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FOR PARALLEL COMPUTATIONS

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On Implicit Runge-Kutta Methods for Parallel Computations

Stephen L. Keeling*

Abstract. Implicit Runge-Kutta methods which are well-suited for parallel computations are characterized. It is claimed that such methods are first of all, those for which the associated rational approximation to the exponential has distinct poles, and these are called *multiply implicit* (MIRK) methods. Also, because of the so-called *order reduction* phenomenon, there is reason to require that these poles be real. Then, it is proved that a necessary condition for a q-stage, real MIRK to be A-stable with maximal order $q + 1$ is that $q = 1, 2, 3,$ or 5. Nevertheless, it is shown that for every positive integer q, there exists a q-stage, real MIRK which is A_0-stable with order $q + 1$, and for every even q, there is a q-stage, real MIRK which is I-stable with order q. Finally, some useful examples of algebraically stable MIRK's are given.

1 Introduction.

This paper is concerned with the characterization and construction of implicit Runge-Kutta methods (IRKM's) which are especially well-suited for the approximate solution of evolution equations on a parallel machine with a modest number of processors. For a precise discussion of the issues, IRKM's and their properties are now introduced. Given an integer $q \geq 1$, a q-stage IRKM is determined by a set of constants:

$$
\begin{array}{ccc|c}
a_{11} & \cdots & a_{1q} & \tau_1 \\
\vdots & & \vdots & \vdots \\
a_{q1} & \cdots & a_{qq} & \tau_q \\
\hline
b_1 & \cdots & b_q &
\end{array}
$$

and it is convenient to make the following definitions:

$$
A \equiv \{a_{ij}\}_{i,j=1}^q, \quad b^T \equiv \langle b_1, b_2, \ldots, b_q \rangle, \quad B \equiv \operatorname*{diag}_{1 \leq i \leq q}\{b_i\}, \quad M \equiv BA + A^T B - bb^T,
$$

$$
T \equiv \operatorname*{diag}_{1 \leq i \leq q}\{\tau_i\}, \quad V \equiv \{\tau_i^{j-1}\}_{i,j=1}^q, \quad R \equiv \operatorname*{diag}_{1 \leq i \leq q}\{i^{-1}\}, \quad e^T \equiv \langle 1, 1, \ldots, 1 \rangle.
$$

For the IRKM formulation used in this work, choose arbitrarily, $t_0 \in \mathbf{R}$, $\mathbf{y}_0 \in \mathbf{R}^n$, $\mathbf{F} : \mathbf{R}^{n+1} \to \mathbf{R}^n$ sufficiently smooth, and $k > 0$ sufficiently small, so that for $t_0 \leq t \leq t_0 + k$, smooth functions $\mathbf{y}, \hat{\mathbf{y}} : \mathbf{R} \to \mathbf{R}^n$ are well-defined by:

$$
(1.1) \qquad \begin{cases} D_t \mathbf{y}(t) &= \mathbf{F}(t, \mathbf{y}(t)) \\ \mathbf{y}(t_0) &= \mathbf{y}_0, \end{cases}
$$

and:

$$
(1.2) \qquad \begin{cases} \mathbf{y}^i(t) &= \mathbf{y}_0 + (t - t_0) \displaystyle\sum_{j=1}^q a_{ij} \mathbf{F}(t_0 + \tau_j(t - t_0), \mathbf{y}^j(t)), \quad 1 \leq j \leq q \\ \hat{\mathbf{y}}(t) &= \mathbf{y}_0 + (t - t_0) \displaystyle\sum_{i=1}^q b_i \mathbf{F}(t_0 + \tau_i(t - t_0), \mathbf{y}^i(t)). \end{cases}
$$

The method is described as *explicit* if $a_{ij} = 0$, $i \leq j$ and *implicit* if for any i, $a_{ii} \neq 0$.

As usual, there are three criteria by which a method is judged in this work: order of consistency, stability, and implementability. First, an IRKM is said to have *order ν* if for every $\mathbf{y}$ and $\hat{\mathbf{y}}$ defined as above, $D_t^l \mathbf{y}(t_0) = D_t^l \hat{\mathbf{y}}(t_0)$, $0 \leq l \leq \nu$. Nevertheless, when these methods are used for stiff problems, they suffer from an *order reduction* phenomenon. Specifically, if p is the largest integer for which the following holds:

$$
T[e; Ae; \ldots; A^{p-2}e] = [Ae; 2A^2 e; \ldots; (p-1)A^{p-1}e]
$$

then it often happens that only a $k^{\min(\nu, p)}$ type convergence can be proved or demonstrated computationally. (See e. g., [6], [7], [4], [10], [12], [15], and [11]) Also, note the barrier: $p \leq q + 1$.

With regard to stability, let $r(z)$ be a rational approximation to the exponential e^{-z} defined by:

$$
(1.3) \qquad r(z) \equiv 1 - z b^T (I + zA)^{-1} e.
$$

1

An IRKM is said to be A_0-*stable* if:

$$|r(z)| \le 1 \qquad \forall z \ge 0,$$

I-stable if:

$$|r(z)| \le 1 \qquad \forall \Re\{z\} = 0,$$

A-stable if:

$$|r(z)| \le 1 \qquad \forall \Re\{z\} \ge 0,$$

and *algebraically stable* if:

B and M are positive semidefinite.

Note that the last notion of stability is the strongest among these. [7] In fact, for the methods which are algebraically stable with B actually positive, there exist results for certain parabolic equations which guarantee decay of approximations with respect to the time step. [10]

Now, concerning implementability, there has been much effort devoted to the development of IRKM's for which the eigenvalues of A are identical and real. ([8], [9]) As indicated in the next section, these so-called *singly implicit* (SIRK) methods offer a computational advantage over other IRKM's on serial machines. However, it is explained in section 2 that in a parallel environment the preferred methods are those for which the eigenvalues of A are distinct. In this work, the latter are referred to as *multiply implicit* (MIRK) methods. Further, they are called real if $\sigma(A) \subset \mathbf{R}$, and otherwise complex.

It can be seen in section 2, that real MIRK's permit a greater degree of parallelism than those which are complex. However, if the eigenvalues of A are real, then $\nu \le q + 1$. [14] Nevertheless, while the classical order can be increased at the cost of introducing complex eigenvalues, the order reduction phenomenon enforces the $p \le q + 1$ barrier for the problems which motivate this work. Hence, the principal interest here is in real MIRK's.

In this connection, it is important for certain parabolic problems that for every positive integer q, there exists a q-stage, real MIRK which is A_0-stable with maximal order $\nu = q + 1$ and $p = q + 1$. This fact follows from results in [2],* but an independent and direct proof is given in section 4. Also, for hyperbolic problems, it is shown in section 5 that for every even integer q, there is a q-stage, real MIRK which is *I*-stable with order $\nu = q$. For a related result, see Bales, Karakashian, and Serbin.[†]

Concerning methods which are more stable, Wanner, Hairer, and Nørsett [16] have established that if an A-stable SIRK has order $\nu = q + 1$, then $q = 1, 2, 3,$ or 5. Also, for SIRK's which are actually algebraically stable, the limit $p = q + 1$ is achievable only for $q \le 2$. [3] Nevertheless, it is shown in section 3, that for a wide range of problems, an IRKM can be modified in such a way that the order reduction is no worse than $k^{\min(\nu, q+1)}$ even if $p < q + 1$. Hence, without regard for the value of p, one is led to ask about the existence of real MIRK's which are A-stable with maximal order $\nu = q + 1$. In section 4, it is shown that a necessary condition on such methods is that $q = 1$, $2, 3,$ or 5, i.e., the result of [16] is generalized to the case of real, distinct eigenvalues. Then in section 6, some useful examples of algebraically stable MIRK's are presented.

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*Bales, Karakashian, and Serbin, private communication.

[†]Bales, L. A., Karakashian, O. A., Serbin, S. M., *On the Stability of Rational Approximations to the Cosine with Only Real Poles.* (To appear.)

