leq (2/(1-r)) \|A - B\|^2$ as well as $\|B_2 - A_{22}\| \leq ((2/(1-r)) \|A - B\| + 1) \|A - B\| \leq (5/4) \|A - B\|$. \square

Our assumption (H3) implies that 1 is an eigenvalue of multiplicity m for the matrix

$$Q_0 = \begin{pmatrix} 0 & I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & I & 0 \\ -\frac{\alpha_0}{\alpha_k} I & & \cdots & & -\frac{\alpha_{k-1}}{\alpha_k} I \end{pmatrix}$$

The corresponding eigenspace is $Z_1 = \{(x, \dots, x) : x \in \mathbb{R}^m\}$. A complementary Q_0 -invariant subspace is given by

$$Z_2 = \left\{ (x_0, \dots, x_{k-1}) : \sum_{j=0}^{k-1} \gamma_j x_j = 0 \right\} \quad \text{where} \quad \sum_{j=0}^k \alpha_j z^j = (z-1) \sum_{j=0}^{k-1} \gamma_j z^j.$$

As all other eigenvalues of Q_0 lie inside the unit circle, we find that

$$T_0 = \begin{pmatrix} I & \\ \vdots & T_2 \\ I & \end{pmatrix}, \quad T_0^{-1} Q_0 T_0 = \begin{pmatrix} I & 0 \\ 0 & Q_2 \end{pmatrix}$$

and a norm on $\mathbb{R}^{m(k-1)}$ such that $\|Q_2\| \leq r < 1$.

Applying Lemma 4.4 to

$$A = T_0^{-1}Q_0T_0 \quad \text{and} \quad B_h = T_0^{-1}Q_hT_0 = \begin{pmatrix} B_{h11} & B_{h12} \\ B_{h21} & B_{h22} \end{pmatrix}$$

we find

$$h_0 > 0 \quad \text{and} \quad \Gamma_h = \begin{pmatrix} I & W_h \\ V_h & I \end{pmatrix}$$

which satisfy

$$(4.19) \quad \Gamma_h^{-1}T_0^{-1}Q_hT_0\Gamma_h = \begin{pmatrix} E_{hu} & 0 \\ 0 & E_{hs} \end{pmatrix} \quad \text{for } h \leq h_0$$

and $V_h = O(h)$, $W_h = O(h)$, $E_{hs} = Q_2 + O(h)$, $E_{hu} = B_{h11} + O(h^2)$. By the definition of B_{h11} we have

$$(B_{h11}, \dots, B_{h11})^T + T_2B_{h21} = \left(I, \dots, I, -\sum_{j=0}^{k-1} D_{hk}^{-1}D_{hj} \right)^T.$$

We multiply from the left by $(\gamma_0I, \dots, \gamma_{k-1}I)$ and use (H1)

$$\begin{aligned} B_{h11} &= \sum_{j=0}^{k-1} \gamma_j B_{h11} = \left(\sum_{j=0}^{k-2} \gamma_j \right) I - \gamma_{k-1} D_{hk}^{-1} \sum_{j=0}^{k-1} D_{hj} \\ &= I - \gamma_{k-1} D_{hk}^{-1} \sum_{j=0}^k D_{hj} = I - \alpha_k D_{hk}^{-1} \left(-h \sum_{j=0}^k \beta_j f'(0) \right) = I + h\alpha_k D_{hk}^{-1} f'(0) \\ &= I + hf'(0) + O(h^2). \end{aligned}$$

Hence the block diagonalization (4.19) satisfies

$$\Gamma_h = I + O(h), \quad E_{hu} = I + hf'(0) + O(h^2), \quad \|E_{hs}\| \leq \frac{1+r}{2} < 1 \quad \text{for } h \leq h_0.$$

