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Stability of the method of lines*

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Summary. It is well known that a necessary condition for the Lax-stability of the method of lines is that the eigenvalues of the spatial discretization operator, scaled by the time step k, lie within a distance $O(k)$ of the stability region of the time integration formula as $k \to 0$. In this paper we show that a necessary and sufficient condition for stability, except for an algebraic factor, is that the ε-pseudo-eigenvalues of the same operator lie within a distance $O(\varepsilon)+O(k)$ of the stability region as k, $\varepsilon \to 0$. Our results generalize those of an earlier paper by considering: (a) Runge-Kutta and other one-step formulas, (b) implicit as well as explicit linear multistep formulas, (c) weighted norms, (d) algebraic stability, (e) finite and infinite time intervals, and (f) stability regions with cusps.

In summary, the theory presented in this paper amounts to a transplantation of the Kreiss matrix theorem from the unit disk (for simple power iterations) to an arbitrary stability region (for method of lines calculations).

Mathematics Subject Classification (1991): 65M20, 15A18

1 Introduction

Since the early work of von Neumann, Lax, and Richtmyer, it has been recognized that analysis of eigenvalues gives necessary but not sufficient conditions for the (Lax-) stability of discretizations of linear initial-value problems [30]. Eigenvalue analysis is so convenient, however, that the tendency among engineers has been to ignore this pitfall and assume that a discretization is stable if it passes an eigenvalue test, with results usually more or less correct but sometimes considerably in error [3, 11, 24, 25, 36]. Theoretical numerical ana-

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lysts, on the other hand, too mathematically conscientious to gloss over a gap in the theory, have tended to dismiss eigenvalue analysis as of merely heuristic value except in the well-known special case where the operators involved are normal.

The purpose of this paper is to show that this gap between necessary and sufficient – or between theory and practice – can be eliminated if one restates the usual arguments in terms of *ε-pseudo-eigenvalues* instead of eigenvalues. For each $\varepsilon \geqq 0$, the ε-pseudospectrum of a matrix A is the set of all numbers $z \in \mathbb{C}$ that are eigenvalues of $A+E$ for some perturbation matrix E with $\|E\| \leqq \varepsilon$. Such numbers z are called ε-pseudo-eigenvalues. Our main result gives necessary and sufficient conditions for stability in terms of pseudospectra, and can be roughly stated as follows: a linear method of lines calculation with time step k, spatial discretization operators $\{L_k\}$, and stability region S is Lax-stable, except for an algebraic factor, if and only if all the ε-pseudo-eigenvalues of the operators $\{kL_k\}$ lie within a distance $O(\varepsilon)+O(k)$ of S as $\varepsilon, k \to 0$.

Any statement about the pseudospectra of a matrix A is equivalent to a statement about the norm of its resolvent $(zI-A)^{-1}$, for as is readily shown, a number $z \in \mathbb{C}$ is an ε-pseudo-eigenvalue if and only if $\|(zI-A)^{-1}\| \geqq \varepsilon^{-1}$ [38]. The use of resolvents has a long history in stability theory. Mathematically, what is at issue here is the transplantation of the Kreiss matrix theorem, in a sharpened form established in [21] and [33], from the unit disk to an arbitrary stability region.

In an earlier paper [28], our pseudo-eigenvalue stability criterion was proved for the special case of method of lines calculations on an infinite time interval based on explicit linear multistep formulas with cusp-free stability regions, in the L^2 norm. This paper amounts to an extension of that result to:

(a) Runge-Kutta and other one-step time integration formulas,
(b) implicit as well as explicit linear multistep formulas,
(c) weighted norms,
(d) algebraic stability,
(e) finite and infinite time intervals,
(f) stability regions with cusps.

The paper is organized as follows. Section 2 formulates the problem and defines the notation. Section 3 presents the definition of pseudospectra. Section 4 presents an example which illustrates our main results. Section 5 states a theorem for stability of semidiscrete evolution equations. Section 6 reviews the Kreiss matrix theorem, which gives conditions for power-boundedness of families of matrices, and presents generalizations for algebraic stability and for stability on finite time intervals. Section 7 proves our main stability result for one-step methods. This result is generalized in Sect. 8. Section 9 states our main results for linear multistep methods. The proofs are just sketched, since most of the details are presented already in Sect. 7 and [28]. It is also shown that a modified criterion based on pseudospectra applies to linear multistep methods whose stability regions have cusps. In Sect. 10, the theory is applied to two finite difference discretizations. Section 11 reviews previous and current related work. Our results are reasonably complete for time integration formulas with bounded stability regions and we present partial results for unbounded stability regions.

As the above summary suggests, this paper is rather long. However, we would like to emphasize that the main points of our stability theory are not difficult to follow. The main ideas and results can be understood by first looking at Sects. 2, 3, and 4, which define the notation and illustrate the theory with an example, and then proceeding to the Kreiss matrix theorem in Sect. 6 and to our main results, Theorems 7.1 and 9.1.

The availability of a new stability criterion based on pseudospectra does not imply that analyzing stability will necessarily be easy in particular cases. Like spectra, pseudospectra must often be estimated numerically. Indeed, our theorems suggest that for practical work, a reasonable way to test for stability is to calculate eigenvalues in the usual way *after* modifying the matrix by one or two random perturbations of size, say, 10^{-3} or 10^{-6}.

The application of the results of this paper to questions of stability and stiffness of numerical methods for ordinary differential equations is discussed in [12].

2 Notation

Here is the formulation of the problem [30]. We consider the method of lines approximation of an autonomous linear evolution equation

$$u_t = \mathscr{L} u, \qquad u(x,0) = f(x), \qquad t \in [0, T], \tag{2.1}$$

where $\mathscr{L}$ is a time-independent linear differential operator, which may incorporate boundary conditions, and u is a scalar or vector function of t and of one or more space variables x. Equation (2.1) is first approximated with respect to the space variables by finite differences, finite elements or spectral methods on a discrete grid, transforming the p.d.e. into the system of o.d.e.'s

$$v_t = L_k v, \qquad v(0) = f_k, \tag{2.2}$$

where $v(t)$ is a vector of dimension $N_k \leqq \infty$ and L_k is a matrix or bounded linear operator. At this stage the subscript k is an arbitrary positive real parameter that determines the spatial grid in an unspecified manner. The semidiscretization (2.2) is then approximated with respect to t by a linear multistep, Runge-Kutta, or more general one-step formula with time step k. If we write $v^n \approx v(nk)$, then the resulting full discretization becomes

$$\mathbf{v}^{n+1} = A_k \mathbf{v}^n = G(k L_k)\mathbf{v}^n, \tag{2.3}$$

with appropriate initial conditions. For a one-step time integration formula, $\mathbf{v}^n \equiv v^n$, while for an s-step formula we define

$$\mathbf{v}^n = \begin{bmatrix} v^n \\ v^{n-1} \\ \vdots \\ v^{n-s+1} \end{bmatrix}. \tag{2.4}$$

The function $G(w)$ characterizes the time integration formula. For a linear multistep method, $G(w)$ is a companion matrix. Its entries are affine and rational functions of w for explicit and implicit multistep methods, respectively. For

Runge-Kutta or one-step methods, $G(w)$ is a polynomial or rational function that approximates e^w for $w \approx 0$.

The full discretization (2.3) is defined to be Lax-stable if

$$\|A_k^n\| \leqq C \quad \text{for all } n \text{ and } k \text{ with } 0 \leqq nk \leqq T, \tag{2.5}$$

for some constant C and all sufficiently small k. The Lax Equivalence Theorem states that (2.5) is a necessary and sufficient condition for convergence of the discrete approximation as $k \to 0$, assuming that the initial-value problem (2.1) is well-posed and that the discretization (2.3) is consistent [30].

Throughout this paper, $\|\cdot\|$ denotes the weighted 2-norm defined by a non-singular weight matrix W.[1] The matrix W depends on the grid, and hence on k, in a fashion that in principle is arbitrary. In applications, if W is not the identity, it will typically be a discrete diagonal approximation to a smooth weight function such as a Jacobi or Laguerre weight.

3 Pseudospectra

Let A be a real or complex square matrix of dimension N. Here is the definition of pseudospectra.

Definition. Given $\varepsilon \geqq 0$, a number $z \in \mathbb{C}$ is an *ε-pseudo-eigenvalue* of A if any of the following equivalent conditions is satisfied:

(i) z is an eigenvalue of $A+E$ for some E with $\|E\| \leqq \varepsilon$;
(ii) $\exists u \in \mathbb{C}^N$ with $\|u\| = 1$ such that $\|(A - zI)u\| \leqq \varepsilon$;
(iii) $\|(zI - A)^{-1}\| \geqq \varepsilon^{-1}$.

The *ε-pseudospectrum* of A, denoted by $\Lambda_\varepsilon(A)$, is the set of all ε-pseudo-eigenvalues of A.

The vector u in (ii) is called a normalized *ε-pseudo-eigenvector*. The function $(zI - A)^{-1}$ is the resolvent. The proof of the equivalence of the three conditions is given in [38].

If $\mathscr{H}$ is a Hilbert space and $A: \mathscr{H} \to \mathscr{H}$ is a bounded linear operator, then conditions (i)–(iii) are not quite equivalent. Let $\Lambda(A)$ denote the spectrum of A. In this case, z is defined to be a ε-pseudo-eigenvalue if $z \in \Lambda(A)$ or if $z \in \mathbb{C} \backslash \Lambda(A)$ and $\|(zI - A)^{-1}\| \geqq \varepsilon^{-1}$.

For a normal[2] matrix or operator A, $\Lambda_\varepsilon(A)$ is simply the union of the closed ε-balls around the spectrum of A. On the other hand, if A is non-normal, then $\Lambda_\varepsilon(A)$ may be much larger than the spectrum, even if $\varepsilon \ll 1$. It is in these cases that considering the spectrum alone may be misleading. Highly non-normal matrices arise in many areas in numerical analysis. In previous work we have examined the pseudospectra of non-normal matrices arising in spectral discretizations of partial differential equations [28] and have also obtained results on pseudospectra of Toeplitz matrices [29]. An introduction to the idea of pseudospectra can be found in [37], and a longer survey is in preparation [38].

[1] This norm is defined by $\|x\| \equiv \|x\|_W = \|Wx\|_2$ and $\|E\| \equiv \|E\|_W = \|WEW^{-1}\|_2$ for vectors x and matrices E, respectively

[2] An operator A is normal if $A^+A = AA^+$, where A^+ is the adjoint of A. If $\|\cdot\|$ is the usual 2-norm, then A^+ is simply the Hermitian conjugate A^*. For our weighted 2-norm the adjoint is given by the more complicated expression $A^+ = W^{-1}(W^{-1})^* A^* W^* W$

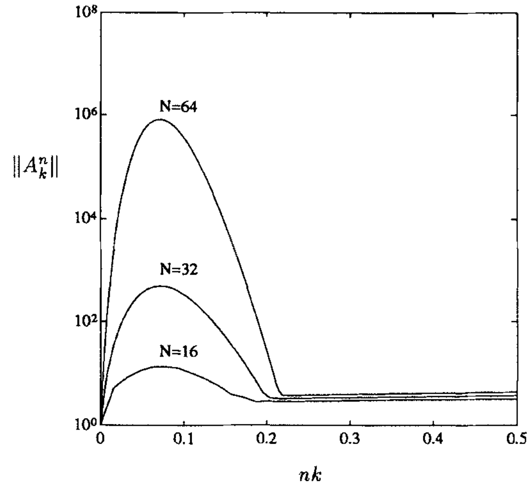

Fig. 1. Powers of $A_k = G(k\,L_k)$ for the problem (4.1) with $k = 0.25/(N-1)$

Our stability theorems are based on resolvents and make frequent use of the following result. Let $V \subseteq \mathbb{C}$ be an open set with boundary ∂V and closure $\bar{V}$. If $\Lambda_\varepsilon(A) \subseteq \bar{V}$ for some $\varepsilon > 0$, then

$$(3.1) \qquad \|(zI - A)^{-1}\| \leqq \varepsilon^{-1} \qquad \forall z \in \partial V.$$

For $z \in \mathbb{C} \setminus \bar{V}$, the same estimate holds with a strict inequality. In general the set V will depend on ε.

Our stability analysis via pseudospectra and resolvents is related to previous work by Bakhvalov, Godunov and Ryabenkii, Di Lena and Trigiante, Lenferink and Spijker, Lubich and Nevanlinna, Kreiss and Wu, and others (see Sect. 11).