2 Parallel Implementation.

The primary purpose of this section is to support the claim that among IRKM's, MIRK's are the preferred methods in a parallel computing environment. For definiteness, let S_h be a finite dimensional function space and suppose that an approximation is required for the solution $u : [0, t^*] \rightarrow S_h$, to the initial value problem:

$$\begin{cases} D_t u & = & -L_h(t)u + f(t, u) \qquad 0 \leq t \leq t^* \\ u(0) & = & u^0 \end{cases}$$

where h amounts to a stiffness parameter, and for simplicity, $f(t, u)$ is assumed to be smooth and independent of h. Also $L_h(t)$ is assumed to be linear and selfadjoint with positive spectrum. Such a problem could of course arise from the semidiscretization of a semilinear parabolic initial boundary value problem. For its temporal discretization, let $t^* \equiv kn^*$, $t^n \equiv kn$, and make the following definitions:

$$L_h^n \equiv L_h(t^n), \qquad \mathcal{L}_h^n \equiv \operatorname*{diag}_{q \times q}\{L_h^n\}, \qquad \tilde{\mathcal{L}}_h^n \equiv \operatorname*{diag}_{1 \leq i \leq q}\{L_h(t^n + k\tau_i)\}.$$

It is well-known that implementing (1.2) as it stands can be very expensive because of the burden involved in computing the stages. Nevertheless, for simplicity here, assume that for the first $\nu - 1$ time steps, the stages are indeed computed exactly. Then, moving toward a cheaper procedure, given $\{f(t^{n-m}, U^{n-m})\}_{m=0}^{\nu-1}$, define approximate stages $\bar{U}^n = \langle U^{n,1}, U^{n,2}, \ldots, U^{n,q} \rangle^T$ according to:

$$\bar{U}^n = [I + kA\tilde{\mathcal{L}}_h^n]^{-1}\{eU^n + kA\mathcal{E}^n f\}$$

where:

$$\mathcal{E}^n f \equiv \{\sum_{m=0}^{\nu-1} \alpha_{jm} f^{n-m}\}_{1 \leq j \leq q},$$

$$\sum_{m=0}^{\nu-1} \alpha_{jm} m^l = (-1)^l \hat{e}_j^T T^l e \qquad 0 \leq l \leq \nu - 1, \quad 1 \leq j \leq q, \quad (m^l|_{m=l=0} \equiv 1),$$

and terms such as $A\tilde{\mathcal{L}}_h^n$ for example, are understood in the sense of composition of operators defined on $[S_h]^q$. Even though this extrapolation circumvents the need for solving a system of nonlinear algebraic equations at every time step, inverting the full operator $[I + kA\tilde{\mathcal{L}}_h^n]$ could still be very costly. Hence, suppose:

$$A = S^{-1} \Lambda S,$$

$$\Lambda = \operatorname*{diag}_{1 \leq i \leq q}\{\lambda_i\} + \operatorname*{subdiag}_{2 \leq i \leq q}\{\theta_i\} \qquad \lambda_i > 0, \quad 1 \leq i \leq q, \quad \theta_i = 0 \text{ or } 1, \quad 2 \leq i \leq q$$

so that $\bar{V}_{l_n}^n \approx \bar{U}^n$ can be obtained by the (outer) iterations:

$$[I + k\Lambda \mathcal{L}_h^n](S\bar{V}_l^n) = \{SeU^n + kSA(\mathcal{L}_h^n - \tilde{\mathcal{L}}_h^n)\bar{V}_{l-1}^n + kSA\mathcal{E}^n f\} \equiv R_l^n \qquad 1 \leq l \leq l_n$$

where:

$$\bar{V}_0^n \equiv \sum_{m=1}^{\min(n,\nu)} (-1)^{m+1} \binom{\min(n,\nu)}{m} \tilde{U}^{n-m} \qquad 1 \leq n \leq n^* - 1, \qquad \bar{V}_0^0 \equiv eU^0 = eu^0,$$

3

and $\{\tilde{U}^{n-m}\}_{m=1}^{\min(n,\nu)}$ are computed as indicated below. Now, consider the simple but important observation that if $\lambda_i \neq \lambda_j$, $i \neq j$ and $\theta_i = 0$, $2 \leq i \leq q$, then for arbitrarily large q, the block system above completely decouples into the following equations which can be solved in parallel:

$$[I + k\lambda_i L_h^n](S\bar{V}_l^n)_i = (R_l^n)_i \qquad 1 \leq i \leq q.$$

On the other hand, if a SIRK is used for which $\lambda_i = \lambda$, $1 \leq i \leq q$ and $\theta_i = 1$, $2 \leq i \leq q$, then at each time step, the approximate solution is required of systems involving only a single new coefficient matrix with the dimension d_h of S_h. However, Karakashian and Rust [*] have compared a two-stage MIRK and a two-stage SIRK on a two-processor IBM-3081D at the University of Tennessee, and a four-processor CRAY-XMP48 at the supercomputing center in Pittsburgh. This work suggests that as the dimension d_h increases, making the solution of the time stepping equations the dominant operation, the speed-up quickly exceeds unity and then approaches the ideal factor of q. Therefore, if a certain sufficiently large d_h (high spatial accuracy) is not required for a given problem, it could of course happen that the serial calculation would offer superior performance for a fixed q. Nevertheless, the temporal accuracy requirement could be satisfied by taking q large enough that a dramatic reduction in execution time is achieved with parallel computations.

Finally, in any of these cases, the factorization of new coefficient matrices at every time step can be avoided by using a preconditioned iterative method to approximate $\bar{V}_l^n$ with (inner) iterates, say $\{\tilde{V}_{l,j}^n\}_{0 \leq j \leq j_n}$. Further, for certain problems, it can be shown [10] that there exist integers m_n and j_n such that:

$$\frac{1}{n^*} \sum_{n=0}^{n^*-1} m_n j_n \leq c \neq c(h,k)$$

while the convergence order obtained for the scheme:

$$\begin{cases} U^{n+1} &= (1 - b^T A^{-1} e)U^n + k b^T A^{-1} \tilde{U}^n \\ \tilde{U}^n &= \tilde{V}_{l_n, j_n}^n \end{cases} \qquad 0 \leq n \leq n^* - 1$$

is the same as that obtained by using any additional outer or inner iterations.

Studying methods similar to those discussed above, certain authors have proved convergence estimates for partial and stiff ordinary differential equations obtaining $\mathcal{O}(k^{\min(\nu,p)})$ for the temporal discretization. (See e. g., [6], [10], and [4].) However, as advertised in the Introduction, for a wide range of evolution equations, there is a systematic way of modifying an IRKM so that order reduction can be avoided. Specifically, it is shown in [12] that for semilinear parabolic equations with time independent coefficients, order reduction can be completely eliminated by computing the stages using an extrapolation procedure in which the constants $\{\alpha_{jm}\}_{1 \leq j \leq q}^{0 \leq m \leq \nu-1}$ are defined by:

$$\sum_{m=0}^{\nu-1} \alpha_{jm} m^l = (-1)^l l! \, \hat{e}_j^T A^l e \qquad 0 \leq l \leq \nu - 1, \quad 1 \leq j \leq q.$$

It is also shown in [12] that for linear parabolic equations with time dependent coefficients, the order reduction can be rendered no worse that $\mathcal{O}(k^{\min(\nu,q+1)})$ by computing the stages as indicated

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[*]KARAKASHIAN, O. A., RUST, W., *On the Parallel Implementation of Implicit Runge-Kutta Methods.* (To Appear.)

at the beginning of this section but with $\tilde{\mathcal{L}}_h^n$ replaced by:

$$\bar{\mathcal{L}}_h^n \equiv \sum_{m=0}^{\min(\nu-1,q)} \Gamma_m \mathcal{L}_h^{n-m}$$

where:

$$\sum_{m=0}^{\min(\nu-1,q)} \Gamma_m m^l = (-1)^l D^l \qquad 0 \le l \le \min(\nu-1,q)$$

and:

$$D[e; Ae; \ldots; A^{q-1}e] \equiv [Ae; 2A^2e; \ldots; qA^qe].$$

Finally, in [12] it is shown that an approach similar to this can be used for quasilinear problems to obtain comparable results. Note that in each case, a special starting scheme is used to initiate the indicated extrapolation but the details are not provided here.

Now consider the case that $\sigma(A) \not\subset \mathbf{R}$, but assume that A can be transformed to quasidiagonal form:

$$A = S^{-1}\Lambda S, \qquad \Lambda = \operatorname*{diag}_{1 \le i \le m}\{\Lambda_i\}, \quad 1 \le m < q$$

and either:

$$\Lambda_i = \lambda_i > 0 \quad \text{or} \quad \Lambda_i = \begin{bmatrix} \alpha_i & -\beta_i \\ \beta_i & \alpha_i \end{bmatrix} \qquad \alpha_i, \beta_i > 0 \qquad 1 \le i \le m.$$

Then, the block linear systems discussed above decouple to equations of the form:

$$[I + k\lambda L_h^n]\psi = \phi$$

and:

$$\begin{bmatrix} I + k\alpha L_h^n & -k\beta L_h^n \\ k\beta L_h^n & I + k\alpha L_h^n \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}.$$

Again the subordinate equations can in principle, be solved simultaneously. Further, the solutions ψ_1 and ψ_2 for the 2×2 system can be computed in parallel according to:

$$[I + 2\alpha k L_h^n + (\alpha^2 + \beta^2)(kL_h^n)^2]\psi_1 = [I + k\alpha L_h^n]\phi_1 + k\beta L_h^n\phi_2 \equiv \chi_1$$

and:

$$[I + 2\alpha k L_h^n + (\alpha^2 + \beta^2)(kL_h^n)^2]\psi_2 = [I + k\alpha L_h^n]\phi_2 - k\beta L_h^n\phi_1 \equiv \chi_2.$$

Following Baker, Bramble and Thomée [1], since for $x \in \mathbf{R}$:

$$\frac{1}{1 + 2\alpha x + (\alpha^2 + \beta^2)x^2} = \Re\left[\frac{z_1}{1 + z_2 x}\right] \qquad z_1 \equiv 1 - \alpha\beta^{-1}i, \quad z_2 \equiv \alpha + \beta i,$$

complex arithmetic can be used to obtain:

$$\psi_i = \Re\{z_1[I + z_2 kL_h]^{-1}\chi_i\} \qquad i = 1, 2.$$

Note that as mentioned in the Introduction, the depth of decoupling which the real MIRK's allow is greater than their complex counterparts. Nevertheless, examples of each are given in sections 4-6.