It remains to separate E_{hu} into stable and unstable blocks. Let us first put $f'(0)$ into block diagonal form

$$(4.20) \quad U^{-1}f'(0)U = \begin{pmatrix} J_1 & 0 \\ 0 & J_2 \end{pmatrix}$$

where J_2 is of dimension $d = \dim X_s$ and relates to the stable eigenvalues of $f(0)$. By Lemma 3.4 we have constants $\alpha, h_0 > 0$ and norms on \mathbb{R}^d and \mathbb{R}^{m-d} such that $\|I + hJ_2\| \leq 1 - \alpha h$, $\|(I + hJ_1)^{-1}\| \leq 1 - \alpha h$ for $h \leq h_0$. Now we use Lemma 4.4 with $A = (1 - \alpha h)U^{-1}(I + hf'(0))U$ and $B = (1 - \alpha h)U^{-1}E_{hu}U$. This gives us a transformation

$$(4.21) \quad R_h^{-1}U^{-1}E_{hu}UR_h = \begin{pmatrix} L_{hu} & 0 \\ 0 & L_{hs} \end{pmatrix}$$

where $R_h = I + O(h^2)$, $L_{hu} = I + hJ_1 + O(h^2)$, $L_{hs} = I + hJ_2 + O(h^2)$. Summing up (4.21) and (4.19), we obtain (4.5) with

$$(4.22) \quad \begin{aligned} T_h &= T_0 \begin{pmatrix} U & 0 \\ 0 & I \end{pmatrix} + O(h), \quad Q_{hu} = I + hJ_1 + O(h^2), \\ Q_{hs} &= \begin{pmatrix} L_{hs} & 0 \\ 0 & E_{hs} \end{pmatrix} = \begin{pmatrix} I + hJ_2 + O(h^2) & 0 \\ 0 & Q_2 + O(h) \end{pmatrix}. \end{aligned}$$

These matrices have the desired properties. \square

Proof of Theorem 4.3. For $x \in K_\varepsilon \subset \Omega$, ε sufficiently small, we define

$$S(x) = (\bar{x}(0; x), \dots, \bar{x}((k-1)h; x)), \quad S_h(x) = (x^h(0; x), \dots, x^h((k-1)h; x)).$$

Assumptions (H4) and (H5) yield the convergence of the starting procedure, i.e., for some $\varepsilon > 0$

$$(4.23) \quad S_h(x) = S(x) + O(h^r) \quad \text{uniformly for } x \in K_\varepsilon.$$

Now we consider the mapping $\Lambda_h(x) = P_{hu}S_h(x) - q_h(P_{hs}S_h(x))$ where P_{hu}, P_{hs} are the projectors from (4.6) and q_h determines the stable manifold M_s^h of the multi-step method (see (4.11)). For fixed but small $x_s \in X_s$, we want to find a solution $x_u \in X_u$ of the equation

$$(4.24) \quad \Lambda_h(x_s, x_u) = 0.$$

Suppose $x = (x_s, x_u)$ is a solution, then

$$S_h(x) = P_{hs}S_h(x) + P_{hu}S_h(x) = P_{hs}S_h(x) + q_h(P_{hs}S_h(x)) \in M_s^h$$

and hence x is on the stable manifold of the complete method (4.1), (4.14).

Let us apply Theorem 3.2 to (4.24). We take $X = X_u, Y = Z_{hu} \subset \mathbb{R}^{mk}, x_0 = 0$ and use the decomposition $\Lambda_h(x_s, x_u) = \tilde{A}_h x_u + \tilde{F}_h(x_s, x_u)$ with $\tilde{A}_h x_u = P_{hu}(x_u, \dots, x_u)$. We write $x_u = U_1 x_1, x_1 \in \mathbb{R}^{m-d}$ where $U = (U_1, U_2)$ is compatible with (4.20). Then (4.22) implies $T_h(x_1, 0) = (x_u, \dots, x_u) + O(h\|x_1\|)$ and hence $\tilde{A}_h x_u = (x_u, \dots, x_u) + O(h\|x_u\|)$ by (4.6). Therefore, we have a uniform bound $\tilde{\sigma}^{-1} \cong \|\tilde{A}_h^{-1}\|, h \leq h_0$. As for the Lipschitz bound on \tilde{F}_h , we estimate for $x_s \in K_{\varepsilon,s}$ and $x_u, y_u \in K_{\varepsilon,u}$ as follows