4 An example

Our analysis of stability via pseudospectra was originally motivated by investigations of spectral methods on bounded domains [36, 39]. Before proceeding to our results we present an example of this type which illustrates the main points of our theory.

We consider a discretization of the initial boundary value problem

$$(4.1) \qquad u_t = -x\,u_x, \qquad -1 \leqq x \leqq 1, \qquad u(x, 0) = f(x).$$

The method combines collocation at the Chebyshev points for the spatial discretization with the third-order Adams-Bashforth formula (AB3) for time integration (see [28, 36, 39] for the details).

The standard eigenvalue criterion for stability requires the eigenvalues of the operators $\{k\,L_k\}$ to lie in the stability region of the time integration formula. It is straightforward to show that the eigenvalues of L_k are the integers $-(N-1), -(N-2), \ldots, 0$, where $N \equiv N_k$. Hence, a necessary condition for stability is that $k \leqq C/(N-1)$, where $C \approx 0.6$ for AB3.

In actuality, the above stability condition leads to an exponential instability. To show this numerically, we set $k = 0.25/(N-1)$ and attempt to verify the definition of stability (2.5). Figure 1 plots the powers $\|A_k^n\|$ for the unweighted 2-norm

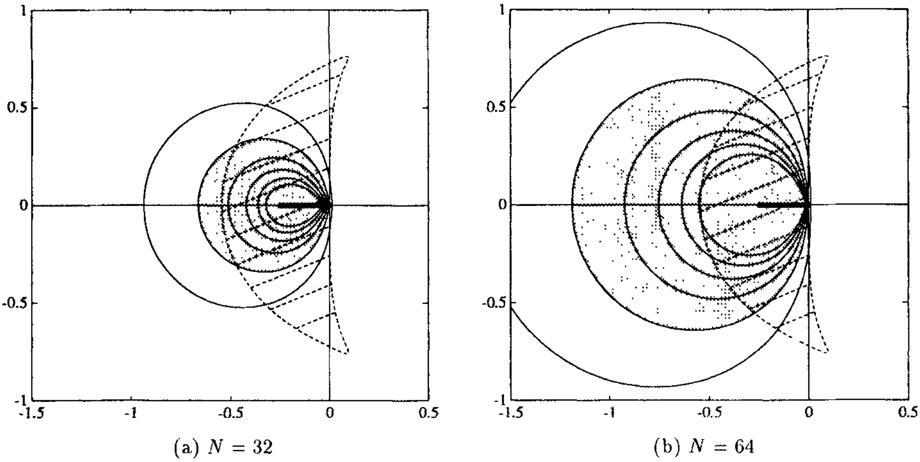

Fig. 2. Pseudospectra of the Chebyshev spectral discretization matrix for problem (4.1). The *striped region* is the stability region. The *solid line* on the negative real axis marks the spectrum $\Lambda(kL_k)$. The *shaded region* is the ε-pseudospectrum for $\varepsilon = 10^{-3}$ and the *curves* (from outer to inner) are boundaries of the ε-pseudospectra for $\varepsilon = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}$

for several values of N. For fixed dimension N, and therefore fixed k, $\|A_k^n\|$ is bounded as a function of n. Thus, the discretization is time-stable. However, as the plot indicates, $\sup_{0 \leq nk \leq T} \|A_k^n\|$ grows exponentially with the dimension N; the discretization is not Lax-stable. This exponential instability exists for any choice of time step of the form $k = C/N$. In practical calculations, it can lead to large errors in the computed values of $u(x, t)$.

The reason for the instability becomes apparent upon examining the pseudospectra for this problem. Figure 2 compare the pseudospectra of the operators kL_k for $N = 32$ and $N = 64$. The thick solid line on the negative real axis marks the spectrum. The shaded region is the ε-pseudospectrum for $\varepsilon = 10^{-3}$, and the curves are the boundaries of the pseudospectra for this and various other values of ε. The plots show that the spectrum lies comfortably within the stability region, regardless of N. However, for each fixed $\varepsilon > 0$, $\Lambda_\varepsilon(kL_k)$ grows as $k \to 0$ and $N \to \infty$; it has radius approximately $O(N)$, violating our stability criterion (Theorem 9.1). A quantitative investigation of the resolvent shows that for every fixed $u \in \mathbb{C}$, the resolvent norm $\|(\mu I - kL_k)^{-1}\|$ grows exponentially with N. This accounts for the exponential growth seen in Fig. 1.

In [28] we showed that a sufficient condition for algebraic stability for this spectral discretization is $k = O(N^{-2})$. For any choice of time step satisfying this condition, the ε-pseudospectra of the operators $\{kL_k\}$ remain bounded as $k \to 0$, ensuring stability.

5 Stability of semidiscretizations

Before examining the stability of the full discretization (2.3), we first present a stability (or well-posedness) result for the semidiscretization (2.2).

The solution of (2.2) is

$$v(t)=\mathrm{e}^{L_k t} f_k, \tag{5.1}$$

where $\mathrm{e}^{L_k t}$ can be defined by a Taylor series. The family of semidiscretizations $\{\mathrm{e}^{L_k t}\}$ is defined to be stable if

$$\|\mathrm{e}^{L_k t}\| \leqq C(t) \qquad \forall t \geqq 0, \tag{5.2}$$

where $C(t)$ is some function independent of k [10, Chapter 5]. The fundamental result for stability of the family of semidiscretizations is the continuous version of the Kreiss matrix theorem [35, Lemma 4.1]. The following result is a restatement of a sharpened version of one part of this theorem [21, 33].

Theorem 5.1. *Let $\{L_k\}$ be a family of matrices or bounded linear operators of dimensions $N_k \leqq \infty$. If*

$$\|\mathrm{e}^{L_k t}\| \leqq C\,\mathrm{e}^{\omega t} \qquad \forall t \geqq 0 \tag{5.3}$$

for some constants C and ω, then the ε-pseudo-eigenvalues $\{\mu_\varepsilon\}$ of the operators $\{L_k\}$ satisfy

$$\operatorname{Re} \mu_\varepsilon \leqq \omega + C\varepsilon \qquad \forall \varepsilon \geqq 0. \tag{5.4}$$

Conversely, (5.4) *implies*

$$\|\mathrm{e}^{L_k t}\| \leqq \mathrm{e}\, C N_k\, \mathrm{e}^{\omega t} \qquad \forall t \geqq 0. \tag{5.5}$$

Proof. The relationship between pseudospectra and resolvents presented in Sect. 3 implies that (5.4) is equivalent to the condition

$$\|(\mu I - L_k)^{-1}\| \leqq \frac{C}{\operatorname{Re} \mu - \omega}, \qquad \operatorname{Re} \mu > \omega. \tag{5.6}$$

If (5.3) holds, then (5.6) follows readily from the Laplace transform formula

$$(\mu I - L_k)^{-1} = \int_0^\infty \mathrm{e}^{-\mu t}\, \mathrm{e}^{L_k t}\, dt \qquad \operatorname{Re} \mu > \omega. \tag{5.7}$$

Conversely, a more complicated argument based on a resolvent integral shows that (5.6) implies (5.5) [21, 33]. □

If $C=1$ in (5.4), then $\|\mathrm{e}^{L_k t}\| \leqq \mathrm{e}^{\omega t}$ for all $t \geqq 0$ by the Hille-Yosida theorem [13].

6 The Kreiss matrix theorem

Now we turn to fully discrete problems. Our Lax-stability results for method of lines discretizations are based on a sharpened version of the resolvent condition of the Kreiss matrix theorem [21, 33]. This theorem gives necessary and sufficient conditions for the power-boundedness of a family of matrices in terms of the pseudospectra of these matrices. In the present section we review this result and give three generalizations which give conditions for algebraic stability and for stability on finite time intervals.

Let $\{A_\nu\}$ denote a family of matrices or bounded linear operators of dimensions $N_\nu \leqq \infty$. Let D denote the open unit disk and $\bar{D}$ its closure. The following result is the same as Theorem 1 in [28], except that since the publication of that paper, Spijker has sharpened the result by eliminating a troublesome factor of 2 [33]. For a simple derivation of Spijker's result see [41].

Theorem 6.1. *If the operators* $\{A_\nu\}$ *satisfy*

$$\|A_\nu^n\| \leqq C \qquad \forall n \geqq 0 \tag{6.1}$$

for some constant C*, then the* ε*-pseudo-eigenvalues* $\{\lambda_\varepsilon\}$ *of these operators satisfy*

$$\operatorname{dist}(\lambda_\varepsilon, D) \leqq C\varepsilon \qquad \forall \varepsilon \geqq 0. \tag{6.2}$$

Conversely, (6.2) *implies*

$$\|A_\nu^n\| \leqq \mathrm{e}\, C \min\{N_\nu, n+1\} \qquad \forall n \geqq 0. \tag{6.3}$$

Proof. The relationship between pseudospectra and resolvents implies that (6.2) is equivalent to

$$\|(\lambda I - A_\nu)^{-1}\| \leqq \frac{C}{\operatorname{dist}(\lambda, D)} \qquad \forall \lambda \in \mathbb{C} \backslash \bar{D}. \tag{6.4}$$

With (6.2) replaced by (6.4), the theorem becomes the sharp form of the Kreiss matrix theorem proved in [33]. □

It is well known that the resolvent condition (6.4) is necessary for power-boundedness. The sufficiency of this condition for power-boundedness with an additional factor of only $O(N_\nu)$ was first proved by Tadmor [34] and appears to be less well known. The question of to what extent the factors N_ν and n in (6.3) are sharp has not yet been fully settled. McCarthy and Schwartz [23] showed that (6.4) does not imply power-boundedness by constructing a family of operators $\{A_\nu\}$ satisfying (6.4) for a fixed C with $\sup_{n \geqq 0} \|A_\nu^n\|_2 \geqq C' \log^\beta N_\nu$, for some constant C' and $\beta < 1/4$. On the other hand the results of LeVeque and Trefethen [21] and Spijker [33] show that the factor $\mathrm{e}\, N_\nu$ is sharp if one requires uniformity over all constants $C > 0$.

If $C = 1$ in (6.2), then the algebraic factors in (6.3) can be deleted. In this case, the pseudo-eigenvalue condition implies that the field of values $\mathscr{F}(A_\nu)$ lies in the closed unit disk [38], which in turn implies that $\|A_\nu^n\| \leqq 2$ for all $n \geqq 0$ [26, 30]. This result is analogous to the Hille-Yosida theorem in the semi-discrete case.

The simple relationships between the conditions (6.1), (6.2) and (6.3) immediately yield the following corollary, which gives conditions for algebraic stability with respect to the dimension N_ν.

Corollary 6.2. *If the operators* $\{A_\nu\}$ *satisfy*

$$\|A_\nu^n\| \leqq C N_\nu^\beta \qquad \forall n \geqq 0 \tag{6.5}$$

for some constants C and $\beta>0$, then the ε-pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of these operators satisfy

$$\operatorname{dist}(\lambda_\varepsilon, D) \leqq C N_\nu^\beta \varepsilon \qquad \forall \varepsilon \geqq 0. \tag{6.6}$$

Conversely, (6.6) *implies*

$$\|A_\nu^n\| \leqq \mathrm{e}\, C N_\nu^\beta \min\{N_\nu, n+1\} \qquad \forall n \geqq 0. \tag{6.7}$$

Results for algebraic stability with respect to the power n can be derived by modifying the pseudo-eigenvalue condition (6.2). The following theorem is a restatement, in the language of pseudospectra, of results in [8] and [34].

Theorem 6.3. *If the operators $\{A_\nu\}$ satisfy*

$$\|A_\nu^n\| \leqq C_1 n^\alpha \qquad \forall n>0 \tag{6.8}$$

for some constants C_1 and $\alpha>0$, then the ε-pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of these operators satisfy

$$\operatorname{dist}(\lambda_\varepsilon, D) \leqq C_2(\varepsilon^{\frac{1}{\alpha+1}} + \varepsilon) \qquad \forall \varepsilon \geqq 0. \tag{6.9}$$

Conversely, (6.9) *implies*

$$\|A_\nu^n\| \leqq C_3 n^\alpha \min\{N_\nu, n\} \qquad \forall n>0. \tag{6.10}$$

The relationships between the constants C_i depend only on α.