5

3 A Barrier for A-Stable Real MIRK's with Maximal Order.

In this section, it is proved that a necessary condition for a q-stage, real MIRK to be A-stable with maximal order $\nu = q + 1$, is that $q = 1, 2, 3$, or 5. The plan of the proof is roughly as follows. According to the work of Nørsett and Wanner [13], for a real MIRK to be A-stable with maximal order, the eigenvalues of A must be linked to a certain type of hypersurface near the middle of the so-called real-pole sandwich. However, it is shown below that when constrained to such hypersurfaces, the rational function (1.3) has absolute value bounded by unity for infinite argument only if $q = 1, 2, 3$, or 5. The latter claim is established by considering this absolute value as a function depending on (the reciprocals of) the eigenvalues of A, and showing that it is minimized over (the positive part of) a maximal order hypersurface of the real-pole sandwich at the point where the eigenvalues are the same. Then since such points have been studied carefully for SIRK's, the remainder of the proof follows from the work of Wanner, Hairer, and Nørsett. [16]

Before proceeding with the details, the appropriate notation is developed. First, define the so-called symmetric polynomials for $\mathbf{x} \in \mathbf{R}^m$:

$$S_0(\mathbf{x}) \equiv 1, \qquad S_l(\mathbf{x}) \equiv \sum_{i_1 < i_2 < \cdots < i_l \leq m} x_{i_1} \cdot x_{i_2} \cdot \cdots \cdot x_{i_l} \quad 1 \leq l \leq m, \qquad S_{m+1}(\mathbf{x}) \equiv 0.$$

Next, some relevant properties of these polynomials are enumerated. By direct calculation:

$$
\begin{aligned}
S_l(\mathbf{x}) &= x_i \sum_{\substack{i_1 < \cdots < i_{l-1} \leq m \\ i_j \neq i, 1 \leq j \leq l-1}} x_{i_1} \cdot \cdots \cdot x_{i_{l-1}} + \sum_{\substack{i_1 < \cdots < i_l \leq m \\ i_j \neq i, 1 \leq j \leq l}} x_{i_1} \cdot \cdots \cdot x_{i_l} \\
&= x_i \partial_{x_i} S_l(\mathbf{x}) + \partial_{x_i} S_{l+1}(\mathbf{x}) \qquad 1 \leq i \leq m, \quad 0 \leq l \leq m \qquad \forall \mathbf{x} \in \mathbf{R}^m.
\end{aligned}
$$

(3.1)

Thus:

$$(3.2) \qquad \partial_{x_i} S_{l+1}(\mathbf{x}) = S_l(\mathbf{x})|_{x_i=0} \qquad 1 \leq i \leq m, \quad 0 \leq l \leq m \qquad \forall \mathbf{x} \in \mathbf{R}^m.$$

Also with $e^m \in \mathbf{R}^m$ having all unit coordinates:

$$(3.3) \qquad S_l(xe^m) = x^l \sum_{i_1 < i_2 < \cdots < i_l \leq m} 1 = x^l \binom{m}{l}$$

since the sum is the number of combinations of m distinct integers taken l at a time. Finally with $\mathbf{x}^{-1} \equiv \langle x_1^{-1}, x_2^{-1}, \ldots, x_m^{-1} \rangle^T$:

$$(3.4) \qquad \frac{S_l(\mathbf{x})}{S_m(\mathbf{x})} = S_{m-l}(\mathbf{x}^{-1}) \qquad 0 \leq l \leq m \qquad \forall \mathbf{x}^{-1} \in \mathbf{R}^m.$$

Now according to [13] and (3.4), the rational function (1.3) has real poles and order of approximation to e^{-z} equal to at least q,* if and only if it has the form:

$$(3.5) \qquad r(z) = \frac{\displaystyle\sum_{l=0}^{q}(-z)^l \sum_{m=0}^{l} \frac{(-1)^m}{(l-m)!} S_m(\mathbf{x}^{-1})}{\displaystyle\sum_{l=0}^{q} S_l(\mathbf{x}^{-1}) z^l} = \frac{\displaystyle\sum_{l=0}^{q}(-z)^l \sum_{m=0}^{l} \frac{(-1)^m}{(l-m)!} S_{q-m}(\mathbf{x})}{\displaystyle\sum_{l=0}^{q} S_{q-l}(\mathbf{x}) z^l}$$

---

*This notion of order is of course weaker than that described in the Introduction for IRKM's, but the distinction should be clear from the context.

for some $\mathbf{x}^{-1} \in \mathbf{R}^q$. Also since:

$$\sum_{l=0}^{q} S_{q-l}(\mathbf{x}) z^l = \prod_{m=1}^{q} (x_m + z)$$

the poles of $r(z)$ are $\{-x_m\}_{m=1}^q$. So it follows from work in [13] that a q-stage, real MIRK can be A-stable with maximal order $q+1$ only if $\mathbf{x}$ is contained in one of the q hypersurfaces of the set:[†]

$$W \equiv \{\mathbf{x} \in \mathbf{R}^q : \quad x_i > 0, \quad \sum_{l=0}^{q} \frac{(-1)^l}{(l+1)!} S_l(\mathbf{x}) = 0\}.$$

For convenience, these sheets or connected components of W are ordered as follows. First, define the Laguerre polynomial of degree m:

$$L_m(x) \equiv \sum_{l=0}^{m} (-1)^l \binom{m}{l} \frac{x^l}{l!}$$

and the values $\{x_i^m\}_{1 \le i \le m}^{m \ge 1}$ by:

$$L_{m+1}^l(x_i^m) = 0, \qquad 0 < x_1^m < x_2^m < \cdots < x_m^m.$$

Then using (3.3):

$$W \equiv W_1 \cup W_2 \cup \ldots \cup W_q \quad \text{with} \quad e x_i^q \in W_i, \quad 1 \le i \le q.$$

Now, the following is an adaptation of Theorem 10 of [13].

Lemma 3.1 *Let an A-stable, q-stage IRKM be given with a rational function (1.3) having only real poles and maximal order $q+1$. Then (1.3) must have the form (3.5) and it is necessary that:*

$$\mathbf{x} \in W_{\frac{q+1}{2}} \cup W_{\frac{q-1}{2}} \quad \text{if } q \text{ is odd, or} \qquad \mathbf{x} \in W_{\frac{q}{2}} \quad \text{if } q \text{ is even}$$

where $W_0 \equiv \emptyset$. ∎

The next lemma is proved in section 5 of [16].

Lemma 3.2 *For m, $i \ge 1$, $|L_m(x_i^m)| \le 1$ only if:*

$$m \ge \begin{cases} 1, & i = 1 \\ 5, & i = 2 \\ 9, & i = 3 \\ 6i - 10, & i \ge 4. \end{cases}$$

∎

[†]The maximal order hypersurfaces of the real-pole sandwich are defined in [13] as the sheets of $M \equiv \{\mathbf{y} \in \mathbf{R}^q : \sum_{l=0}^{q} \frac{(-1)^l}{(l+1)!} S_{q-l}(\mathbf{y}) = 0\}$; so by (3.4), to every point in W there corresponds a point in M with reciprocal coordinates.