$$(4.25) \quad \begin{aligned} \|\tilde{F}_h(x_s, x_u) - \tilde{F}_h(x_s, y_u)\| &\leq \|q_h(P_{hs}S_h(x_s, y_u)) - q_h(P_{hs}S_h(x_s, x_u))\| \\ &\quad + \|P_{hu}[S_h(x_s, x_u) - S_h(x_s, y_u) - (x_u - y_u, \dots, x_u - y_u)]\|. \end{aligned}$$

Putting $S_h(x)$ into (4.14), differentiating with respect to x and using (H4) we find

$$(4.26) \quad S'_h(x) = (I, \dots, I) + O(h) \quad \text{uniformly for } x \in K_\varepsilon.$$

Hence, the second term in (4.25) may be estimated by $(\tilde{\sigma}/6)\|x_u - y_u\|$ for h sufficiently small.

The first term is more difficult to handle. Let us first choose δ_0, h_0 so small that F_h from (4.8) has a Lipschitz constant $(\sigma/4) \text{Min}(1, \sigma\tilde{\sigma}/12\tilde{C}^2)$ in K_{δ_0} for $h \leq h_0$ (see (4.6), (4.9)). Then by (4.7), (4.10), any two vectors $z, w \in K_{\delta_0} \subset Z_{hs}$ satisfy

$$\begin{aligned} \|\gamma(z) - \gamma(w) - A_h^{-1}(z - w, 0)\|_\infty &\leq 2\sigma^{-1}\|F_h(\gamma(w)) - F_h(\gamma(z)) \\ &\quad + F_h(\gamma(z) - \gamma(w)) - F_h(A_h^{-1}(z - w, 0))\|_\infty \\ &\leq \frac{\sigma\tilde{\sigma}}{24\tilde{C}^2}\|\gamma(z) - \gamma(w)\|_\infty \\ &\quad + \frac{1}{2}\|\gamma(z) - \gamma(w) - A_h^{-1}(z - w, 0)\|_\infty. \end{aligned}$$

Thus

$$\begin{aligned} \|\gamma(z) - \gamma(w) - A_h^{-1}(z - w, 0)\|_\infty &\leq (\sigma\tilde{\sigma}/12\tilde{C}^2)\|\gamma(z) - \gamma(w)\|_\infty \\ &\leq (\tilde{\sigma}/6\tilde{C}^2)\|P_{hs}(z - w)\| \leq (\tilde{\sigma}/6\tilde{C})\|z - w\| \end{aligned}$$

and because of $P_{hu}(A_h^{-1}(z - w, 0))(0) = 0$ we have

$$(4.27) \quad \|q_h(z) - q_h(w)\| = \|P_{hu}[(\gamma(z) - \gamma(w))(0)]\| \leq (\tilde{\sigma}/6\tilde{C})\|z - w\|.$$

Combining this with (4.26) and (4.6), we have a bound $(\bar{\sigma}/6)(1 + O(h))\|x_u - y_u\|$ for the first term in (4.25). Summing up, we obtain $\tilde{\delta}_0, h_0 > 0$ such that $\tilde{F}_h(x_s, \cdot)$ is Lipschitz in $K_{\tilde{\delta}_0, u}$ with constant $\bar{\sigma}/2$ for all $x_s \in K_{\tilde{\delta}_0, s}, h \leq h_0$. Finally, Λ_h is uniformly Lipschitz and $\Lambda_h(0) = 0$ so that there exists a $\tilde{\delta} > 0$ satisfying $\|\Lambda_h(x_s, 0)\| \leq \tilde{\delta}_0(\bar{\sigma}/2)$ for $x_s \in K_{\tilde{\delta}, s}, h \leq h_0$. Theorem 3.2 then assures a unique solution $x_u = p^h(x_s) \in K_{\tilde{\delta}_0, u}$ of (4.24) if $x_s \in K_{\tilde{\delta}, s}$. For the corresponding element $\tilde{x} = (x_s, p(x_s)) \in M_s$, the stability inequality (3.7) yields