Proof. It can readily be shown that (6.9) is equivalent to the condition

$$\|(\lambda I - A_\nu)^{-1}\| \leqq \frac{\bar{C}_2(1+\operatorname{dist}(\lambda, D))^\alpha}{\operatorname{dist}(\lambda, D)^{\alpha+1}} \qquad \forall \lambda \in \mathbb{C}\setminus\bar{D} \tag{6.11}$$

for some constant $\bar{C}_2$. The proof that (6.8) implies (6.11) is given in [8]. Conversely, it can be shown that (6.11) implies (6.10) by using a resolvent integral as in [21] or [34]. □

The crucial feature of the estimate (6.9) is the behavior of the ε-pseudospectra as $\varepsilon \to 0$. Theorem 6.3 is still true if (6.9) is replaced by the condition that the ε-pseudo-eigenvalues satisfy

$$\operatorname{dist}(\lambda_\varepsilon, D) \leqq C_2' \varepsilon^{\frac{1}{\alpha+1}} \qquad 0 \leqq \varepsilon \leqq \varepsilon_0 \tag{6.12}$$

for some $\varepsilon_0 < \infty$. The $O(\varepsilon)$ behavior of the ε-pseudospectra for large ε implied in (6.9) follows as a corollary of (6.12), as is shown below in Lemma 7.2.

We now establish conditions for power-boundedness of the operators $\{A_\nu\}$ when the powers satisfy $0 \leqq n\nu \leqq T$ for some $T>0$. The following result is an extension of Theorem 6.1. The mathematics of such an extension is straightforward [30, Sect. 4.9]. For this result we assume that $0<\nu<\nu_0$ for some $\nu_0<\infty$.

Theorem 6.4. *If the operators $\{A_\nu\}$ satisfy*

$$\|A_\nu^n\| \leqq C_1 \qquad 0 \leqq n\nu \leqq T \tag{6.13}$$

for some constant C_1, *then the* ε*-pseudo-eigenvalues* $\{\lambda_\varepsilon\}$ *of these operators satisfy*

$$\text{(6.14)} \qquad \operatorname{dist}(\lambda_\varepsilon, D) \leqq C_2\,\varepsilon + C_3\,v \qquad \forall\,\varepsilon \geqq 0.$$

Conversely, (6.14) *implies*

$$\text{(6.15)} \qquad \|A_v^n\| \leqq C_4(T) \min\{N_v, n\} \qquad 0 < n\,v \leqq T.$$

The relationships between the constants C_i *depend only on* v_0 *and* T.

Proof. It is convenient to rewrite (6.14) in the equivalent form

$$\text{(6.16)} \qquad \Lambda_\varepsilon(A_v) \subseteq D_{C_2\varepsilon + C_3 v} \qquad \forall\,\varepsilon \geqq 0,$$

where D_δ denotes the closed disk of radius $1+\delta$ centered at the origin. First assume that (6.16) holds. Scaling both sets by $e^{-C_3 v}$, we obtain

$$\text{(6.17)} \qquad e^{-C_3 v} \Lambda_\varepsilon(A_v) \subseteq e^{-C_3 v} D_{C_2\varepsilon + C_3 v} \subseteq D_{C_2 \varepsilon e^{-C_3 v}} \qquad \forall\,\varepsilon \geqq 0,$$

since $e^{-C_3 v}(1 + C_2\,\varepsilon + C_3\,v) \leqq 1 + C_2\,\varepsilon\, e^{-C_3 v}$. It is easily shown that the ε-pseudospectra of an operator L satisfy the scaling identity [38]

$$\text{(6.18)} \qquad \Lambda_{|a|\varepsilon}(a\,L) = a\,\Lambda_\varepsilon(L) \qquad \forall\,a \in \mathbb{C}.$$

Applying this result to (6.17) with $a = e^{-C_3 v}$, we obtain

$$\text{(6.19)} \qquad \Lambda_{\varepsilon e^{-C_3 v}}(e^{-C_3 v} A_v) \subseteq D_{C_2 \varepsilon e^{-C_3 v}} \qquad \forall\,\varepsilon \geqq 0.$$

Condition (6.19) is equivalent to the power-boundedness condition (6.2) for the family of operators $\{e^{-C_3 v} A_v\}$. Hence, by Theorem 6.1, (6.15) holds with $C_4 = e\,C_2\,e^{C_3 T}$.

Conversely, suppose that (6.13) holds. It is easily shown that the family $\{e^{-C_3' v} A_v\}$, with $C_3' = \log(C_1)/T$, is power-bounded by C_1 [30, Sect. 4.9]. Hence, Theorem 6.1 implies

$$\text{(6.20)} \qquad \Lambda_\varepsilon(e^{-C_3' v} A_v) \subseteq D_{C_1 \varepsilon} \qquad \forall\,\varepsilon \geqq 0.$$

We now proceed by reversing the steps in the first part of the proof. Applying the scaling identity with $a = e^{-C_3' v}$ to (6.20) we obtain

$$\text{(6.21)} \qquad e^{-C_3' v} \Lambda_{\varepsilon e^{C_3' v}}(A_v) \subseteq D_{C_1 \varepsilon} \qquad \forall\,\varepsilon \geqq 0.$$

Multiplying both sets in (6.21) by $e^{C_3' v}$ and applying the inequality $e^{C_3' v} \leqq 1 + C_3\,v$ with $C_3 = (e^{C_3' v_0} - 1)/v_0$ yields (6.16) with $C_2 = C_1$. □

7 Stability of one-step time integration formulas

We now prove our main stability result for method of lines discretizations based upon one-step time integration formulas.

It is convenient to rewrite the full discretization (2.3) in the standard form

$$\text{(7.1)} \qquad v^{n+1} = \phi(k\,L_k)\,v^n = A_k\,v^n, \qquad v^0 = f_k,$$

where $\phi(w)=p(w)/q(w)$ is a rational function of type (r, s). (We will assume that the polynomial $q(w)$ is monic.) Following the spectral theory for bounded linear operators described, for example, in [7] and [14], we assume that $\phi(w)$ is analytic in some neighborhood of the spectrum of kL_k. This condition ensures that $\phi(kL_k)$ is well defined. The spectral mapping theorem states that the spectra of A_k and kL_k, which we denote by $\Lambda(A_k)$ and $\Lambda(kL_k)$, are related by $\Lambda(A_k) = \phi(\Lambda(kL_k))$.

The stability region S of the time integration formula is defined by

$$S=\{w\in\mathbb{C}\colon \phi(w)\in\bar{D}\}.$$

If $\Lambda(kL_k)\subseteq S$, and kL_k has no defective eigenvalues on ∂S, then $\Lambda(A_k)\subseteq\bar{D}$ and A_k has no defective eigenvalues of unit modulus. This condition implies that A_k is power-bounded and is the well-known eigenvalue condition for stability. We make the following assumption about the stability region:

(A.1) S is bounded and $\phi'(w)\neq 0$ for $w\in\partial S$.

This condition excludes A-stable and other common implicit formulas with unbounded stability regions. Note that the boundedness of S implies that $r\geqq s$. The derivative condition is equivalent to the statement that $|\phi(w)|$ has no saddle points on ∂S.

Our main result for stability of one-step formulas on the infinite time interval is analogous to our earlier stability result for multistep formulas [28, Theorem 2]. The family of operators $\{A_k\}$ is stable, except for an algebraic factor, if the ε-pseudo-eigenvalues of the operators $\{kL_k\}$ lie within a distance $O(\varepsilon)$ of S as $\varepsilon\to 0$. For one-step methods, however, the converse need not hold unless the operators $\{kL_k\}$ satisfy an additional hypothesis, as demonstrated by an example below. The hypothesis we shall make is the following:

(A.2) There exists a non-empty domain $V\subseteq\mathbb{C}$ and a constant $M<\infty$ such that $\|(\mu I-kL_k)^{-1}\|\leqq M$ for all $\mu\in V$ and all k.

For their necessary condition for stability of the method of lines, Di Lena and Trigiante [6] assume that the family $\{kL_k\}$ satisfies a uniform boundedness condition $\|kL_k\|\leqq C$. This uniform boundedness assumption implies (A.2) (take V to be a set sufficiently far from the origin).

Here is our main result for stability on the infinite time interval.

Theorem 7.1. *Let* (7.1) *be the method of lines discretization of* (2.1) *based upon a one-step time integration formula satisfying Assumptions* (A.1) *and* (A.2). *If*

$$\|A_k^n\|\leqq C_1 \qquad \forall n\geqq 0, \tag{7.2}$$

then the ε-pseudo-eigenvalues $\{\mu_\varepsilon\}$ of the operators $\{kL_k\}$ satisfy

$$\operatorname{dist}(\mu_\varepsilon, S)\leqq C_2\,\varepsilon \qquad \forall \varepsilon\geqq 0. \tag{7.3}$$

Conversely, (7.3) *implies*

$$\|A_k^n\|\leqq C_3\min\{N_k, n\} \qquad \forall n>0. \tag{7.4}$$

The relationship between the constants C_i can be chosen to depend only on the one-step formula and on the constant M and the set V of Assumption (A.2).

Before proving this theorem we give the contrived example mentioned above to show that if Assumption (A.2) is omitted, then (7.2) does not imply (7.3). Suppose that the second-order Runge-Kutta formula, defined by the polynomial $\phi(w)=\frac{1}{2}w^2+w+1$, is applied to the family of matrices $\{kL_k\}$ defined by

(7.5) $$kL_k=\begin{bmatrix} -1+c(k) & 1/c(k) \\ 0 & -1+c(k) \end{bmatrix},$$

for $0<k\leqq 1$. Here $c(k)$ is any function satisfying $0<|c(k)|\leqq\frac{1}{2}$ and $\lim_{k\to 0} c(k)=0$. A simple calculation shows that

(7.6) $$A_k=\begin{bmatrix} \frac{1}{2}(1+c^2) & 2 \\ 0 & \frac{1}{2}(1+c^2) \end{bmatrix}.$$

The family $\{A_k\}$ satisfies (7.2) but not (7.3), and it can be shown that for any fixed $\mu\notin S$, $\|(\mu I-kL_k)^{-1}\|\to\infty$ as $k\to 0$.

Theorem 7.1 can be proved by the same arguments used in the proof of Theorem 2 in [28]. Here we take a more general approach and introduce three lemmas which can also be applied to our subsequent results for algebraic stability and for stability on finite time intervals. First, however, we simplify the statement of the theorem by an application of the Kreiss matrix theorem. Theorem 6.1 implies that Theorem 7.1 holds if (7.3) is replaced by the condition that the ε-pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of the operators $\{A_k\}$ satisfy

(7.7) $$\operatorname{dist}(\lambda_\varepsilon, D)\leqq C_2'\varepsilon \qquad \forall\varepsilon\geqq 0$$

for some constant C_2'. Hence, it is enough to show the equivalence of (7.3) and (7.7). That is to say, it is enough to show the equivalence of

(7.8) $$\|(\mu I-kL_k)^{-1}\|\leqq\frac{C_2}{\operatorname{dist}(\mu, S)} \qquad \forall\mu\in\mathbb{C}\setminus\bar{S}$$

and

(7.9) $$\|(\lambda I-A_k)^{-1}\|\leqq\frac{C_2'}{\operatorname{dist}(\lambda, D)} \qquad \forall\lambda\in\mathbb{C}\setminus\bar{D}.$$

This will be our goal for the next few pages.

The first lemma encapsulates the following observation. Suppose, say, that $\Lambda(A_k)\subseteq\bar{D}$ and that (7.9) is known to hold for λ satisfying $0<\operatorname{dist}(\lambda, D)<\tau$ for some $\tau>0$. Then (7.9) must hold for *all* $\lambda\in\mathbb{C}\setminus\bar{D}$. The reason is that for λ with $\operatorname{dist}(\lambda, D)\geqq\tau$, the resolvent $(\lambda I-A_k)^{-1}$ can be expressed by the integral

(7.10) $$(\lambda I-A_k)^{-1}=\frac{1}{2\pi i}\int_\Gamma(\lambda-z)^{-1}(zI-A_k)^{-1}\,dz,$$

where Γ is any closed contour enclosing the spectrum of A_k [7]. To be precise, let us define $\Gamma = \{z \in \mathbb{C}: \operatorname{dist}(\lambda, D) = \frac{1}{2}\tau\}$. On this contour $\|(zI - A_k)^{-1}\| \leqq 2C_2/\tau$ by (7.9) and $|\lambda - z|^{-1} \leqq 2/\operatorname{dist}(\lambda, D)$. These last two estimates and (7.10) imply

$$\|(\lambda I - A_k)^{-1}\| \leqq \frac{4C_2(1+\frac{1}{2}\tau)}{\tau \operatorname{dist}(\lambda, D)} \tag{7.11}$$

since the length of Γ is $2\pi(1+\frac{1}{2}\tau)$. This bound in fact holds for all $\lambda \notin \bar{D}$.