Recalling (3.5), define:

$$\mathcal{R}(\mathbf{x}) \equiv \sum_{l=0}^{q} \frac{(-1)^l}{l!} S_l(\mathbf{x}) = r(\infty).$$

Next, let an IRKM be given as specified in Lemma 3.1, so that in particular, $|r(\infty)| \leq 1$. Now suppose that the following has been established:

$$(3.6) \qquad\qquad \inf_{\mathbf{x} \in W_i} |\mathcal{R}(\mathbf{x})| = |L_q(x_i^q)| \qquad 1 \leq i \leq q.$$

Then according to Lemma 3.1, one of the following must hold:

$$
\left.
\begin{array}{lll}
q \text{ is odd}, \quad \mathbf{x} \in W_{\frac{q+1}{2}}, & \text{and:} & |L_q(x_{\frac{q+1}{2}}^q)| \leq \\[2ex]
q \text{ is odd}, \quad \mathbf{x} \in W_{\frac{q-1}{2}}, & \text{and:} & |L_q(x_{\frac{q-1}{2}}^q)| \leq \\[2ex]
q \text{ is even} \quad \mathbf{x} \in W_{\frac{q}{2}}, & \text{and:} & |L_q(x_{\frac{q}{2}}^q)| \leq
\end{array}
\right\} \quad |\mathcal{R}(\mathbf{x})| \leq 1.
$$

Finally according to Lemma 3.2, the first case implies that $q = 1$, the second that $q = 3$ or 5, and the third that $q = 2$. This is the advertised result and what remains is to establish (3.6).

Lemma 3.3 *The constrained critical points of $\mathcal{R}(\mathbf{x})$ on W are precisely those points in W with identical coordinates.*

Proof: First, form the Lagrangian:

$$F(\mathbf{x}, \lambda) \equiv \sum_{l=0}^{q} \frac{(-1)^l}{l!} S_l(\mathbf{x}) - \lambda \sum_{l=0}^{q} \frac{(-1)^l}{(l+1)!} S_l(\mathbf{x})$$

so that if $\mathcal{R}(\mathbf{x})$ has a constrained critical point at $\mathbf{x}^* \in W$, then:

$$(3.7) \quad 0 = \partial_{x_i} F(\mathbf{x}^*, \lambda) = -\sum_{l=0}^{q-1} \frac{(-1)^l}{(l+1)!} \partial_{x_i} S_{l+1}(\mathbf{x}^*) + \lambda \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+2)!} \partial_{x_i} S_{l+1}(\mathbf{x}^*) \qquad 1 \leq i \leq q.$$

Also by (3.1):

$$
\begin{aligned}
0 &= \sum_{l=0}^{q} \frac{(-1)^l}{(l+1)!} S_l(\mathbf{x}^*) = x_i^* \sum_{l=1}^{q} \frac{(-1)^l}{(l+1)!} \partial_{x_i} S_l(\mathbf{x}^*) + \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+1)!} \partial_{x_i} S_{l+1}(\mathbf{x}^*) \\[2ex]
(3.8) \qquad\qquad\qquad &= -x_i^* \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+2)!} \partial_{x_i} S_{l+1}(\mathbf{x}^*) + \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+1)!} \partial_{x_i} S_{l+1}(\mathbf{x}^*)
\end{aligned}
$$

$$1 \leq i \leq q.$$

Now for the sake of contradiction suppose that for some j:

$$(3.9) \qquad\qquad \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+2)!} \partial_{x_j} S_{l+1}(\mathbf{x}^*) = 0.$$

8

Then it follows from (3.8) that in addition:

$$(3.10) \qquad \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+1)!} \partial_{x_j} S_{l+1}(\mathbf{x}^*) = 0.$$

Using (3.2) and (3.4), it follows that if the coordinates of $\mathbf{y}^* \in \mathbf{R}^{q-1}$ are reciprocal to those of $\mathbf{x}^*$ other that x_j^*, then:

$$\frac{\partial_{x_j} S_{l+1}(\mathbf{x}^*)}{\partial_{x_j} S_q(\mathbf{x}^*)} = \frac{S_l(\mathbf{y}^{*-1})}{S_{q-1}(\mathbf{y}^{*-1})} = S_{q-1-l}(\mathbf{y}^*).$$

So, dividing (3.9) and (3.10) by $\partial_{x_j} S_q(\mathbf{x}^*)$ gives the following conditions:

$$\sum_{l=0}^{q-1} \frac{(-1)^l}{(l+2)!} S_{q-1-l}(\mathbf{y}^*) \quad = \quad 0 \quad = \quad \sum_{l=0}^{q-1} \frac{(-1)^l}{(l+1)!} S_{q-1-l}(\mathbf{y}^*).$$

However, as indicated in [13], with:

$$(3.11) \qquad N_0(t; \mathbf{y}) \equiv \sum_{l=0}^{n} (-1)^{n-l} S_{n-l}(\mathbf{y}) \frac{t^l}{l!}, \qquad N_{m+1}(t; \mathbf{y}) \equiv \int_0^t N_m(s; \mathbf{y}) ds \qquad \mathbf{y} \in \mathbf{R}^n$$

the following must be satisfied:

$$\{\mathbf{y} \in \mathbf{R}^n : N_1(1; \mathbf{y}) = 0\} \quad \cap \quad \{\mathbf{y} \in \mathbf{R}^n : N_2(1; \mathbf{y}) = 0\} \quad = \quad \emptyset.$$

Hence, (3.9) and (3.10) cannot hold simultaneously. Therefore, by (3.7) and (3.8), $x_i^* = \lambda = x_j^*$, $1 \le i, j \le q$. ∎

Now in order to capture the global minima of $|\mathcal{R}(\mathbf{x})|$ on the components of W, the following corollary is concerned with constrained critical points on the boundary of W. Its proof involves only appropriate adjustments in the dimensions of the above argument.

Corollary 3.1 *Given a multi-index* $\mathbf{m} \equiv \langle m_1, m_2, \ldots, m_q \rangle$ *where* $m_i = 0$ *or* 1, $1 \le i \le q$, *and* $|\mathbf{m}| \equiv \sum_{i=1}^q m_i$, $1 \le |\mathbf{m}| \le q$, *define:*

$$\mathbf{R}_+^{\mathbf{m}} \equiv \{\mathbf{x} \in \mathbf{R}^q : \quad x_i = 0, \text{ if } m_i = 0, \quad x_j > 0, \text{ if } m_j = 1, \quad 1 \le i, j \le q\}.$$

Then the constrained critical points of $\mathcal{R}(\mathbf{x})$ *on* $\overline{W} \cap \mathbf{R}_+^{\mathbf{m}}$ *are precisely those points in* $\overline{W} \cap \mathbf{R}_+^{\mathbf{m}}$ *with identical coordinates.* ∎

The next lemma is not actually contained in Theorem 8 of [13], but the argument required is essentially the same. Nevertheless, a brief proof is offered for completeness.

Lemma 3.4 *Let* $m = |\mathbf{m}|$, $1 \le m \le q$, *and suppose* $e^{\mathbf{m}} \in \mathbf{R}_+^{\mathbf{m}}$ *has only unit nonzero coordinates. Then the points of* $\overline{W} \cap \mathbf{R}_+^{\mathbf{m}}$ *with identical coordinates are precisely:*

$$x_i^m e^{\mathbf{m}} \in \overline{W}_i \qquad 1 \le i \le m,$$

and:

$$\mathcal{R}(x_i^m e^{\mathbf{m}}) = L_m(x_i^m) \qquad 1 \le i \le m.$$

Proof. Fix $\mathbf{m}$, $m = |\mathbf{m}|$, with $2 \leq m \leq q$, and $\mathbf{n}$, $n = |\mathbf{n}|$, with $n = m - 1$. Also, suppose $\mathbf{R}_+^\mathbf{n} \subset \overline{\mathbf{R}}_+^\mathbf{m}$ and that $e^\mathbf{m} \in \mathbf{R}_+^\mathbf{m}$ and $e^\mathbf{n} \in \mathbf{R}_+^\mathbf{n}$ have only unit nonzero coordinates. Next, with $X(0) \equiv \{\mathbf{x} \in \mathbf{R}_+^\mathbf{m} : \mathbf{x} = xe^\mathbf{m}, x > 0\}$ and $X(1) \equiv \{\mathbf{x} \in \mathbf{R}_+^\mathbf{n} : \mathbf{x} = xe^\mathbf{n}, x > 0\}$, suppose that for $\theta \in [0, 1)$, $X(\theta)$ is a ray from the origin into $\mathbf{R}^\mathbf{m}$ passing smoothly from $X(0)$ to $X(1)$. With (3.3), it follows that $X(0) \cap \overline{W} = \{x_i^m e^\mathbf{m}\}_{i=1}^m$ and $X(1) \cap \overline{W} = \{x_i^n e^\mathbf{n}\}_{i=1}^n$. So for $\theta \in [0, 1)$, let $\{\mathbf{x}_i(\theta)\}_{i=1}^m$ denote the points of $X(\theta) \cap \overline{W}$ ordered according to increasing magnitude. That these points remain separated, preserved in number and order, and bounded for θ in compact subintervals of $[0, 1)$, can be seen by noting that the explicit calculation of their coordinates involves the roots of a polynomial which has degree m while $\theta < 1$. Since the components of W never intersect, [13] these roots can never coalesce to become multiple or complex or to change relative positions. Now, since their number decreases by one as θ passes to 1, it only remains to determine whether $\mathbf{x}_m$ escapes to ∞ or $\mathbf{x}_1$ passes through the origin. Since $\overline{W} \cap \mathbf{0} = \emptyset$, the indicated alignment between the points $\{x_i^m e^\mathbf{m}\}_{1 \leq i \leq m}^{1 \leq m \leq q}$ and $\{\overline{W}_i\}_{1 \leq i \leq q}$ is established. Finally, the values for $\mathcal{R}(\mathbf{x})$ are obtained with (3.3). ∎

Now the following shows that the constrained critical values of $\mathcal{R}(\mathbf{x})$ determine the constrained global minima of $|\mathcal{R}(\mathbf{x})|$.