$$\begin{aligned} \|p(x_s) - p^h(x_s)\| &\leq 2\bar{\sigma}^{-1}\|\Lambda_h(\tilde{x})\| \leq 2\bar{\sigma}^{-1}\{\|P_{hu}\|(\|S_h(\tilde{x}) - S(\tilde{x})\| \\ &\quad + \|S(\tilde{x}) - [\gamma(P_{hs}S(\tilde{x}))](0)\|) + \|q_h(P_{hs}S(\tilde{x})) - q_h(P_{hs}S_h(\tilde{x}))\|\} \end{aligned}$$

and hence by (4.23), (4.27), (4.12)

$$(4.28) \quad \|p(x_s) - p^h(x_s)\| = O(h^r) \text{ uniformly for } x_s \in K_{\tilde{\delta}, s}.$$

Using (4.26) and (4.23) again, $\tilde{x}_h := (x_s, p^h(x_s))$ satisfies

$$(4.29) \quad \|S_h(\tilde{x}_h) - S(\tilde{x})\| = O(h^r).$$

For $n \geq k$ we employ (4.12) with $y = \gamma(P_{hs}S(\tilde{x}))(0), x_0 = \tilde{x}$ as well as $x^h(nh; \tilde{x}_h) = \gamma(P_{hs}S_h(\tilde{x}_h))(n)$ to obtain

$$\|x^h(nh; \tilde{x}_h) - \bar{x}(nh; \tilde{x})\| \leq \|\gamma(P_{hs}S_h(\tilde{x}_h)) - \gamma(P_{hs}S(\tilde{x}))\|_\infty + O(h^r).$$

The uniform Lipschitz boundedness of γ together with (4.29) then proves our assertion.

Remark. Our proof shows that, in addition to Theorem 4.3, the complete multi-step method (4.1), (4.14) has a stable manifold which approximates that of the differential equation as in Theorem 3.1.

5. Numerical experiments in the global case. Perhaps the simplest nonlocal situation occurs if the system (1.1) has two stationary points in Ω , one stable and one unstable. We then compute numerically trajectories that start near the unstable point and converge to the stable point. The one-dimensional model equation for this situation is the logistic equation

$$x' = x(1 - x).$$

For $x_0, y_0 > 0$, we set

$$\rho_h(x_0, y_0) = \sup_{n \in \mathbb{N}} |\bar{x}(nh; x_0) - x^h(nh; y_0)|.$$

This sup was evaluated numerically by using the explicit formula for \bar{x} and the fact that both sequences approach 1 as $n \rightarrow \infty$ if $x_0 > 0$ and $y_0 > 0$. Since the adapted initial values are not unique and cannot be evaluated explicitly (see the remark at the end of § 3) we computed the quantities

$$\varepsilon_h(x_0) = \text{Min}_{y_0 \in [0, 1]} \rho_h(x_0, y_0) \quad \text{and} \quad \delta_h(y_0) = \text{Min}_{x_0 \in [0, 1]} \rho_h(x_0, y_0)$$

by numerical optimization. We expect $O(h^r)$ -behaviour for both numbers if (1.3) holds for $\Omega = [0, 1]$. This is confirmed by Tables 1 and 2 for $\varepsilon_h = \varepsilon_h(0.05)$ and $\delta_h = \delta_h(0.05)$. We have included the values of the standard error $\rho_h = \rho_h(0.05, 0.05)$, the estimated order of convergence

$$\text{ord}(\varepsilon_h) = \ln \left(\frac{\varepsilon_h}{\varepsilon_{h/2}} \right) / \ln 2$$