Analogously, it is enough to consider the estimate (7.8) for μ near S. These observations can be generalized by the following lemma, which is similar to [7, Lemma VII.6.11]. Let A be a matrix or bounded linear operator and let the set $U \subseteq \mathbb{C}$ be the union of a finite number of bounded connected domains. Define Γ to be the contour $\Gamma = \{z \in \mathbb{C}: \operatorname{dist}(z, U) = \frac{1}{2}\tau\}$. The proof of the following lemma follows from the resolvent integral (7.10).

Lemma 7.2. *If Γ encloses $\Lambda(A)$ and $\|(zI - A)^{-1}\| \leqq B$ uniformly for all $z \in \Gamma$, then*

$$\|(\lambda I - A)^{-1}\| \leqq \frac{CB}{\operatorname{dist}(\lambda, U)} \quad \forall \lambda \text{ satisfying } \operatorname{dist}(\lambda, U) \geqq \tau. \tag{7.12}$$

The constant C depends only on the set U and on τ.

As a consequence of Lemma 7.2, we need only show that (7.8) implies (7.9) for $\lambda \in \mathbb{C} \setminus \bar{D}$ satisfying $0 < \operatorname{dist}(\lambda, D) < \tau_z$ for some $\tau_z > 0$ and conversely, that (7.9) implies (7.8) for $\mu \in \mathbb{C} \setminus \bar{S}$ satisfying $0 < \operatorname{dist}(\mu, S) < \tau_w$ for some $\tau_w > 0$. We can define appropriate constants τ_w and τ_z depending only on the one-step formula. Let $\{\mu_i\}$ be the roots of $\phi(w) = \lambda$ and define the annulus

$$\Omega_z = \{z \in \mathbb{C}: 0 < \operatorname{dist}(z, D) < \tau_z\}, \tag{7.13}$$

where $\tau_z < \infty$ is chosen so that if $\lambda \in \bar{\Omega}_z$, then $|\mu_i|$ is bounded and $\phi'(\mu_i) \neq 0$. This is possible by Assumption (A.1). Define a corresponding set

$$\Omega_w = \{w \in \mathbb{C}: 0 < \operatorname{dist}(w, S) < \tau_w\}, \tag{7.14}$$

where $\tau_w > 0$ is chosen so that if $\mu \in \bar{\Omega}_w$, then $\phi(\mu) \in \bar{\Omega}_z$.

The next two lemmas are the key results which relate the resolvents $(\lambda I - A_k)^{-1}$ and $(\mu I - kL_k)^{-1}$.

Lemma 7.3. *Suppose that $\Lambda(A_k) \subseteq \bar{D}$. Choose $\lambda \in \Omega_z$ and let $\{\mu_i\}$ denote the roots of $\phi(w) = \lambda$. Then*

$$\|(\lambda I - A_k)^{-1}\| \leqq M_1 \sum_{i=1}^{r} \|(\mu_i I - kL_k)^{-1}\| + M_2, \tag{7.15}$$

where the constants M_1 and M_2 depend only on the one-step formula.

Proof. If $\Lambda(A_k) \subseteq \bar{D}$, then $\Lambda(kL_k) \subseteq S$ by the spectral mapping theorem. Therefore any number $\lambda \in \Omega_z$ lies in the resolvent set of A_k, and thus $(\lambda I - A_k)^{-1}$ is well defined. The roots $\{\mu_i\}$ lie outside of S and hence in the resolvent set of kL_k,

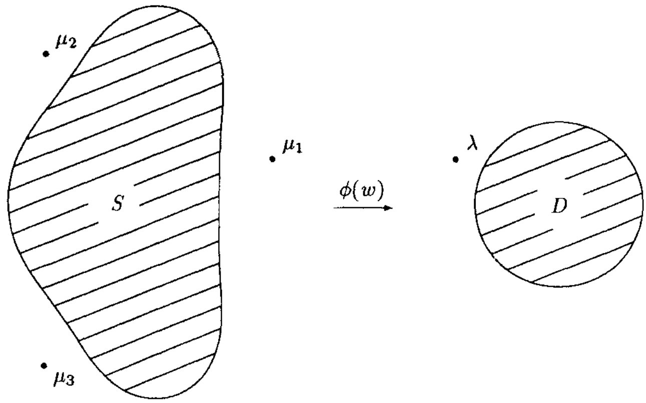

Fig. 3. Lemma 7.3 relates the resolvent $(\lambda I - A_k)^{-1}$ to the resolvents $(\mu_i I - k L_k)^{-1}$ (case $r=3$)

so $(\mu_i I - k L_k)^{-1}$ is well defined also (see Fig. 3). We start with the relation $(\lambda I - A_k)^{-1} = (\lambda I - \phi(k L_k))^{-1}$. The resolvent $(\lambda I - A_k)^{-1}$ can be related to the resolvent $(\mu I - k L_k)^{-1}$ by using the partial fraction decomposition

$$(\lambda - \phi(w))^{-1} = \sum_{i=1}^{r} (\phi'(\mu_i))^{-1} (\mu_i - w)^{-1} + (\lambda - \rho)^{-1}, \tag{7.16}$$

where $\rho = \lim_{w \to \infty} \phi(w)$ [22]. The last term in (7.16) is 0 if $\rho = \infty$. Equation (7.16) can be derived by an appropriate contour integral. The relation (7.16) still holds if the scalar w is replaced by the operator $k L_k$. We then obtain

$$(\lambda I - A_k)^{-1} = \sum_{i=1}^{r} \frac{(\mu_i I - k L_k)^{-1}}{\phi'(\mu_i)} + \frac{I}{\lambda - \rho}. \tag{7.17}$$

(This last result can also be derived by expressing $(\lambda I - A_k)^{-1}$ in terms of a resolvent integral of $(w I - k L_k)^{-1}$ as in [28].) Taking the norm of (7.17) yields (7.15) with M_1 and M_2 defined by

$$M_1 = [\inf_{\mu \in \phi^{-1}(\bar{\Omega}_z)} |\phi'(\mu)|]^{-1} \tag{7.18}$$

and

$$M_2 = [\inf_{\lambda \in \bar{\Omega}_z} |\lambda - \rho|]^{-1}. \tag{7.19}$$

The definitions of Ω_w and Ω_z guarantee that M_1 and M_2 are finite. □

The converse result is similar to Lemma 7.3 but is more difficult to derive. To show that $(\mu I - k L_k)^{-1}$ can be bounded in terms of $(\lambda I - A_k)^{-1}$, we rely on the additional Assumption (A.2). (If $\phi(w)$ is affine or rational of type (1, 1), then Assumption (A.2) is not required.) The proof of the following lemma makes use of several lemmas proved in Appendix A and can possibly be simplified.

Lemma 7.4. *Suppose that $\Lambda(kL_k) \subseteq S$. Choose $\mu \in \Omega_w$ and let $\lambda = \phi(\mu)$. Then*

$$\|(\mu I - kL_k)^{-1}\| \leqq M_3 \|(\lambda I - A_k)^{-1}\|, \tag{7.20}$$

where the constant M_3 depends on the one-step formula, on $\|A_k\|$, and on the constant M and the set V in Assumption (A.2).

Proof. If $\Lambda(kL_k) \subseteq S$, then $\Lambda(A_k) \subseteq \tilde{D}$. Therefore if $\mu \in \Omega_w$ lies in the resolvent set of kL_k, $\lambda = \phi(\mu)$ lies in the resolvent set of A_k. For the proof of the lemma we start with the expression $\lambda I - A_k = \lambda I - \phi(kL_k)$. The function $\lambda - \phi(w)$ has the factorization

$$\lambda - \phi(w) = \frac{(\mu - w)\,\bar{p}(w)}{q(w)}, \tag{7.21}$$

where $\bar{p}$ and q are relatively prime polynomials of degrees $r-1$ and s, respectively. The polynomial $\bar{p}$ depends on the choice of μ, and the family of these polynomials for $\mu \in \Omega_w$ is bounded in the sense that if $\bar{K} \subseteq \mathbb{C}$ is a compact set, then $|\bar{p}(w)| \leqq \bar{C}$ for all $w \in \bar{K}$ for some constant $\bar{C}$ independent of μ. Now Eq. (7.21) is valid if w is replaced by kL_k. The operators $(\lambda I - A_k)$ and $(\mu I - kL_k)$ are both invertible, so we obtain

$$(\mu I - kL_k)^{-1} = \bar{p}(kL_k)\, q^{-1}(kL_k)(\lambda I - A_k)^{-1}. \tag{7.22}$$

Taking the norm of this last expression gives

$$\|(\mu I - kL_k)^{-1}\| \leqq \|\bar{p}(kL_k)\, q^{-1}(kL_k)\|\ \|(\lambda I - A_k)^{-1}\|. \tag{7.23}$$

First, suppose that $r > s$. Lemma A.1 shows that Assumption (A.2) implies $\|kL_k\| \leqq M_4$, where the constant M_4 depends on the one-step formula, on $\|A_k\|$, on M, and on the set V. Since $|\bar{p}(w)|$ is bounded, it follows that $\|\bar{p}(kL_k)\|$ is also bounded by a constant which depends on the same factors. Lemma A.2 shows that if w_i is a root of $q(w)$, then $\|(w_i I - kL_k)^{-1}\|$ is bounded by a constant which again depends on the same factors. Combining these last results yields (7.20) with

$$M_3 = \|\bar{p}(kL_k)\, q^{-1}(kL_k)\|. \tag{7.24}$$

Now suppose that $r = s$. In this case, the function $\bar{p}/q$ can be written as a product of terms of the form $(w_i I - kL_k)^{-1}$ and $(\bar{\mu}_i I - kL_k)(w_i I - kL_k)^{-1}$, where $\bar{\mu}_i$ is a root of $\bar{p}$. Using Lemmas A.1 and A.2, it can be shown that $\|(\bar{\mu}_i I - kL_k)(w_i I - kL_k)^{-1}\| \leqq M_5$, where the constant M_5 depends on the same factors as the constant M_4. This last result and Lemma A.2 imply (7.20) with M_3 defined in (7.24). □

We now complete the proof of Theorem 7.1, making use of the Lemmas 7.2, 7.3, and 7.4.

Proof of Theorem 7.1. As mentioned above, we must show the equivalence of the resolvent conditions (7.8) and (7.9).

We first show that (7.8) implies (7.9). Condition (7.8) implies that $\Lambda(kL_k)\subseteq S$. The spectral mapping theorem implies that $\Lambda(A_k)\subseteq\bar{D}$. Now choose $\lambda\in\Omega_z$. The estimate (7.15) in Lemma 7.3 and (7.8) imply that

$$\|(\lambda I-A_k)^{-1}\|\leqq M_1\sum_{i=1}^{r}\frac{C_2}{\operatorname{dist}(\mu_i, S)}+M_2. \tag{7.25}$$

By Assumption (A.1), there is a constant E_1 such that

$$\operatorname{dist}(\lambda, D)\leqq E_1\operatorname{dist}(\mu_i, S)\qquad\forall\lambda\in\Omega_z. \tag{7.26}$$

Multiplying (7.25) by $\operatorname{dist}(\lambda, D)$ and applying this last bound yields (7.9) with $C_2=rM_1E_1C_2+\tau_zM_2$. Finally, Lemma 7.2 extends this conclusion from $\lambda\in\Omega_z$ to arbitrary $\lambda\in\mathbb{C}\backslash\bar{D}$.

The converse implication is proved in a similar manner. Condition (7.9) implies that $\Lambda(A_k)\subseteq\bar{D}$. The spectral mapping theorem implies $\Lambda(kL_k)\subseteq S$. Now choose $\mu\in\Omega_w$ and define $\lambda=\phi(\mu)$. Lemma 7.4 and (7.9) yield the bound

$$\|(\mu I-kL_k)^{-1}\|\leqq\frac{M_3C_2'}{\operatorname{dist}(\lambda, D)}. \tag{7.27}$$

The constant M_3 depends on $\|A_k\|$ and hence on C_1 by (7.2). Assumption (A.1) implies that there is a constant E_2 such that

$$\operatorname{dist}(\mu, S)\leqq E_2\operatorname{dist}(\lambda, D)\qquad\forall\mu\in\Omega_w. \tag{7.28}$$

Condition (7.27) and this last result yield (7.8) with $C_2=M_3E_2C_2'$. Again, Lemma 7.2 extends this conclusion from $\mu\in\Omega_w$ to arbitrary $\mu\in\mathbb{C}\backslash\bar{S}$. □

The relationship between Theorem 7.1 and the Kreiss matrix theorem is similar to the relationship between a method of lines stability result proved by Di Lena and Trigiante [5] and the Godunov-Ryabenkii criterion [9, 30]. The Godunov-Ryabenkii criterion states that a family of matrices $\{A_k\}$ can be stable only if the spectrum of the family [3], denoted by $P(\{A_k\})$, satisfies $P(\{A_k\})\subseteq\bar{D}$. The Di Lena/Trigiante result states that a method of lines calculation with a bounded family of scaled discretization matrices $\{kL_k\}$ can be stable only if $P(\{kL_k\})\subseteq S$. This result is proved by demonstrating that $P(\{A_k\})=\phi(P(\{kL_k\}))$.