Lemma 3.5 *The constrained global minima of $|\mathcal{R}(\mathbf{x})|$ on the components of W are given as follows:*

$$\inf_{\mathbf{x} \in W_i} |\mathcal{R}(\mathbf{x})| = \min_{i \leq m \leq q} \{|L_m(x_i^m)|\} \qquad 1 \leq i \leq q.$$

Proof. First, note that $\mathcal{R}(\mathbf{x})$ never vanishes on W, because the rational function (3.5) cannot have degree $q - 1$ in the numerator and order $q + 1$ simultaneously. [14] Hence, on each $\overline{W}_i \cap \mathbf{R}_+^\mathbf{m}$, $|\mathcal{R}(\mathbf{x})|$ is a smooth, positive polynomial with exactly one critical point where it must be minimized. The rest of the result follows with Corollary 3.1 and Lemma 3.4. ∎

Now, the following lemma yields (3.6).

Lemma 3.6 *The Laguerre polynomials $\{L_m(x)\}_{m \geq 1}$, and the values $\{x_i^m\}_{1 \leq i \leq m}^{m \geq 1}$ satisfy:*

(3.12) $$|L_m(x_i^m)| < |L_{m-1}(x_i^{m-1})| \qquad 1 \leq i \leq m - 1, \quad m \geq 2.$$

Proof. By the identity:
(3.13) $$L_m(x) = L_{m+1}(x) - \frac{x}{m+1} L_{m+1}'(x)$$

the inequalities of (3.12) are equivalent to:

$$|L_{m+1}(x_i^m)| < |L_m(x_i^{m-1})| \qquad 1 \leq i \leq m - 1, \quad m \geq 2$$

which can be established by showing that:

(3.14) $$L_m(x_i^{m-1}) < L_m(x_i^m) = L_{m+1}(x_i^m) < 0 \quad \text{for odd } i \leq m - 1$$

and:

(3.15) $$0 < L_{m+1}(x_i^m) = L_m(x_i^m) < L_m(x_i^{m-1}) \quad \text{for even } i \leq m - 1.$$

10

First note that since $L_{m+1}(x)$ has exactly $m+1$ simple real roots, it has exactly m local extrema which must be associated with the m simple real roots of $L'_{m+1}(x)$. Therefore since $L_{m+1}(0) = 1$:

(3.16) $(-1)^i L_{m+1}(x_i^m) > 0$, $(-1)^{i+1} L''_{m+1}(x_i^m) > 0$ $1 \leq i \leq m$.

So using this with (3.13):

$$(-1)^i L'_m(x_i^m) = \frac{(-1)^{i+1} x_i^m}{m+1} L''_{m+1}(x_i^m) = |\frac{x_i^m}{m+1} L''_{m+1}(x_i^m)| > 0 \qquad 1 \leq i \leq m.$$

Now assume that $i \leq m-1$ is odd. Then on the interval $[x_i^m, x_{i+1}^m]$, $L_m(x)$ is decreasing at the beginning and increasing at the end, while $L'_m(x)$ vanishes only at $x_i^{m-1} \in (x_i^m, x_{i+1}^m)$ where $L_m(x)$ is minimized. Combining this fact with (3.13) and (3.16) gives (3.14). Also (3.15) follows similarly.   ∎

Finally, the result of this section is summarized in the following.

Theorem 3.1 *Let an A-stable, q-stage IRKM be given with a rational function (1.3) having only real poles and maximal order $q + 1$. Then $q = 1, 2, 3$, or 5.*   ∎

4   A Family of High Order A_0-Stable Real MIRK's.

In spite of the barrier established above, a family of IRKM's is constructed in this section, which contains for every positive integer q, a q-stage, real MIRK which is A_0-stable with maximal order $q + 1$. Such methods are useful for parabolic equations, since the following is pivotal in the stability analysis:

$$\|r(kL_h^n)\| \leq 1$$

where $\| \cdot \|$ is an appropriate norm. [10] Note that if $L_h(t)$ is selfadjoint and positive definite, then this inequality follows from A_0-stability and a spectral argument. Otherwise, a restrictive relationship between h and k must be imposed.

Toward the goal of this section, recall the functions $\{N_m(t; \mathbf{y})\}_{m \geq 0}$ defined in (3.11). Then let $\hat{e} \equiv \langle e_1, e_2, \ldots, e_q \rangle^T$ be a unit vector chosen so that:

$$e_i > 0 \quad \text{and} \quad e_i \neq e_j \qquad 1 \leq i \neq j \leq q.$$

According to [13], there are exactly q positive solutions to:

$$N_1(1, y\hat{e}) = 0.$$

So if y^* is the largest, set $\mathbf{y}^* \equiv y^* \hat{e}$. Then it follows that the function:

$$G(t) \equiv \frac{N_1(t, \mathbf{y}^*)}{N'_1(0, \mathbf{y}^*)} = \frac{t^{q+1} N_1(1, t^{-1}\mathbf{y}^*)}{(-1)^q S_q(\mathbf{y}^*)}$$

vanishes at $t = 0$ and $t = 1$ but for no $t \in (0, 1)$. Further, since $G'(0) = 1$, it follows that for every $t \in [0, 1]$, $G''(t) < 0$. Finally, note that by (3.4):

$$G'(1) = \sum_{l=0}^{q} \frac{(-1)^l}{l!} \frac{S_{q-l}(\mathbf{y}^*)}{S_q(\mathbf{y}^*)} = \mathcal{R}(\mathbf{y}^{*-1}).$$

Lemma 4.1 $|G'(1)| < 1$.

Proof. As explained in the proof of Lemma 3.5, $\mathcal{R}(\mathbf{x})$ never vanishes on W. Also, from the proof of Lemma 3.4, it can be seen that $\overline{W}_1$ is compact. So, the global maximum of $|\mathcal{R}(\mathbf{x})|$ on W_1 is determined by the constrained critical values of $\mathcal{R}(\mathbf{x})$ given by Corollary 3.1 and Lemma 3.4. Hence by Lemma 3.6:

$$\sup_{\mathbf{x} \in W_1} |\mathcal{R}(\mathbf{x})| = \max_{1 \le m \le q} \{|L_m(x_1^m)|\} = |L_1(x_1^1)|.$$

Then since some calculations show that $\mathbf{y}^{*-1} \in W_1$, $|G'(1)| \le |L_1(x_1^1)| = \sqrt{2} - 1$. ∎

Now set:

$$R(z) \equiv \frac{\displaystyle\sum_{l=0}^{q} (-z)^l \sum_{m=0}^{l} \frac{(-1)^m}{(l-m)!} S_m(\mathbf{y}^*)}{\displaystyle\sum_{l=0}^{q} S_l(\mathbf{y}^*) z^l}$$

taking $Q(z)$ as the denominator.

Theorem 4.1 *Any IRKM for which (1.3) is equal to $R(z)$ above, must be A_0-stable.*

Proof. First, note the error formula of [13]:

$$R(z) = e^{-z} \left[1 - \frac{(-z)^{q+1}}{Q(z)} \int_0^1 e^{zt} N_1'(t; \mathbf{y}^*) dt \right].$$

With $x \ge 0$, integration by parts gives:

$$
\begin{aligned}
e^x R(x) &= 1 + \frac{(-x)^q}{Q(x)} \left[e^x N_1'(1; \mathbf{y}^*) - N_1'(0; \mathbf{y}^*) - \int_0^1 e^{xt} N_1''(t; \mathbf{y}^*) dt \right] \\
&= 1 + \frac{x^q S_q(\mathbf{y}^*)}{Q(x)} \left[(e^x - 1) + \int_0^1 (e^x - e^{xt}) G''(t) dt \right]
\end{aligned}
$$

or:

$$R(x) = e^{-x}(1 - \theta) + \theta(1 + J)$$

where:

$$\theta \equiv \frac{x^q S_q(\mathbf{y}^*)}{\displaystyle\sum_{l=0}^{q} S_l(\mathbf{y}^*) x^l} \in [0, 1), \quad \text{and} \quad J \equiv \int_0^1 (1 - e^{-x(1-t)}) G''(t) dt.$$

As indicated above, $G''(t) < 0$ and $|G'(1)| < 1$, so:

$$-J = |J| \le -\int_0^1 G''(t) dt = 1 - G'(1) < 2.$$

Hence:

$$|R(x)| = R(x) = e^{-x}(1 - \theta) + \theta(1 + J) \le 1 \qquad \forall x \ge 0.$$

∎

Now the next three theorems show that $R(z)$ can be used to construct a q-stage, real MIRK which is A_0-stable with order $q + 1$. The first is due to Bales, Karakashian, and Serbin [2].