TABLE 1
Euler.

h	ρ_h	ε_h	ord(ε_h)	Δ_h	δ_h	ord(δ_h)
1	1.82E-1	3.92E-2	1.04	2.73E-2	4.51E-2	1.22
$\frac{1}{2}$	9.92E-2	1.91E-2	1.07	1.48E-2	1.94E-2	1.10
$\frac{1}{4}$	5.12E-2	9.09E-3	1.03	7.81E-3	9.06E-3	1.02
$\frac{1}{8}$	2.59E-2	4.44E-3	1.01	4.00E-3	4.47E-3	1.01
$\frac{1}{16}$	1.30E-2	2.20E-3	1.01	2.02E-3	2.22E-3	1.01
$\frac{1}{32}$	6.48E-3	1.09E-3		1.02E-3	1.10E-3	

TABLE 2
Fourth order Runge-Kutta.

h	ρ_h	ε_h	ord(ε_h)	Δ_h	δ_h	ord(δ_h)
1	1.35E-3	6.86E-4	4.40	3.8E-4	7.38E-4	4.48
$\frac{1}{2}$	1.09E-4	3.24E-5	4.10	2.5E-5	3.31E-5	4.14
$\frac{1}{4}$	7.84E-6	1.89E-6	4.03	1.6E-6	1.88E-6	4.06
$\frac{1}{8}$	5.25E-7	1.16E-7	4.04	1.1E-7	1.13E-7	4.01
$\frac{1}{16}$	3.40E-8	7.05E-9	4.02	6.6E-9	6.99E-9	4.00
$\frac{1}{32}$	2.16E-9	4.36E-10		4.1E-10	4.37E-10	

and the values Δ_h where the minimum $\varepsilon_h(x_0)$ was attained at $y_0 = x_0 + \Delta_h$. If x_0 moves towards the unstable point 0, then ρ_h increases whereas ε_h, δ_h remain almost unchanged. For instance, at $x_0 = 5E-8, h = \frac{1}{8}$ we have

$$\rho_h = 0.231, \quad \varepsilon_h = 0.444E-2, \quad \delta_h = 0.461E-2 \quad \text{for Euler's method, and}$$

$$\rho_h = 0.677E-5, \quad \varepsilon_h = 0.115E-6, \quad \delta_h = 0.113E-6 \quad \text{for the RK-method.}$$

Similar results were obtained for a 3-step Adams Bashforth method with Runge-Kutta starting procedure.

In fact it is not very difficult to establish relation (1.3) for one-dimensional systems (1.1) if Ω is a finite interval containing only finitely many simple zeros of f . Only the initial values near unstable points have to be adjusted. Once a trajectory leaves the neighbourhood of an unstable point, either standard results on finite time intervals or the stable case of Theorem 3.1 are applicable. For higher-dimensional systems, however, one is immediately led to impose some structural stability condition on (1.1).

We consider a typical two-dimensional example (cf. [2] for the underlying cell model)

$$(5.1) \quad \begin{aligned} x'_1 &= -2x_1 + x_2 + 1 - \mu f(x_1, \lambda), \\ x'_2 &= x_1 - 2x_2 + 1 - \mu f(x_2, \lambda), \end{aligned} \quad f(x, \lambda) = x(1 + x + \lambda x^2)^{-1}.$$

For $\mu = 15$ this system shows a hysteresis effect with respect to λ . We take, for example, $\lambda = 57$ and find two stable and one unstable stationary points in the relevant region $0 \leq x_1, x_2 \leq 1$. In contrast to our first example we now have a nontrivial stable manifold M_s for the unstable point which separates the basins of attraction for the two stable points. Our numerical results are intended to show that the approximation of M_s and of the phase portrait by a one-step method is valid in a more global sense than it was actually proved in Theorem 3.1. Figure 1 gives a partial phase portrait obtained by some standard code at high accuracy (we used the Routine DO2BBF from the NAG