8 Generalizations of Theorem 7.1

Theorem 7.1 can be generalized to give necessary and sufficient conditions for algebraic stability and for stability on finite time intervals.

First, let us consider algebraic stability with respect to the dimension N_k. Suppose that the ε-pseudo-eigenvalues $\{\mu_\varepsilon\}$ of the operators $\{kL_k\}$ satisfy

$$\operatorname{dist}(\mu_\varepsilon, S)\leqq C_2N_k^{\beta}\varepsilon\qquad\forall\varepsilon\geqq 0 \tag{8.1}$$

[3] Let $\{A_v\}$ be a family of matrices. A number $z\in\mathbb{C}$ is in the spectrum of the family if and only if $\|(\lambda I-A_v)^{-1}\|$ is unbounded with respect to v [9] (see Sect. 11)

for some $\beta > 0$. Then Lemmas 7.2 and 7.3 imply that the ε-pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of the operators $\{A_k\}$ satisfy

$$\text{(8.2)} \qquad \operatorname{dist}(\lambda_\varepsilon, D) \leqq C_2' N_k^\beta \varepsilon \quad \forall \varepsilon \geqq 0,$$

where the ratio C_2'/C_2 depends only on the one-step formula. By Corollary 6.2, this last condition yields the stability estimate

$$\text{(8.3)} \qquad \|A_k^n\| \leqq \mathrm{e}\, C_2' N_k^\beta \min\{N_k, n+1\} \quad \forall n \geqq 0.$$

A converse result cannot be deduced from the results of the previous section.

Algebraic stability with respect to the power n follows from Theorem 6.3.

Theorem 8.1. *Let* (7.1) *be the method of lines discretization of* (2.1) *based upon a one-step time integration formula satisfying Assumptions* (A.1) *and* (A.2). *If*

$$\|A_k^n\| \leqq C_1 n^\alpha \quad \forall n > 0$$

for some $\alpha > 0$, *then the* ε*-pseudo-eigenvalues* $\{\mu_\varepsilon\}$ *of the operators* $\{k L_k\}$ *satisfy*

$$\text{(8.4)} \qquad \operatorname{dist}(\mu_\varepsilon, S) \leqq C_2 (\varepsilon^{\frac{1}{\alpha+1}} + \varepsilon) \quad \forall \varepsilon \geqq 0.$$

Conversely, (8.4) *implies*

$$\text{(8.5)} \qquad \|A_k^n\| \leqq C_3 n^\alpha \min\{N_k, n\} \quad \forall n > 0.$$

The relationships between the constants C_i *depend only on the one step formula, on* α, *and on the constant* M *and the set* V *of Assumption* (A.2).

Proof. By Theorem 6.3, the result holds if (8.4) is replaced by the estimate that the ε-pseudo-eigenvalues $\{\lambda_\varepsilon\}$ of the operators $\{A_k\}$ satisfy

$$\text{(8.6)} \qquad \operatorname{dist}(\lambda_\varepsilon, D) \leqq C_2' (\varepsilon^{\frac{1}{\alpha+1}} + \varepsilon) \quad \forall \varepsilon \geqq 0$$

for some constant C_2'. Hence, the theorem can be proved by showing the equivalence of (8.4) and (8.6). The relationship between pseudospectra and resolvents implies that it is enough to show the equivalence of the resolvent conditions

$$\text{(8.7)} \qquad \|(\mu I - k L_k)^{-1}\| \leqq \frac{\bar{C}_2 (1 + \operatorname{dist}(\mu, S))^\alpha}{\operatorname{dist}(\mu, S)^{\alpha+1}} \quad \forall \mu \in \mathbb{C} \setminus \bar{S}$$

and

$$\text{(8.8)} \qquad \|(\lambda I - A_k)^{-1}\| \leqq \frac{\bar{C}_2' (1 + \operatorname{dist}(\lambda, D))^\alpha}{\operatorname{dist}(\lambda, D)^{\alpha+1}} \quad \forall \lambda \in \mathbb{C} \setminus \bar{D}.$$

The proof of the equivalence of (8.7) and (8.8) is similar to the proof of Theorem 7.1. □

We now consider stability on finite time intervals. Theorem 8.2 differs from Theorem 8.1 in that $\Lambda(k L_k)$ need not lie in the stability region. However, if μ lies in the spectrum of $k L_k$, then we must have $\operatorname{dist}(\mu, S) = O(k)$ as $k \to 0$. For this result we assume that $\Lambda(k L_k)$ lies sufficiently close to the stability region, and this implies an upper bound on the maximum time step k_0.

Theorem 8.2. *Let* (7.1) *be the method of lines discretization of* (2.1) *based upon a one-step time integration formula satisfying Assumptions* (A.1) *and* (A.2) *and having a sufficiently small time step k. If*

$$\|A_k^n\| \leqq C_1 \qquad 0 \leqq nk \leqq T, \tag{8.9}$$

then the ε-pseudo-eigenvalues $\{\mu_\varepsilon\}$ *of the operators* $\{kL_k\}$ *satisfy*

$$\operatorname{dist}(\mu_\varepsilon, S) \leqq C_2\,\varepsilon + C_3\,k \qquad \forall\,\varepsilon \geqq 0. \tag{8.10}$$

Conversely, (8.10) *implies*

$$\|A_k^n\| \leqq C_4 \min\{N_k, n\} \qquad 0 < nk \leqq T. \tag{8.11}$$

The relationships between the constants C_i depend only on the one-step formula, on T, and on the constant M and the set V of Assumption (A.2).

Proof. First we rewrite the pseudo-eigenvalue condition (8.10) in the form

$$\operatorname{dist}(\mu_{\varepsilon/C_2}, S) \leqq \varepsilon + C_3\,k \qquad \forall\,\varepsilon \geqq 0. \tag{8.12}$$

By Theorem 6.4 the result holds if (8.12) is replaced by the statement that the pseudo-eigenvalues $\{\lambda_{\varepsilon/C_2'}\}$ of the operators $\{A_k\}$ satisfy

$$\operatorname{dist}(\lambda_{\varepsilon/C_2'}, D) \leqq \varepsilon + C_3'\,k \qquad \forall\,\varepsilon \geqq 0 \tag{8.13}$$

for some constants C_2' and C_3'. Therefore it is enough to show the equivalence of (8.12) and (8.13). The proof of this equivalence is similar to the proof of Theorem 7.1. Suppose that $\mu \in \Lambda(kL_k)$ and $\lambda \in \Lambda(A_k)$. First, the spectral mapping theorem and Assumption (A.1) are used to show that

$$\operatorname{dist}(\mu, S) \leqq C_3\,k \Leftrightarrow \operatorname{dist}(\lambda, D) \leqq C_3'\,k.$$

Then, Lemma 7.2 and slightly modified versions of Lemmas 7.3 and 7.4 are used to relate the resolvents $(\mu I - kL_k)^{-1}$ for μ satisfying $\operatorname{dist}(\mu, S) > C_2\,k$ and $(\lambda I - A_k)^{-1}$ for λ satisfying $\operatorname{dist}(\lambda, D) > C_2'\,k$. We omit the details. □

We have been able to extend the above stability results to one-step formulas with unbounded stability regions in some special cases. It can be shown that Lemma 7.3 is also valid for the class of one-step formulas with unbounded S and bounded ∂S. The extension of this lemma follows since Ω_w is bounded for this class of formulas. Using this result the sufficiency parts of Theorems 7.1, 8.1, and 8.2 can be extended to this restricted class of one-step formulas. Also, it can be shown that Theorem 7.1 is valid for the trapezoid formula defined by $\phi(w) = (1 + \frac{1}{2}w)/(1 - \frac{1}{2}w)$, which has the left half-plane as a stability region [27, Sect. 5.5]. The generalization of our results to arbitrary unbounded stability regions, however, has not been worked out yet.

9 Stability of linear multistep formulas

We now turn our attention to Lax-stability for method of lines discretizations based upon linear multistep time integration formulas. Our previous paper [28] presented a result on the infinite time interval for explicit formulas whose stability regions do not have cusps. In the present section we generalize that result to implicit formulas, to algebraic stability, to finite time intervals, and, with a suitable modification of the pseudo-eigenvalue condition, to stability regions with cusps.

An s-step linear multistep method approximation to the semidiscretization (2.2) can be written in the form

$$\sum_{j=0}^{s} \alpha_j v^{n+j} - k \sum_{j=0}^{s} \beta_j L_k v^{n+j} = 0 \tag{9.1}$$

and is characterized by the polynomials

$$\rho(z) = \sum_{j=0}^{s} \alpha_j z^j, \qquad \sigma(z) = \sum_{j=0}^{s} \beta_j z^j, \tag{9.2}$$

with the convention $\alpha_s = 1$ and $|\alpha_0| + |\beta_0| \neq 0$. By introducing the vector $\mathbf{v}$ in (2.4), the full discretization (9.1) can be written in the compact form (2.3) with

$$A_k = G(k L_k) = \begin{bmatrix} a_{s-1} & \dots & a_1 & a_0 \\ I & & & \\ & \ddots & & \\ & & I & \end{bmatrix}. \tag{9.3}$$

Here $a_j = (I - \beta_s k L_k)^{-1} (\beta_j k L_k - \alpha_j I)$ for $0 \leqq j \leqq s-1$ and $I \equiv I_{N_k}$ is the identity operator of dimension N_k.[4]

The stability region S of the linear multistep formula is the set of numbers $w \in \mathbb{C}$ for which all roots z of the stability polynomial $\pi_w(z) = \rho(z) - w\sigma(z)$ satisfy $|z_i| \leqq 1$, with only simple roots for $|z| = 1$. If $\mu \in \Lambda(k L_k)$, then each root λ of π_μ lies in the spectrum of A_k. Conversely, $\mu \in \Lambda(k L_k)$ only if there is a $\lambda \in \Lambda(A_k)$ such that $\pi_\mu(\lambda) = 0$. This result follows trivially for matrices. See [27, Sect. 5.10] for a proof of this result for bounded linear operators. If $\Lambda(k L_k) \subseteq S$ and there are no defective eigenvalues on ∂S, then $\Lambda(A_k) \subseteq \bar{D}$ with no defective eigenvalues of unit modulus. This is the familiar eigenvalue criterion for power-boundedness. As described in [28], the stability region can be characterized in terms of the image of the unit circle under the rational function

$$r(z) = \frac{\rho(z)}{\sigma(z)}. \tag{9.4}$$

We restrict our attention to multistep formulas satisfying:

(B.1) S is bounded, with $r(z) \neq \infty$ for $z \in \partial D$;

(B.2) $r'(z) \neq 0$ for $z \in \partial D$.

---

[4] The weighted norm for vectors of length $s N_k$ is defined in terms of the block diagonal matrix $W_s = I_s \otimes W$, where W is the weight matrix for vectors of length N_k. If B and L are $s \times s$ and $N_k \times N_k$ matrices, respectively, and $A = B \otimes L$, then it can be shown that $\|A\|_{W_s} \leqq \|B\|_2 \, \|L\|_W$

For explicit formulas the condition $r(z) \neq \infty$ for $z \in \partial D$ implies that S is bounded, but this does not hold for implicit methods. Condition (B.2) implies that the stability region does not have cusps [5] and is necessary for Theorems 9.1, 9.5 and 9.6 below. A stability theorem for multistep formulas with cusps is given at the end of this section.

Here is our fundamental result for stability on infinite time intervals. The statement of this theorem is precisely the same as Theorem 2 in [28], but applies here to implicit as well as explicit methods.