Theorem 4.2 *If the coordinates of* $\mathbf{y}^* \in \mathbf{R}^q$ *are distinct and nonzero, then* $N_0(t; \mathbf{y}^*)$ *has* q *distinct real roots* $\{\tau_i\}_{i=1}^q$. ∎

Theorem 4.3 *Given distinct real roots* $\{\tau_i\}_{i=1}^q$ *of* $N_0(t; \mathbf{y}^*)$, *the following are well-defined:*

$$A \equiv TVRV^{-1} \quad and \quad b \equiv (V^T)^{-1}Re.$$

and the resulting IRKM has order at least q. *Furthermore, if* $N_1(1, \mathbf{y}^*) = 0$, *then the order is* $q + 1$.

Proof. With the conditions of Butcher:

$$B(\xi): \quad lb^T T^{l-1}e = 1 \quad 1 \le l \le \xi,$$

$$C(\xi): \quad lAT^{l-1}e = T^l e \quad 1 \le l \le \xi,$$

conditions $B(\nu)$ and $C(\mu)$ imply order ν if $\nu \le \mu + 1$. [5] Now the first statement follows since the assumptions amount to conditions $C(q)$ and $B(q)$. Then if $N_1(1, \mathbf{y}^*) = 0$, by $B(q)$:

$$\frac{1}{q+1} = \int_0^1 t^q = q! \int_0^1 [N_0(t; \mathbf{y}^*) - \sum_{l=0}^{q-1} (-1)^{q-l} S_{q-l}(\mathbf{y}^*) \frac{t^l}{l!}]$$

$$= q! N_1(1, \mathbf{y}^*) - q! \sum_{l=0}^{q-1} \frac{(-1)^l}{l!} S_{q-l}(\mathbf{y}^*) \sum_{i=1}^q b_i \tau_i^l$$

$$= \sum_{i=1}^q b_i [\tau_i^q - q! N_0(\tau_i, \mathbf{y}^*)] = b^T T^q e$$

and the second statement follows with $B(q+1)$ and $C(q)$. ∎

Finally, the next theorem follows from Theorems 2 and 4 of [13].

Theorem 4.4 *Given an IRKM constructed as described in Theorem 4.3, the rational function (1.3) must have the form (3.5) with* $\mathbf{x}^{-1} = \mathbf{y}^*$. ∎

5   A Family of High Order I-Stable Real MIRK's.

In this section, a family of IRKM's is constructed which contains for every even q, a q-stage, real MIRK which is I-stable with order q. As briefly indicated below, such methods are useful for hyperbolic problems.

Suppose that an approximation is required for the solution $u : [0, t^*] \to S_h$, to the initial value problem:

$$\begin{cases} D_t^2 u &= -L_h(t)u + f(t, u) \quad\quad 0 \le t \le t^* \\ u(0) &= u^0 \\ D_t u(0) &= u^1 \end{cases}$$

13

where $L_h(t)$ and $f(t, u)$ are assumed to have the same properties as mentioned in section 2. Note that this problem can be expressed in first order form as follows:

$$\begin{cases} D_t \begin{pmatrix} u \\ D_t u \end{pmatrix} = -\begin{pmatrix} 0 & -I \\ L_h(t) & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ f(t, u) \end{pmatrix} & 0 \leq t \leq t^* \\ \begin{pmatrix} u(0) \\ D_t u(0) \end{pmatrix} = \begin{pmatrix} u^0 \\ u^1 \end{pmatrix}. \end{cases}$$

As opposed to the parabolic case, with:

$$\mathbf{L}_h^n \equiv \begin{pmatrix} 0 & -I \\ L_h^n & 0 \end{pmatrix}$$

the pivotal stability inequality here is:

$$|||r(k\mathbf{L}_h^n)||| \leq 1$$

where $||| \cdot |||$ is an appropriate norm. Since $\mathbf{L}_h^n$ has only imaginary eigenvalues, a certain spectral argument shows that I-stability is crucial. [11]

Now in the sequel, q is implicitly assumed to be even. Toward the goal of this section, recall the functions $\{N_m(t; \mathbf{y})\}_{m \geq 0}$ defined in (3.11). Then let $\hat{e} \equiv \langle e_1, e_2, \ldots, e_q \rangle^T$ be a unit vector chosen so that:

$$e_i = -e_{i+\frac{q}{2}} > 0 \quad \text{and} \quad e_i \neq e_j \qquad 1 \leq i \neq j \leq \tfrac{q}{2}.$$

According to [13], there are q real solutions to:

$$N_0(1, y\hat{e}) = 0$$

and exactly $\frac{q}{2}$ of them are positive. So if y_0 is the largest, choose $y^* \geq y_0$ and set $\mathbf{y}^* \equiv y^*\hat{e}$. Then it follows that:

$$G(t) \equiv \frac{N_0(t, \mathbf{y}^*)}{N_0(0, \mathbf{y}^*)} = \frac{t^q N_0(1, t^{-1}\mathbf{y}^*)}{(-1)^{\frac{q}{2}} |S_q(\mathbf{y}^*)|}$$

decreases in a strictly monotonic fashion from 1 to $G(1) \geq 0$ as t passes from 0 to 1. Now set:

$$Q(z) \equiv \prod_{m=1}^{\frac{q}{2}} [1 - (y_m^* z)^2] = \sum_{l=0}^{q} S_l(\mathbf{y}^*) z^l, \qquad P(z) \equiv \sum_{l=0}^{q} (-z)^l \sum_{m=0}^{l} \frac{(-1)^m}{(l-m)!} S_m(\mathbf{y}^*)$$

and take $R(z) \equiv P(z)/Q(z)$.

Theorem 5.1 *Any IRKM for which (1.3) is equal to $R(z)$ above, must be I-stable.*

Proof: First, recall the error formula of [13]:

$$R(z) = e^{-z} \left[1 - \frac{(-z)^{q+1}}{Q(z)} \int_0^1 e^{zt} N(t; \mathbf{y}^*) dt \right].$$

So with $z = iy$:

$$|R(iy)| = \left| 1 - iy \left[\prod_{m=1}^{\frac{q}{2}} \frac{(yy_m^*)^2}{[1 + (yy_m^*)^2]} \right] \int_0^1 e^{-iyt} G(t) dt \right|.$$

14

Integration by parts gives:

$$|R(iy)| = |(1 - \theta) + \theta(e^{-iy}G(1) - J)|$$

where:

$$\theta \equiv \prod_{m=1}^{\frac{q}{2}} \frac{(yy_m^*)^2}{[1 + (yy_m^*)^2]} \in [0, 1) \quad \text{and} \quad J \equiv \int_0^1 e^{-iyt}G'(t)dt.$$

By construction, $G'(t) < 0$, so:

$$|J| \leq -\int_0^1 G'(t)dt = 1 - G(1).$$

Further, since $G(1) \geq 0$:

$$|R(z)| \leq (1 - \theta) + \theta G(1) + \theta(1 - G(1)) \leq 1.$$

$\blacksquare$

Now, in view of Theorems 4.2 - 4.4, for every even integer q, the rational function $R(z)$ above can be used to construct a q-stage, real MIRK which is I-stable with order q.

6   Examples of Algebraically Stable MIRK's.

In this section, certain methods are presented which have the properties discussed in previous sections. In the discussion, use is made of Theorem 6.1 below, which is due to Hairer and Wanner [9]. For this, some relevant constructions are now provided. Given $B > 0$, let C be determined by the Cholesky decomposition:

$$V^T BV \equiv C^T C.$$

Then take:

$$W \equiv VC^{-1}$$

so that:

$$W^T BW = I.$$

Finally with:

$$\delta_{i \leq m} \equiv \begin{cases} 1, & i \leq m \\ 0, & \text{otherwise} \end{cases}$$

let $I_m \equiv \{\delta_{ij}\delta_{i \leq m}\}_{i,j=1}^q$, $H \equiv \{(i + j - 1)^{-1}\}_{i,j=1}^q$, and:

$$X_G \equiv \underset{q \times q}{\text{diag}}\{\tfrac{1}{2}, 0, 0, \ldots, 0\} + \underset{1 \leq i \leq q-1}{\text{subdiag}}\{\xi_i\} - \underset{1 \leq i \leq q-1}{\text{supdiag}}\{\xi_i\}, \qquad \xi_i \equiv \frac{1}{2\sqrt{4i^2 - 1}}.$$

Now the following can be stated.