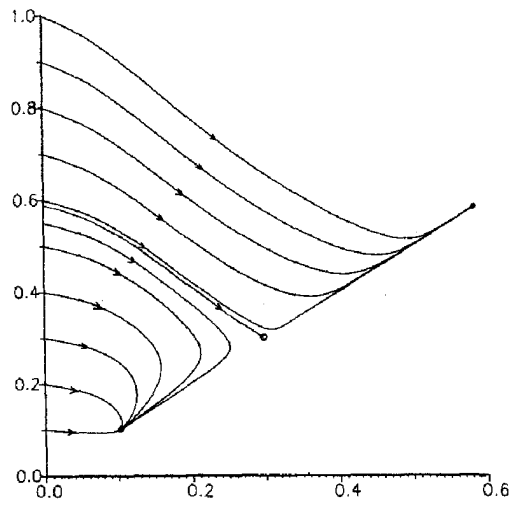


FIG. 1

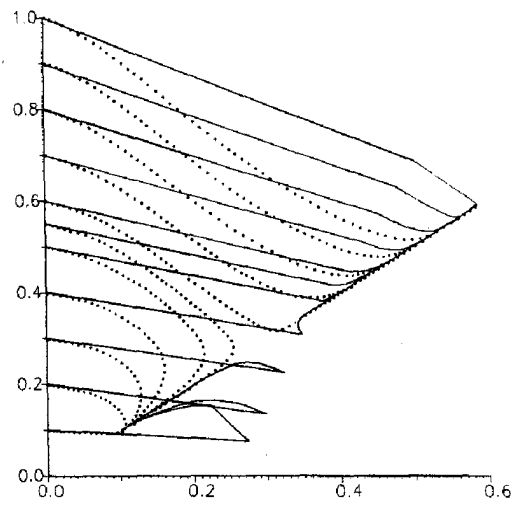


FIG. 2(a). Euler, $h = \frac{1}{4}$.

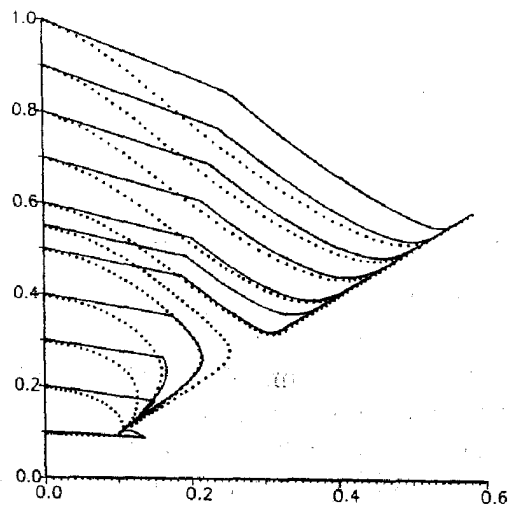


FIG. 2(b). Euler, $h = \frac{1}{8}$.

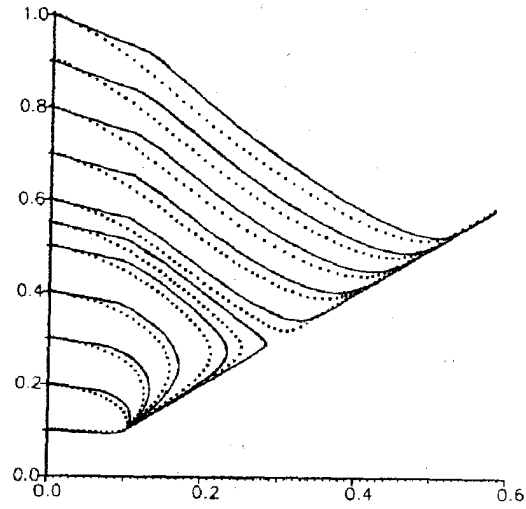


FIG. 2(c). Euler, $h = \frac{1}{16}$.