Theorem 9.1. *Let* (9.1) *be the method of lines discretization of* (2.1) *based upon a multistep formula satisfying* (B.1) *and* (B.2). *If*

$$\|A_k^n\| \leqq C_1 \qquad \forall n \geqq 0, \tag{9.5}$$

then the ε*-pseudo-eigenvalues* $\{\mu_\varepsilon\}$ *of the operators* $\{k L_k\}$ *satisfy*

$$\operatorname{dist}(\mu_\varepsilon, S) \leqq C_2 \varepsilon \qquad \forall \varepsilon \geqq 0. \tag{9.6}$$

Conversely, (9.6) *implies*

$$\|A_k^n\| \leqq C_3 \min\{N_k, n\} \qquad \forall n > 0. \tag{9.7}$$

The constants C_i *are independent of* k *and the ratios* C_2/C_1 *and* C_3/C_2 *can be chosen to depend only on the multistep formula.*

Theorem 9.1 differs from the corresponding Theorem 7.1 for one-step methods in two respects. First, no additional condition analogous to (A.2) needs to be imposed on the operators $\{k L_k\}$. This is a consequence of the fact that each entry of $G(w)$ is either affine or a rational function of type (1, 1). (See the remarks preceding Lemma 7.4.) Second, the relationship between the constants C_i is particularly simple in this case. This fact implies the following corollary, which gives a pseudo-eigenvalue condition that is both necessary and sufficient for algebraic stability.

Corollary 9.2. *Let* (9.1) *be the method of lines discretization of* (2.1) *based upon a multistep formula satisfying* (B.1) *and* (B.2). *If*

$$\|A_k^n\| \leqq C_1 N_k^\beta \qquad \forall n \geqq 0 \tag{9.8}$$

for some $\beta > 0$, *then the* ε*-pseudo-eigenvalues* $\{\mu_\varepsilon\}$ *of the operators* $\{k L_k\}$ *satisfy*

$$\operatorname{dist}(\mu_\varepsilon, S) \leqq C_2 N_k^\beta \varepsilon \qquad \forall \varepsilon \geqq 0. \tag{9.9}$$

Conversely, (9.9) *implies*

$$\|A_k^n\| \leqq C_3 N_k^\beta \min\{N_k, n\} \qquad \forall n > 0. \tag{9.10}$$

The constants C_i *are independent of* k, *and the ratios* C_2/C_1 *and* C_3/C_2 *can be chosen to depend only on the multistep formula.*

We will only sketch the proof of Theorem 9.1 since it is given in [28] and is similar to the proof of Theorem 7.1. Theorem 6.1 and the relationship between

[5] *Let* S be a region in $\mathbb{C}$ with boundary ∂S. A point $w_0 \in \partial S$ is a cusp if at most one ray from w_0 leads into S [4]

pseudospectra and resolvents imply that the theorem can be proved by showing the equivalence of the resolvent conditions (7.8) and (7.9). The proof of this equivalence is similar to the corresponding proof for one-step methods. The only difference is that we require multistep analogs of Lemmas 7.3 and 7.4 to relate the resolvents $(\lambda I - A_k)^{-1}$ and $(\mu I - kL_k)^{-1}$ for λ near D and μ near S.

First, let us define the appropriate sets Ω_z and Ω_w. Let Ω_z be the annulus defined in (7.13), where $\tau_z < \infty$ is now chosen so that $r(z) \neq \infty$ for all $z \in \bar{\Omega}_z$. Let Ω_w be the set defined in (7.14) with $\tau_w < \infty$ chosen so that for all $\mu \in \Omega_w$, the number λ with maximum modulus satisfying $r(\lambda) = \mu$ satisfies $\lambda \in \Omega_z$. The following two results relate the resolvents.

Lemma 9.3. *Suppose that $\Lambda(A_k) \subseteq \bar{D}$. Choosing $\lambda \in \Omega_z$ and defining $\mu = r(\lambda)$ yields the estimate*

$$\|(\lambda I - A_k)^{-1}\| \leqq M_1 \|(\mu I - kL_k)^{-1}\| + M_2. \tag{9.11}$$

The constants M_1 and M_2 are finite and depend only on the multistep formula, which is assumed to satisfy (B.1).

Proof. This estimate (9.11) can be derived using the contour integral

$$(\lambda I - A_k)^{-1} = \frac{1}{2\pi i} \int_\Gamma (\lambda - G(w))^{-1} \otimes (wI - kL_k)^{-1}\, dw, \tag{9.12}$$

where the symbol $\otimes$ denotes a tensor product and Γ is any closed contour enclosing $\Lambda(kL_k)$. The details are given in [28]. Alternatively, (9.11) can be verified by directly expressing $(\lambda I - A_k)^{-1}$ in terms of $(\mu I - kL_k)^{-1}$ [27]. □

Lemma 9.4. *Suppose that $\Lambda(kL_k) \subseteq S$. Choose $\mu \in \Omega_w$ and let λ_m denote the root of $r(z) = \mu$ of maximum modulus. We then have the estimate*

$$\|(\mu I - kL_k)^{-1}\| \leqq M_3 \|(\lambda_m I - A_k)^{-1}\| + M_4. \tag{9.13}$$

The constants M_3 and M_4 are finite and depend only on the multistep formula, which is assumed to satisfy (B.1).

Proof. The resolvent bound (9.13) also follows from the integral (9.12) [28] (see also [27]). □

These results differ slightly from the corresponding lemmas for one-step methods. In contrast to Lemma 7.3, $(\lambda I - A_k)^{-1}$ is related to $(\mu I - kL_k)^{-1}$ at only one point in Lemma 9.3. The result in Lemma 9.4 does not require any additional assumptions analogous to (A.2) about the operator kL_k.

The proof of the equivalence of (7.8) and (7.9) for multistep methods is accomplished using Lemmas 7.2, 9.3, and 9.4 and is similar to the proof of Theorem 7.1.

Theorem 9.1 can be extended to give conditions for algebraic stability and for stability on finite time intervals. The following theorems are similar to Theorems 8.1 and 8.2 for one-step formulas. For stability on finite time intervals we once again assume that k is sufficiently small so that $\Lambda(kL_k)$ and $\Lambda(A_k)$ are close to S and D, respectively. The proofs of these theorems are similar to the proofs of the corresponding results for one-step formulas.

Theorem 9.5. *Let* (9.1) *be the method of lines discretization of* (2.1) *based upon a multistep formula satisfying* (B.1) *and* (B.2). *If*

$$\|A_k^n\| \leqq C_1 n^\alpha \qquad \forall n > 0$$

for some $\alpha > 0$, *then the* ε*-pseudo-eigenvalues* $\{\mu_\varepsilon\}$ *of the operators* $\{k L_k\}$ *satisfy*

$$\operatorname{dist}(\mu_\varepsilon, S) \leqq C_2 (\varepsilon^{\frac{1}{\alpha+1}} + \varepsilon) \qquad \forall \varepsilon \geqq 0. \tag{9.14}$$

Conversely, (9.14) *implies*

$$\|A_k^n\| \leqq C_3 n^\alpha \min\{N_k, n\} \qquad \forall n > 0.$$

The constants C_i *are independent of* k.

Theorem 9.6. *Let* (9.1) *be the method of lines discretization of* (2.1) *based upon a multistep formula satisfying* (B.1) *and* (B.2) *and having a sufficiently small time step* k. *If*

$$\|A_k^n\| \leqq C_1 \qquad 0 \leqq n k \leqq T, \tag{9.15}$$

then the ε*-pseudo-eigenvalues* $\{\mu_\varepsilon\}$ *of the operators* $\{k L_k\}$ *satisfy*

$$\operatorname{dist}(\mu_\varepsilon, S) \leqq C_2 \varepsilon + C_3 k \qquad \forall \varepsilon \geqq 0. \tag{9.16}$$

Conversely, (9.16) *implies*

$$\|A_k^n\| \leqq C_4(T) \min\{N_k, n\} \qquad 0 < n k \leqq T. \tag{9.17}$$

The constants C_i *are independent of* k.

These above stability theorems do not apply to linear multistep formulas whose stability regions have cusps. If $w_0 \in \Lambda(k L_k)$ for some cusp $w_0 \in S$, then A_k has a defective eigenvalue of unit modulus and hence is not power-bounded. Suppose on the other hand that the pseudo-eigenvalue condition (9.6) is satisfied and $w_0 \notin \Lambda(k L_k)$ for any k, but that w_0 is an accumulation point of $\bigcup_k \Lambda(k L_k)$. In this case, each operator A_k is individually power-bounded but the family $\{A_k\}$ is not uniformly power-bounded. If (9.6) is satisfied and the spectra of the operators $\{k L_k\}$ are bounded away from w_0, then the operators $\{A_k\}$ are power bounded. A theorem to this effect is proved in [4] for the special case in which the operators $\{k L_k\}$ are scalars.

The following example illustrates these ideas. Consider the midpoint rule, $\mathbf{v}^{n+1} = \mathbf{v}^{n-1} + 2 k L_k \mathbf{v}^n$, in the special case where $L_k = l_k$ is a scalar. The stability region is the complex interval $(-\mathrm{i}, \mathrm{i})$, and the two endpoints $\pm\mathrm{i}$ are cusps. Suppose that one of the cusps is an accumulation point of the family $\{k l_k\}$. For example, let $k l_k = \mathrm{i}(1-k)$ for $0 < k \leqq 1$. Since $L_k \equiv k L_k$ is a scalar, the pseudo-eigenvalues of these matrices lie within a distance ε of S. If applicable, Theorem 9.1 would imply that the powers of the matrices $\{A_k\}$ are uniformly bounded since $N_k = 1$. It can be shown that this family of matrices is not uniformly power-bounded; for each power $n > 0$ there is a k_n such that $\|A_k^n\|_2 \geqq n$ for all $k \leqq k_n$.

To adapt our theorems to stability regions with cusps, it is convenient to work with the sets defined by

$$S_\delta = \{w \in \mathbb{C}\colon \text{all roots of } \pi_w(z) \text{ lie in } D_\delta\},$$

where D_δ, defined in Sect. 6, is the closed disk of radius $1+\delta$ centered at the origin. These sets have the property that if w_0 is a cusp, then $\operatorname{dist}(w_0, \partial S_\delta) = O(\delta^2)$ as $\delta \to 0$, whereas if $w \in \partial S$ is not a cusp, then ∂S_δ lies within a distance $O(\delta)$ of w as $\delta \to 0$. The stability result for the infinite time interval can be roughly stated as follows: the method of lines discretization is stable if and only if $\Lambda_\varepsilon(k L_k) \subseteq S_{O(\varepsilon)}$ as $\varepsilon \to 0$ for $0 < \varepsilon < \varepsilon_0$. The following theorem is a modified version of Theorem 9.1.

Theorem 9.7. *Let* (9.1) *be the method of lines discretization of* (2.1) *based upon a linear multistep formula satisfying* (B.1). *If*

$$\|A_k^n\| \leqq C_1 \qquad \forall n \geqq 0, \tag{9.18}$$

then the pseudospectra of the operators $\{k L_k\}$ *satisfy*

$$\Lambda_\varepsilon(k L_k) \subseteq S_{C_2\varepsilon}, \qquad 0 < \varepsilon \leqq \varepsilon_0 \tag{9.19}$$

for some $\varepsilon_0 < \infty$. *Conversely,* (9.19) *implies*

$$\|A_k^n\| \leqq C_3 \min\{N_k, n\} \qquad \forall n > 0. \tag{9.20}$$

The constants C_i *are independent of* k. *The ratios* C_2/C_1 *and* C_3/C_2 *and* ε_0 *can be chosen to depend only on the multistep formula.*

Proof. The proof of Theorem 9.7 is slightly different from the proofs of the corresponding results for multistep formulas without cusps since these previous theorems are stated in terms of distances. First, it is convenient to rewrite (9.19) in the form

$$\Lambda_{\varepsilon/C_2}(k L_k) \subseteq S_\varepsilon, \qquad 0 < \varepsilon \leqq \bar{\varepsilon}_0. \tag{9.21}$$

By Theorem 6.1 and Lemma 7.2, the above result is true if the pseudospectra of the operators $\{A_k\}$ satisfy

$$\Lambda_{\varepsilon/C_2'}(A_k) \subseteq D_\varepsilon, \qquad 0 < \varepsilon < \bar{\varepsilon}_0' \tag{9.22}$$

for some constants C_2' and $\bar{\varepsilon}_0'$. The theorem is proved by showing the equivalence of (9.21) and (9.22), which can be accomplished using Lemmas 9.3 and 9.4. □

This result holds for all linear multistep formulas with bounded stability regions. If Assumption (B.2) holds, then $\operatorname{dist}(w, \partial S_\delta) = O(\delta)$ as $\delta \to 0$ uniformly for all $w \in \partial S$. In this case, the condition on the pseudospectra (9.21) can be expressed in terms of the distance to the stability region as in Theorem 9.1. It is straightforward to extend Theorem 9.7 to algebraic stability and to stability for finite time intervals; see [27] for the precise statements of these theorems.