Theorem 6.1 *Let an IRKM be given for which $B > 0$ and:*

$$I_i V^T BV I_j = I_i H I_j \qquad i + j - 1 = \nu.$$

15

Let $m \equiv \left[\!\left[\frac{1}{2}(\nu - 1)\right]\!\right]$ and suppose X is a $q \times q$ matrix satisfying:

$$XI_m = X_G I_m, \qquad I_m X = I_m X_G$$

and if ν is even:

$$\hat{e}_{m+1}^T X \hat{e}_{m+1} = 0.$$

Then if $A = WXW^{-1}$ the IRKM has order ν. ∎

First, the following family of two-stage methods has been described by Karakashian [10]:

$$
\begin{array}{cc|c}
\dfrac{\tau_1(\tau_2 - \frac{1}{2}\tau_1)}{\tau_2 - \tau_1} & \dfrac{-\frac{1}{2}\tau_1^2}{\tau_2 - \tau_1} & \tau_1 \\[2ex]
\dfrac{\frac{1}{2}\tau_2^2}{\tau_2 - \tau_1} & \dfrac{\tau_2(\frac{1}{2}\tau_2 - \tau_1)}{\tau_2 - \tau_1} & \tau_2 \\[2ex]
\hline
\dfrac{\tau_2 - \frac{1}{2}}{\tau_2 - \tau_1} & \dfrac{\frac{1}{2} - \tau_1}{\tau_2 - \tau_1} &
\end{array}
$$

$$\tau_1 \equiv (\lambda_1 + \lambda_2) - (\lambda_1^2 + \lambda_2^2)^{\frac{1}{2}}$$

$$\tau_2 \equiv (\lambda_1 + \lambda_2) + (\lambda_1^2 + \lambda_2^2)^{\frac{1}{2}}$$

$$\lambda_1 > \frac{1}{2}, \qquad \lambda_2 = \frac{\frac{1}{2}\lambda_1 - \frac{1}{6}}{\lambda_1 - \frac{1}{2}}.$$

The W-transformation leads to:

$$
W = \begin{bmatrix} 1 & 2\sqrt{3}(\tau_1 - \frac{1}{2}) \\ 1 & 2\sqrt{3}(\tau_2 - \frac{1}{2}) \end{bmatrix}
\quad \text{and} \quad
X = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} \\ \frac{1}{2\sqrt{3}} & x \end{bmatrix}
$$

where:

$$x \equiv \lambda_1 + \lambda_2 - \frac{1}{2} > 0.$$

Since $B > 0$ and $V^T B V = H$, by Theorem 6.1, these methods have maximal order $\nu = 3$. In fact, $p = 3$ as well. With regard to stability, since $W^T B W = I$, the algebraic stability matrix M satisfies:

$$
\begin{aligned}
W^T M W &= W^T B W W^{-1} A W + (W^{-1} A W)^T W^T B W + W^T B W [W^{-1} e (W^{-1} e)^T] W^T B W \\[1ex]
&= X + X^T - \hat{e}_1 \hat{e}_1^T = \operatorname{diag}\{0, 2x\}.
\end{aligned}
$$

Hence, these methods are algebraically stable. Also in connection with section 2, note that A has real, distinct eigenvalues:

$$A = S^{-1} \Lambda S, \qquad \Lambda = \operatorname*{diag}_{1 \leq i \leq 2}\{\lambda_i\}, \qquad S^{-1} = \begin{bmatrix} \tau_1 - \lambda_2 & \tau_1 - \lambda_1 \\ \tau_2 - \lambda_2 & \tau_2 - \lambda_1 \end{bmatrix}.$$

Next, the following family of three-stage methods has been described in [12]. First, choose λ_1, λ_2, and λ_3 distinctly and to satisfy:

$$\lambda_1, \lambda_2, \lambda_3 > 0 \qquad \lambda_1 + \lambda_2 + \lambda_3 - \frac{1}{2} > 0 \quad \text{and} \quad \lambda_3 = \frac{\frac{1}{2}\lambda_1 \lambda_2 - \frac{1}{6}(\lambda_1 + \lambda_2) + \frac{1}{24}}{\lambda_1 \lambda_2 - \frac{1}{2}(\lambda_1 + \lambda_2) + \frac{1}{6}}.$$

For example, it is sufficient to choose λ_3 as indicated after taking:

$$\lambda_1 > \tfrac{1}{2} \quad \text{and} \quad \lambda_2 > \frac{\tfrac{1}{2}\lambda_1 - \tfrac{1}{6}}{\lambda_1 - \tfrac{1}{2}}.$$

Now define:

$$x_1 \equiv \lambda_1 + \lambda_2 + \lambda_3 - \tfrac{1}{2}, \qquad x_2 \equiv [(\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3) - \tfrac{1}{2}(\lambda_1 + \lambda_2 + \lambda_3) + \tfrac{1}{6}]^{\frac{1}{2}},$$

and:

$$\alpha_i \equiv \lambda_i - x_1, \quad \beta_i \equiv \tfrac{1}{2} - \lambda_i \qquad 1 \le i \le 3.$$

Also take $\Lambda = \operatorname*{diag}_{1 \le i \le 3}\{\lambda_i\}$,

$$X \equiv \begin{bmatrix} \tfrac{1}{2} & -\tfrac{1}{2\sqrt{3}} & 0 \\[2mm] \tfrac{1}{2\sqrt{3}} & 0 & -x_2 \\[2mm] 0 & x_2 & x_1 \end{bmatrix}, \quad \text{and} \quad Y \equiv \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\[2mm] 2\sqrt{3}\alpha_1\beta_1 & 2\sqrt{3}\alpha_2\beta_2 & 2\sqrt{3}\alpha_3\beta_3 \\[2mm] 2\sqrt{3}x_2\beta_1 & 2\sqrt{3}x_2\beta_2 & 2\sqrt{3}x_2\beta_3 \end{bmatrix}.$$

Then $X = Y\Lambda Y^{-1}$. Now choose τ_1, τ_2, and τ_3 to satisfy:

$$\frac{(\tau_1^2 - \tau_1 + \tfrac{1}{6})(\tau_2^2 - \tau_2 + \tfrac{1}{6})}{\tau_1\tau_2 - \tfrac{1}{2}(\tau_1 + \tau_2) + \tfrac{1}{3}} < 0 \quad \text{and} \quad \tau_3 = \frac{\tfrac{1}{2}\tau_1\tau_2 - \tfrac{1}{3}(\tau_1 + \tau_2) + \tfrac{1}{4}}{\tau_1\tau_2 - \tfrac{1}{2}(\tau_1 + \tau_2) + \tfrac{1}{3}}.$$

For example, it is sufficient to choose τ_3 as indicated after taking:

$$\tau_1 < \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right) \quad \text{and} \quad \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) < \tau_2.$$

Then it can be shown that:

$$\sigma \equiv \tfrac{1}{2}\tau_1\tau_2\tau_3 - \tfrac{1}{3}(\tau_1\tau_2 + \tau_1\tau_3 + \tau_2\tau_3) + \tfrac{1}{4}(\tau_1 + \tau_2 + \tau_3) > \frac{7}{36}$$

so take $r \equiv \left(\sigma - \tfrac{7}{36}\right)^{\frac{1}{2}}$ and define W by:

$$W \equiv \begin{bmatrix} 1 & 2\sqrt{3}(\tau_1 - \tfrac{1}{2}) & (\tau_1^2 - \tau_1 + \tfrac{1}{6})/r \\[2mm] 1 & 2\sqrt{3}(\tau_2 - \tfrac{1}{2}) & (\tau_2^2 - \tau_2 + \tfrac{1}{6})/r \\[2mm] 1 & 2\sqrt{3}(\tau_3 - \tfrac{1}{2}) & (\tau_3^2 - \tau_3 + \tfrac{1}{6})/r \end{bmatrix}.$$