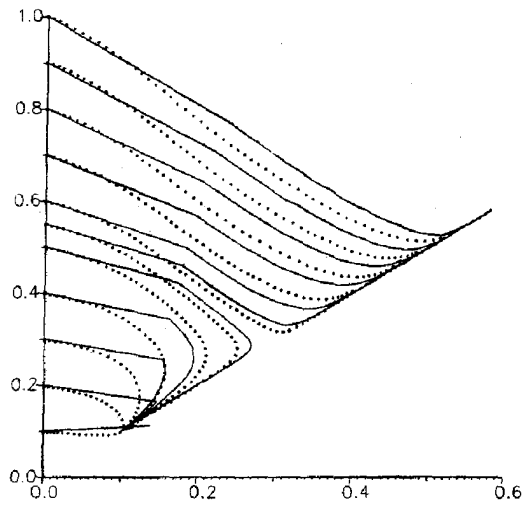


FIG. 3(a). Runge-Kutta, $h = \frac{1}{4}$.

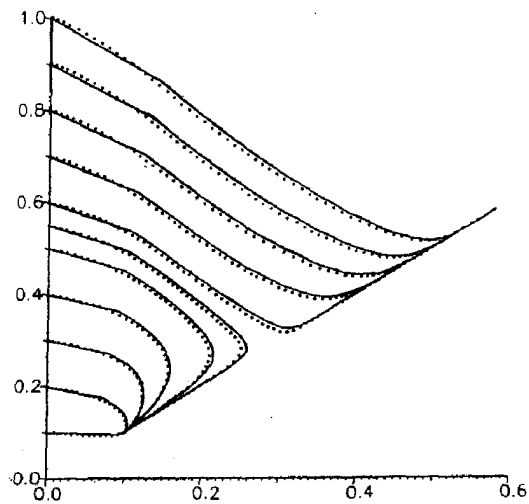


FIG. 3(b). Runge-Kutta, $h = \frac{1}{8}$.

library, distributed by Numerical Algorithms Group, Oxford, United Kingdom), the stable manifold was found by bisection. The resolution in Fig. 1 is sufficient for our purposes. Figures 2 and 3 show how the numerical phase portraits for Euler's method and the fourth order RK-method smooth out as $h \rightarrow 0$ (dotted lines are the trajectories from Fig. 1 whereas solid lines are obtained by linear interpolation of the points from the one-step method).

The most significant change occurs near the stable manifold M_s . We investigated in more detail the intersection $(0, \xi_h)$ of the numerical stable manifold M_s^h with the x_2 -axis. Table 3 gives some values for ξ_h , calculated by a bisection method with sufficient accuracy. Assuming an asymptotic behaviour $\xi_h = \xi_0 + Ch^r + O(h^{r+1})$, the order of convergence was estimated as

$$\text{ord}_h = \ln \left(\frac{\xi_h - \xi_{h/2}}{\xi_{h/2} - \xi_{h/4}} \right) / \ln 2.$$

The results for ord_h are quite satisfactory for Euler's method whereas, for the RK-method, the values of ξ_h still slightly oscillate around ξ_0 for small step size h .

TABLE 3

h	Euler		Runge-Kutta	
	ξ_h	ord_h	ξ_h	ord_h
$\frac{1}{2}$			0.316485	1.82
$\frac{1}{4}$	0.346402	0.94	0.522539	2.96
$\frac{1}{8}$	0.486529	1.98	0.581050	4.78
$\frac{1}{16}$	0.559677	1.67	0.588582	5.83
$\frac{1}{32}$	0.578179	1.21	0.5888568	6.66
$\frac{1}{64}$	0.584009	1.08	0.58886163	4.50
$\frac{1}{128}$	0.586527	1.04	0.588861683	3.05
$\frac{1}{256}$	0.587715		0.58886168093	
$\frac{1}{512}$	0.588293		0.588861680675	

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