Finally, as in the case of one-step formulas, the above results can be partially extended to formulas with unbounded stability regions. In fact, Theorem 9.7

and its generalizations are also valid for multistep formulas with unbounded S and bounded ∂S. This follows from the fact that Lemmas 9.3 and 9.4 can both be extended to this class of multistep formulas.

10 Applications

In this section we reexamine, from the point of view of pseudospectra, two stability results for finite difference approximations that fit into the method of lines framework. First, we consider discretizations of systems of constant-coefficient partial differential equations on infinite or periodic domains. By combining the theory of the previous sections with Fourier analysis we obtain necessary and sufficient conditions for stability that apply even when the amplification matrices involved are not normal. We next consider a specific example: an upwind approximation to the wave equation on a bounded interval. For this problem, analysis based on pseudospectra correctly predicts the stability condition, whereas it is well known that standard analysis, based on eigenvalues alone, gives an incorrect condition.

10.1 Finite difference approximations with constant coefficients

Finite difference approximations of constant-coefficient initial-value problems have been studied extensively. We present a general stability result for approximations fitting into the method of lines framework. The following analysis closely parallels [30, Chapter 4].

Assume that (2.1) is a constant-coefficient initial-value problem, where $u(x, t)$ is a vector function with p components of t and of a single space variable x on an unbounded or periodic domain. The operator $\mathscr{L}$ is a $p \times p$ matrix whose entries $\mathscr{L}_{ij}$ are linear differential operators. This system is first discretized in space at the equally spaced points $x_j = jh$. The spatial discretization operator L_k is a $p \times p$ matrix whose elements l_{ij} are biinfinite Toeplitz operators. Approximating in t with a one-step or multistep formula satisfying our usual assumptions, we obtain the full discretization, which is often written in the form

$$G_1(kL_k)\,\mathbf{v}^{n+1} = G_0(kL_k)\,\mathbf{v}^n, \tag{10.1}$$

where in our notation $G(w) = G_1^{-1}(w)\,G_0(w)$.

Many common finite difference formulas can be derived in the above manner. For the first-order wave equation $u_t = u_x$, the leap frog formula

$$v_j^{n+1} = v_j^{n-1} + \frac{k}{h}(v_{j+1}^n - v_{j-1}^n) \tag{10.2}$$

combines a centered difference in space with the midpoint formula in time. Similarly, the upwind approximation given below as (10.6) combines upwind differences in space and the Euler formula in time.

The stability of the approximation (10.1) is determined by examining the behavior of each Fourier mode $e^{i\xi x_j}$ for $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$. Let $\hat{\mathbf{v}}^n(\xi)$ and $\hat{L}_k(\xi)$ denote the Fourier transforms of $\mathbf{v}^n$ and L_k, respectively. The entries of the $p \times p$ matrix $\hat{L}_k(\xi)$ are the Fourier transforms $\hat{l}_{ij}(\xi)$ of the Toeplitz operators l_{ij}. Taking the Fourier transform of (10.1) and employing the solvability assumption that $G_1(k\hat{L}_k(\xi))$ is invertible, we obtain

$$\hat{\mathbf{v}}^{n+1}(\xi) = G_1^{-1}(k\hat{L}_k(\xi))\, G_0(k\hat{L}_k(\xi))\, \hat{\mathbf{v}}^n(\xi) = G(k\hat{L}_k(\xi))\, \hat{\mathbf{v}}^n(\xi). \tag{10.3}$$

The operator $G(k\hat{L}_k(\xi))$ is the so-called *amplification matrix*. The approximation (10.1) is Lax-stable if

$$\|G^n(k\hat{L}_k(\xi))\| \leqq C \qquad 0 \leqq nk \leqq T, \tag{10.4}$$

uniformly for all $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$, where here $\|\cdot\|$ denotes the unweighted 2-norm.

The von Neumann condition is necessary for stability: the spectra of the amplification matrices, $\Lambda(G(k\hat{L}_k(\xi)))$, must lie within a distance $O(k)$ of the unit disk. The resolvent condition of the Kreiss matrix theorem, Theorem 6.1, strengthens this eigenvalue condition by giving both necessary and sufficient conditions for stability in terms of the pseudospectra of the amplification matrices. On the other hand, the following result, an application of Theorems 8.2 and 9.6, gives conditions for stability in terms of the pseudospectra of the spatial discretization operators $\{k\hat{L}_k(\xi)\}$ themselves.

Theorem 10.1. *The approximation* (10.1) *is Lax-stable if and only if the ε-pseudo-eigenvalues of the operators $\{k\hat{L}_k(\xi)\}$ lie within a distance $O(\varepsilon)+O(k)$ of S as* ε, $k \to 0$, *uniformly for all $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$.*

In contrast to the theorems in the previous sections, the above result does not contain any additional algebraic factors. The reason is that Fourier analysis has reduced the stability analysis to the examination of matrices $\{\hat{L}_k(\xi)\}$ of fixed dimension p.

10.2 Upwind difference approximation of the wave equation

Our second application is a much more specific example in which the presence of boundary conditions precludes the use of Fourier analysis. The upwind finite-difference approximation to the first-order wave equation

$$u_t = u_x, \qquad x \in [0, 1), \qquad u(x, 0) = f(x), \qquad u(1, t) = 0 \tag{10.5}$$

on the infinite time interval is a well-known example of the failure of eigenvalue analysis to predict correctly the stability condition for method of lines discretizations [3, 9, 11, 30].[6] Stability analysis of the discretization via pseudospectra is straightforward and predicts the correct condition.

The upwind discretization of (10.5) is

$$v_j^{n+1} = v_j^n + \frac{k}{h}(v_{j+1}^n - v_j^n), \quad 0 \leqq j < N_k, \quad n > 0, \tag{10.6}$$

where v_j^n is an approximation to $u(jh, nk)$ and $h = 1/N_k$. Setting $\mathbf{v}^n = (v_0^n, v_1^n, \ldots, v_{N_k-1}^n)^{\mathrm{T}}$, we can put (10.6) into the form (2.3) with $G(w) = 1 + w$ and

$$k L_k = \frac{k}{h} \begin{bmatrix} -1 & 1 & & \\ & -1 & \ddots & \\ & & \ddots & 1 \\ & & & -1 \end{bmatrix}. \tag{10.7}$$

For simplicity we assume that $\gamma = k/h$ is a constant and that $\|\cdot\|$ denotes the unweighted 2-norm.

Eigenvalue stability analysis of the full discretization requires that $\Lambda(k L_k) \subseteq S \equiv D(-1, 1)$, where $D(a, b)$ denotes the closed disk of radius b centered at a. Since $\Lambda(k L_k) = \{-\gamma\}$, this in turn implies $\gamma < 2$. This inequality is strict since A_k has a defective eigenvalue of unit modulus if $\gamma = 2$. As mentioned in Sect. 4, the eigenvalue stability condition ensures that $\|A_k^n\| \leqq C$ for all $n > 0$, for *fixed* k and therefore fixed dimension N_k. In general the constant C depends on k, so we must write $C \equiv C(k)$. The discretization is Lax-stable if $C(k)$ is bounded for all k. If $1 < \gamma < 2$, then the discretization is time-stable but not Lax-stable. In fact, for such a choice of γ the discretization is exponentially unstable; it can readily be shown that

$$\max_{n>0} \|A_k^n\| \geqq \gamma^{N_k - 1}. \tag{10.8}$$

See [3, Sect. 10.5] for numerical results.

Where does the above analysis fail? Roughly speaking, eigenvalue analysis is valid only if the spatial discretization operators are normal or close to normal. The operators $\{k L_k\}$ for the upwind approximation are Jordan blocks and are highly non-normal.[7] For these operators $\Lambda(k L_k)$ is the single point $\{-\gamma\}$. Stability is determined by the pseudospectra, which for these operators are much larger than the spectra. The ε-pseudospectra $\Lambda_\varepsilon(k L_k)$ are disks about $-\gamma$ of radius approximately γ. In particular, any $z \in \mathbb{C}$ interior to $D(-\gamma, \gamma)$ is an ε-pseudo-eigenvalue of $k L_k$ for a value of ε decreasing exponentially as $k \to 0$ [29].

These properties of the pseudospectra of the operators $\{k L_k\}$ have the following implications for stability. If $\gamma > 1$, then $D(-\gamma, \gamma)$ is not contained inside

[6] Other examples of the failure of eigenvalue analysis of finite difference discretizations are described, for example, in [11, 24, 25]

[7] The non-normality of these matrices is also pointed out in [3]

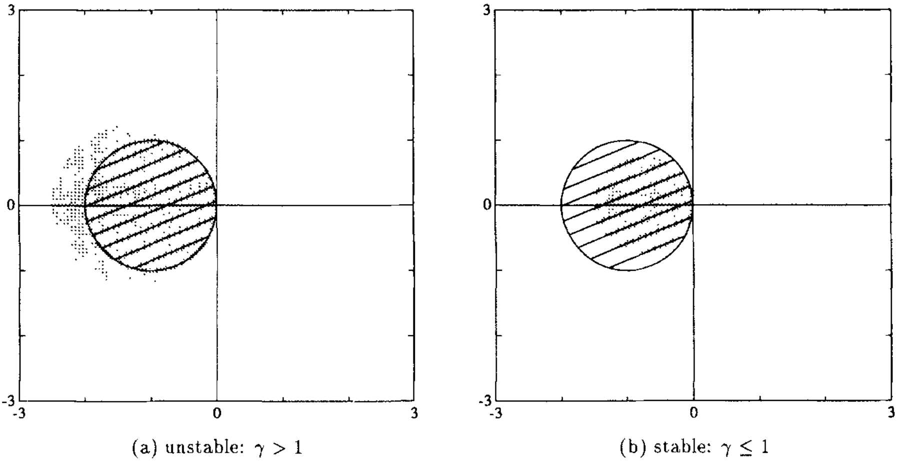

Fig. 4a, b. Upwind finite difference example (10.7). The *shaded disk* is the set $D(-\gamma,\gamma)$ and the *striped region* is the stability region S. For any $\varepsilon > 0$, the ε-pseudospectra of the operators $\{kL_k\}$ approximately fill the disk $D(-\gamma,\gamma)$. If $\gamma > 1$ the ε-pseudo-eigenvalues lie a finite distance, independent of ε, outside of S and the calculation is unstable. If $\gamma \leqq 1$, the ε-pseudo-eigenvalues lie within a distance ε of S and the calculation is stable

the stability region, as shown in Fig. 4a. A number $z \in D(-\gamma,\gamma)\backslash S$, is an ε-pseudo-eigenvalue for a value of ε which goes to 0 as $k \to 0$. This violates the pseudo-eigenvalue condition of Theorem 9.1, and therefore the condition

$$\gamma \leqq 1 \tag{10.9}$$

is necessary for stability. This condition is sufficient for stability also. It can be shown that the ε-pseudo-eigenvalues of the operators $\{kL_k\}$ lie within a distance ε of the disk $D(-\gamma,\gamma)$ for all $\varepsilon \geqq 0$ [29]. As shown in Fig. 4b this last property implies that the ε-pseudo-eigenvalues lie within a distance ε of the stability region. Hence, condition (10.9) gives a necessary and sufficient condition for stability on the infinite time interval. This result can also be proved by directly examining the resolvent $(\mu I - kL_k)^{-1}$, which is easy to compute.

The figure suggests another way of stating the stability condition for the upwind discretization: (10.6) is stable, except for an algebraic factor, if and only if the disk $D(-\gamma,\gamma)$ lies in the stability region. It is clear from our results in the previous sections that this result is also valid if we replace Euler's method with an arbitrary time-integration formula satisfying our usual assumptions. This fact is summarized by the following theorem, which is valid for finite and infinite time intervals.

Theorem 10.2. *Let* (2.1) *be the full discretization of* (10.5) *with an upwind discretization* (10.7) *in space such that* $\gamma = k/h$ *is a constant. Then the discretization is stable, except for an algebraic factor, if and only if the disk* $D(-\gamma,\gamma)$ *lies in the stability region.*

For one-step methods, the disk condition in Theorem 10.2 implies stability without any additional algebraic factors. This result holds because of the remark after Theorem 6.1: if the ε-pseudo-eigenvalues of the operators $\{A_k\}$ lie within a distance ε of the unit disk, then $\|A_k^n\| \leqq 2$ for all $n \geqq 0$. It can be shown that the disk condition imposed on the pseudospectra of the operators $\{k L_k\}$ implies that the pseudospectra of the operators $\{A_k\}$ satisfy the condition above by using standard properties of Toeplitz matrices (see [27] for the details).