Next, since it can be shown that $\tau_i \ne \tau_j$, $i \ne j$, choose the vector b according to:

$$b = (V^T)^{-1}Re.$$

Finally take:

$$A \equiv WXW^{-1} = S^{-1}\Lambda S, \qquad S \equiv Y^{-1}W^{-1}$$

17

and note that A has real, distinct eigenvalues. Concerning stability, note that $B > 0$ since $V^T B V = H + \text{diag}\{0, 0, \sigma - \frac{1}{5}\}$. Also since $W^T B W = I$, the algebraic stability matrix M satisfies:

$$W^T M W = W^T B W W^{-1} A W + (W^{-1} A W)^T W^T B W + W^T B W [W^{-1} e (W^{-1} e)^T] W^T B W$$

$$= X + X^T - \hat{e}_1 \hat{e}_1^T = \text{diag}\{0, 0, 2x_1\}.$$

Hence these methods are algebraically stable. Now since $B > 0$ and $V^T B V$ is as indicated above, it follows from Theorem 6.1 that these methods have maximal order $\nu = 4$. However, $p = 2$. Nevertheless, it is now shown that for each method in the family, there exists a matrix D as defined in section 2:

$$D[e; Ae; A^2 e] = [Ae; 2A^2 e; 3A^3 e]$$

which actually eliminates order reduction since $\nu = 4 = q + 1$. For this, suppose that there are constants $\{c_i\}_{i=1}^3$ such that:

$$c_1 e + c_2 A e + c_3 A^2 e = 0.$$

Since a fourth order method satisfies:

$$l! b^T A^{l-1} e = 1 \qquad 1 \le l \le 4$$

it follows that:

$$c_1 + \tfrac{1}{2} c_2 + \tfrac{1}{6} c_3 = 0$$
$$\tfrac{1}{2} c_1 + \tfrac{1}{6} c_2 + \tfrac{1}{24} c_3 = 0.$$

Therefore $12 c_1 = -2 c_2 = c_3$, and if these constants are nontrivial:

$$[I - 6\Lambda + 12\Lambda^2] S e = 0.$$

However, since $1 - 6t + 12t^2 > 0$, $\forall t \in \mathbf{R}$, it is necessarily the case that $c_1 = c_2 = c_3 = 0$. Thus the matrix $[e; Ae; A^2 e]$ is invertible.

It is also possible to construct similar methods which have five stages and order six, but the details are not provided here. Instead, some useful calculations for some well-known complex MIRK's are given. Recall from section 2 that at least for semilinear problems, order reduction can be eliminated; so for such problems, there is good reason to consider methods of the following form. First, the Gauss-Legendre methods are algebraically stable with $\nu = 2q$. From this family, the three-stage method follows.

$\dfrac{5}{36}$	$\dfrac{80 - 24\sqrt{15}}{360}$	$\dfrac{50 - 12\sqrt{15}}{360}$	$\dfrac{5 - \sqrt{15}}{10}$
$\dfrac{50 + 15\sqrt{15}}{360}$	$\dfrac{2}{9}$	$\dfrac{50 - 15\sqrt{15}}{360}$	$\dfrac{1}{2}$
$\dfrac{50 + 12\sqrt{15}}{360}$	$\dfrac{80 + 24\sqrt{15}}{360}$	$\dfrac{5}{36}$	$\dfrac{5 + \sqrt{15}}{10}$
$\dfrac{5}{18}$	$\dfrac{4}{9}$	$\dfrac{5}{18}$	

Also, the W-transformation leads to:

$$W = \begin{bmatrix} 1 & -\frac{3}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ 1 & 0 & -\frac{\sqrt{5}}{2} \\ 1 & \frac{3}{\sqrt{5}} & \frac{2}{\sqrt{5}} \end{bmatrix} \quad \text{and} \quad X = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} & 0 \\ \frac{1}{2\sqrt{3}} & 0 & -\frac{1}{2\sqrt{15}} \\ 0 & \frac{1}{2\sqrt{15}} & 0 \end{bmatrix}.$$

In connection with section 2, note that:

$$A = S^{-1}\Lambda S \qquad S \equiv Y^{-1}W^{-1}$$

where $X = Y\Lambda Y^{-1}$,

$$\Lambda = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \alpha & -\beta \\ 0 & \beta & \alpha \end{bmatrix}, \qquad Y = \begin{bmatrix} 2\sqrt{15}\lambda & -12\alpha\beta & 12\alpha^2 - 6\alpha + \frac{1}{2} \\ 12\sqrt{5}\lambda(\frac{1}{2}-\lambda) & -\sqrt{3}\beta & -\sqrt{3}\alpha \\ 2\sqrt{3}(\frac{1}{2}-\lambda) & 0 & -\frac{1}{2\sqrt{5}} \end{bmatrix}$$

and the above constants are given by:

$$\lambda \equiv \frac{20^{\frac{1}{3}}}{60}[(5+3\sqrt{5})^{\frac{1}{3}} + (5-3\sqrt{5})^{\frac{1}{3}}] + \frac{1}{6},$$

$$\alpha \equiv \frac{1}{6} - \frac{20^{\frac{1}{3}}}{120}[(5+3\sqrt{5})^{\frac{1}{3}} + (5-3\sqrt{5})^{\frac{1}{3}}], \quad \text{and} \quad \beta \equiv \sqrt{3}\frac{20^{\frac{1}{3}}}{120}[(5+3\sqrt{5})^{\frac{1}{3}} - (5-3\sqrt{5})^{\frac{1}{3}}].$$

Now the Gauss-Legendre methods fail to satisfy $|r(\infty)| < 1$, and the latter condition is required in the analysis of [12] for certain nonlinear problems. On the other hand for example, the Radau IIA methods satisfy this constraint. Also, they are algebraically stable with $\nu = 2q - 1$. From this family, the three-stage method follows.

$\dfrac{88 - 7\sqrt{6}}{360}$	$\dfrac{296 - 169\sqrt{6}}{1800}$	$\dfrac{-2 + 3\sqrt{6}}{225}$	$\dfrac{4 - \sqrt{6}}{10}$
$\dfrac{296 + 169\sqrt{6}}{1800}$	$\dfrac{88 + 7\sqrt{6}}{360}$	$\dfrac{-2 - 3\sqrt{6}}{225}$	$\dfrac{4 + \sqrt{6}}{10}$
$\dfrac{16 - \sqrt{6}}{36}$	$\dfrac{16 + \sqrt{6}}{36}$	$\dfrac{1}{9}$	1
$\dfrac{16 - \sqrt{6}}{36}$	$\dfrac{16 + \sqrt{6}}{36}$	$\dfrac{1}{9}$	

Also, the W-transformation leads to:

$$W = \begin{bmatrix} 1 & \frac{-\sqrt{3}-3\sqrt{2}}{5} & \frac{-2\sqrt{5}+3\sqrt{30}}{25} \\ 1 & \frac{-\sqrt{3}+3\sqrt{2}}{5} & \frac{-2\sqrt{5}-3\sqrt{30}}{25} \\ 1 & \sqrt{3} & \sqrt{5} \end{bmatrix} \quad \text{and} \quad X = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2\sqrt{3}} & 0 \\ \frac{1}{2\sqrt{3}} & 0 & -\frac{1}{2\sqrt{15}} \\ 0 & \frac{1}{2\sqrt{15}} & \frac{1}{10} \end{bmatrix}.$$

In connection with section 2, note that:

$$A = S^{-1}\Lambda S \qquad S \equiv Y^{-1}W^{-1}$$

where $X = Y\Lambda Y^{-1}$,

$$\Lambda = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \alpha & -\beta \\ 0 & \beta & \alpha \end{bmatrix}, \quad Y = \begin{bmatrix} 2\sqrt{15}(\lambda - \frac{1}{10}) & 0 & -\sqrt{5} \\ 12\sqrt{5}(\lambda - \frac{1}{10})(\frac{1}{2} - \lambda) & 2\beta\sqrt{15} & (2\alpha - 1)\sqrt{15} \\ 2\sqrt{3}(\frac{1}{2} - \lambda) & 120\beta(\frac{1}{4} - \alpha) & 1 + 120(\alpha - \frac{1}{4})(\alpha - \frac{1}{10}) \end{bmatrix}$$

and the above constants are given by:

$$\lambda \equiv \frac{1}{10}(3^{\frac{1}{3}} - 3^{-\frac{1}{3}}) + \frac{1}{5}, \qquad \alpha \equiv \frac{1}{5} - \frac{1}{20}(3^{\frac{1}{3}} - 3^{-\frac{1}{3}}), \quad \text{and} \quad \beta \equiv \frac{1}{20}(3^{\frac{5}{6}} + 3^{\frac{1}{6}}).$$

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Final Report

16. Abstract

Implicit Runge-Kutta methods which are well-suited for parallel computations are characterized. It is claimed that such methods are first of all, those for which the associated rational approximation to the exponential has distinct poles, and these are called multiply implicit (MIRK) methods. Also, because of the so-called order reduction phenomenon, there is reason to require that these poles be real. Then, it is proved that a necessary condition for a q-stage, real MIRK to be A-stable with maximal order $q + 1$ is that $q = 1, 2, 3,$ or 5. Nevertheless, it is shown that for every positive integer q, there exists a q-stage, real MIRK which is A_0-stable with order $q + 1$, and for every even q, there is a q-stage, real MIRK which is I-stable with order q. Finally some useful examples of algebraically stable MIRK's are given.

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