The upwind example (10.6) can be correctly analyzed by many alternative methods, as is well known. For example, it can be shown that (10.9) is necessary for stability via the Courant-Friedrichs-Lewy condition [30], the Godunov-Ryabenkii criterion [9, 30], or its transplanted version [5]. It can be shown that (10.9) implies $\|A_k^n\| \leqq 1$ for all $n \geqq 0$ by using the contractivity results in [32]. Furthermore, for this example it is straightforward to verify that (10.9) is sufficient for stability by directly examining the powers of the operators $\{A_k\}$. For more complicated examples, however, the alternative methods for stability analysis are not always applicable.

11 Previous stability results

There have been many previous stability results for method of lines discretizations of linear evolution equations. The majority of these focus on conditions for algebraic stability on the infinite time interval, defined by

$$\|A_k^n\| \leqq C n^{\alpha} N_k^{\beta} \qquad \forall n > 0 \tag{11.1}$$

for some constants α, $\beta \geqq 0$, and apply to one-step time integration formulas with general norms. For the most part, these results are limited to sufficient conditions for Lax-stability, or, when both necessary and sufficient conditions are obtained, to a restricted class of discretization operators $\{L_k\}$.

In one of the early papers [2], Brenner and Thomée prove a stability result for A-stable one-step formulas on finite as well as infinite time intervals. They assume that the operators $\{L_k\}$ satisfy

$$\|e^{L_k t}\| \leqq C_o e^{\omega t} \qquad \forall t \geqq 0 \tag{11.2}$$

for some constants C_0 and $\omega \geqq 0$, and show that if $\omega = 0$, then (11.1) holds with $\alpha = \frac{1}{2}$ and $\beta = 0$. If $\omega > 0$ then this same result only holds on the finite time interval. These results are obtained using the Hille-Phillips operational calculus.

Spijker, Lenferink and Kraaijevanger consider more general one-step time integration formulas [15, 17, 32]. They restrict attention to operators satisfying the *circle condition:*

$$\|k L_k + \rho\| \leqq \rho, \tag{11.3}$$

for some $\rho > 0$. They estimate $\|A_k^n\|$ directly by using a series expansion and show that (11.3) implies (11.1) with $\alpha = \frac{1}{2}$ and $\beta = 0$ if $D(-\rho, \rho) \subseteq S$, where $D(a, b)$ denotes the disk of radius b centered at a. If this disk intersects the boundary of the stability region only at the origin, then (11.1) holds with $\alpha = 0$ and $\beta = 0$. A more restrictive condition on k related to the absolute monotonicity of $\phi(w)$ implies *contractivity* – that is, (11.1) with $\alpha = 0$, $\beta = 0$, and $C = 1$. Their results are applied to convection-diffusion equations.

Sanz-Serna and Verwer derive sufficient conditions for stability with $\alpha=0$ and $\beta=0$ based on contractivity and *C-stability* for more general p.d.e.s, nonlinear as well as linear [31, 40]. Their results are applied to a nonlinear parabolic equation and a cubic Schrödinger equation.

Our theory is most closely related to the results of Di Lena and Trigiante, Lenferink and Spijker, Lubich and Nevanlinna, and Kreiss and Wu, which are also based on resolvents. These stability results are obtained directly by estimating $\|A_k^n\|$ using the resolvent integral

$$A_k^n=\frac{1}{2\pi i}\int_\Gamma \phi^n(w)(wI-kL_k)^{-1}\,dw, \tag{11.4}$$

where Γ is a simple closed curve enclosing $\Lambda(kL_k)$.

Di Lena and Trigiante's results [5, 6] are based on the notion of the *spectrum of a family* of matrices, an idea that goes back to Godunov and Ryabenkii [9] and is also described in [1] and [30]. Let $\{A_\nu\}$ be a family of matrices of dimension $N_\nu<\infty$. The spectrum of the family $\{A_\nu\}$, denoted $P(\{A_\nu\})$, is a set in the complex plane which can be related to pseudospectra as follows: $z\in P(\{A_\nu\})$ if and only if for each $\varepsilon>0$, $z\in\Lambda_\varepsilon(A_\nu)$ for some ν. If $z\notin P(\{kL_k\})$, then $\|(\lambda I-A_\nu)^{-1}\|$ is bounded uniformly as a function of ν. Stability results for one-step formulas with bounded stability regions are obtained by using this idea. Di Lena and Trigiante show that the condition $P(\{kL_k\})\subseteq S$ is necessary for (11.1). This result is a corollary of Theorem 7.1 if $\|\cdot\|$ is a weighted 2-norm. They also show that the condition

$$P(\{kL_k\})\subseteq \operatorname{int}(S) \tag{11.5}$$

is sufficient for (11.1) with $\alpha=0$ and $\beta=0$. This last result is limited since in virtually any application the origin belongs to $P(\{kL_k\})$ and to ∂S, and not to the interior of S.

Lenferink and Spijker [20] obtain several stability results based on the concept of the *M-numerical range* [18]. The M-numerical range of a matrix A, denoted by $\tau_M(A)$, generalizes the usual numerical range in many directions. It is related to the resolvent as follows: if $V\subseteq\mathbb{C}$ is any set with the property that $\tau_M(A)\subseteq V$, then

$$\|(zI-A)^{-k}\|\leq\frac{M}{\operatorname{dist}(z,V)^k}\qquad \forall z\in\mathbb{C}\setminus\bar{V} \tag{11.6}$$

for all integers $k>0$. The set $\tau_M(A)$ is the smallest closed convex set satisfying (11.6). Their first stability results states that if

$$\tau_M(kL_k)\subseteq W\subseteq S, \tag{11.7}$$

where W is a bounded sector in the left half-plane, then (11.1) holds with $\alpha=\beta=0$. If, on the hand, W is an arbitrary compact convex set, then (11.7) implies stability with $\alpha=1$ and $\beta=0$. A more complicated argument based on a generalization of Theorem 6.1 to arbitrary compact convex sets [19] shows that (11.7) implies stability with $\alpha=0$ and $\beta=1$. These last two results can be considered as corollaries of Theorem 7.1 if $\|\cdot\|$ is a weighted 2-norm.

Lubich and Nevanlinna [22] have obtained several results similar to Theorems 7.1 and 9.1 for A-stable one-step and multistep formulas. They show that if the ε-pseudo-eigenvalues of the operators $\{k L_k\}$ lie within a distance $O(\varepsilon)$ of the left half-plane, then (11.1) holds with $\alpha=0$ and $\beta=1$ or with $\alpha=1$ and $\beta=0$.[8] For one-step methods this result is obtained via Theorem 6.1, while for multistep formulas it is proved using a modified version of (11.4). They also prove additional stability results for more restricted classes of time integration formulas.

Finally and most recently, Kreiss and Wu [16] have obtained sufficient conditions for stability of one-step and multistep formulas in exponentially weighted norms. They show that the full discretization is stable on the finite time interval with $\alpha=0$ and $\beta=0$ if the semidiscretization is stable and the full discretization is *locally stable.* A discretization is defined to be locally stable if the open half-disk

$$H=\{w\colon \operatorname{Re} w<0,\ |w|<\|k L_k\|\} \tag{11.8}$$

is a subset of the stability region. The proofs of their results are similar in spirit to the proof of our theorems. Using Parseval's relation, they first relate stability to a bound on the resolvent $(\lambda I-A_k)^{-1}$. They complete the proof by bounding $(\lambda I-A_k)^{-1}$ in terms of bounds on $(\mu I-k L_k)^{-1}$.

A. Appendix

In this appendix we prove two lemmas that are used in the proof of Lemma 7.4. Let $\phi(w)=p(w)/q(w)$ be a rational function of type (r,s) and let $\{k L_k\}$ be a family of bounded linear operators satisfying Assumptions (A.1) and (A.2) in Sect. 7. Denote the family of functions that are analytic in a neighborhood of the spectrum of $k L_k$ by $\mathscr{F}$.

Lemma A.1. *Suppose that $A_k=\phi(k L_k)$, where $\phi\in\mathscr{F}$ is a rational function with $r>s$ and $k L_k$ is a bounded linear operator. Then*

$$\|k L_k\|\leqq C_1\,\|A_k\|+C_2, \tag{A.1}$$

where the constants C_1 and C_2 depend only on the function ϕ, and on the constant M and the set V of Assumption (A.2).

Proof. The proof is by induction. The estimate (A.1) follows trivially if $\phi(w)$ is a polynomial of degree 1.

[8] The result proved by Brenner and Thomée is different from this second result. It can be shown that (11.2) with $\omega=0$ implies that

$$\|(\mu I-k L_k)^{-j}\|\leqq C_0/(\operatorname{Re}\mu)^j \qquad \forall \operatorname{Re}\mu>0 \qquad \forall j>0;$$

this is the Hille-Yosida theorem. The pseudo-eigenvalue condition assumed by Lubich and Nevanlinna is equivalent to this last expression for $j=1$ only

(i) Suppose that $f \in \mathscr{F}$ is a rational function of type (r, s) with $r \geqq s$. We show that there is a rational function $\bar{f} \in \mathscr{F}$ of type $(r-1, s)$ such that

$$\|\bar{f}(kL_k)\| \leqq C_3(\|f(kL_k)\| + C_4), \tag{A.2}$$

where the constants C_3 and C_4 depend only on f, the set V and the constant M. Choose $\lambda \in V$ and let $\gamma = f(\lambda)$. Define the functions $g(w) = (\lambda - w)^{-1}$ and $h(w) = \gamma - f(w)$. The function $\bar{f}(w) = g(w)\, h(w)$ is a rational function of type $(r-1, s)$ and is analytic in a neighborhood of $\Lambda(kL_k)$. We can replace w in this last expression with kL_k. Taking the norm gives (A.2).

(ii) Suppose that $f \in \mathscr{F}$ is a rational function of type (r, s) with $r \geqq s$ and $s \geqq 1$. We show that there is a rational function $\tilde{f} \in \mathscr{F}$ of type $(r-1, s-1)$ such that

$$\|\tilde{f}(kL_k)\| \leqq C_5 \|f(kL_k)\| + C_6, \tag{A.3}$$

where the constants C_5 and C_6 depend only on f, and on the set V and the constant M. First, we apply the procedure (i) to construct a rational function $\bar{f} \in \mathscr{F}$ of type $(r-1, s)$ that satisfies (A.2). If $f(w) = f_1(w)/f_2(w)$, then $\bar{f}(w) = \bar{f}_1(w)/f_2(w)$, where $\bar{f}_1$ is a polynomial of degree $(r-1)$. Suppose that w_0 is a root of f_2. Define α so that $f_1(w_0) + \alpha \bar{f}_1(w_0) = 0$. The function $\tilde{f} = f + \alpha \bar{f}$ is a rational function of type $(r-1, s-1)$ and is analytic in a neighborhood of the spectrum of kL_k. We can replace w by kL_k. Taking the norm, we obtain

$$\|\tilde{f}(kL_k)\| \leqq \|f(kL_k)\| + \|\alpha \bar{f}(kL_k)\|. \tag{A.4}$$

This last bound and (A.2) imply (A.3).

If $\phi(w)$ is a rational function of type (r, s) with $r > s$, then (A.1) follows after applying (ii) s times and (i) $r-s-1$ times. □

The next result gives a bound for the resolvent $(w_0 I - kL_k)^{-1}$, where w_0 is a root of q.

Lemma A.2. *Suppose that $A_k = \phi(kL_k)$, where kL_k is a bounded linear operator and $\phi \in \mathscr{F}$ is a rational function. If w_0 is a root of $q(w)$, then*

$$\|(w_0 I - kL_k)^{-1}\| \leqq C_1 \|A_k\| + C_2. \tag{A.5}$$

The constants C_1 and C_2 depend only on the function ϕ, and on the set V and the constant M of Assumption (A.2).

Proof. By using procedure (ii) of Lemma A.1 it can be shown that there is a rational function $f \in \mathscr{F}$ of type $(r', 1)$ such that $f = f_1(w)/(w_0 - w)$ and

$$\|f(kL_k)\| \leqq C_3 \|A_k\| + C_4. \tag{A.6}$$

The result (A.5) follows after r' applications of procedure (i) of Lemma A.1. □

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