RUNGE-KUTTA METHODS ARE STABLE

EITAN TADMOR

Abstract. We prove that Runge-Kutta (RK) methods for numerical integration of arbitrarily large systems of Ordinary Differential Equations are linearly stable. Standard stability arguments — based on spectral analysis, resolvent condition or strong stability, fail to secure the stability of arbitrarily large RK systems. We explain the failure of different approaches, offer a new stability theory and demonstrate a few examples.

Contents

1. Introduction — the quest for stability

Runge-Kutta (RK) methods are the methods of choice for numerical integration of systems of Ordinary Differential Equations (ODEs). In particular, such methods are used routinely for integration of large systems of ODEs encountered in various applications, for example — in molecular dynamics in Chemistry, in many particle systems in Physics, in phase field dynamics in Materials Science, and in spatial discretization of time-dependent PDEs of increasingly large size, so-called "method of lines". The stability of RK methods encoded in terms of their *region of absolute stability* is well documented, [HNW1993, Ise1996, But2008]. We therefore devote this Introduction to clarify the claim alluded to in the title.

We consider systems of ODEs,

$$\dot{\mathbf{y}} = \mathbf{F}(t, \mathbf{y}),$$

which govern an N-vector of unknown solution, $\mathbf{y}(t) \in \mathbb{R}^N$, subject to prescribed initial data, $\mathbf{y}(t_0) = \mathbf{y}_0$. As a canonical example for one of the most widely used numerical integrators we mention the 4-stage RK method, which computes an approximate solution, $\{\mathbf{u}_n = \mathbf{u}(t_n)\}_{n>0}$,

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at successive time steps $t_{n+1} := t_n + \Delta t$, [HNW1993, §II.1],

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{\Delta t}{6}\big(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4\big), \qquad \left\{\begin{array}{l} \mathbf{k}_1 = \mathbf{F}(t_n, \mathbf{u}_n) \\ \mathbf{k}_2 = \mathbf{F}\big(t_{n+1/2}, \mathbf{u}_n + (\Delta t/2)\mathbf{k}_1\big) \\ \mathbf{k}_3 = \mathbf{F}\big(t_{n+1/2}, \mathbf{u}_n + (\Delta t/2)\mathbf{k}_2\big) \\ \mathbf{k}_4 = \mathbf{F}\big(t_{n+1}, \mathbf{u}_n + \Delta t\mathbf{k}_3\big). \end{array}\right. \tag{1.1}$$

The *linearized stability analysis* examines the behavior of (1.1) for linear systems, $\mathbf{F}(t,\mathbf{y}) = \mathbb{L}_{N}\mathbf{y}$,

$$\dot{\mathbf{y}} = \mathbb{L}_{N}\mathbf{y}, \tag{1.2}$$

where (1.1) is reduced to

$$\mathbf{u}_{n+1} = \left(\mathbb{I} + \Delta t\mathbb{L}_{N} + \frac{1}{2}(\Delta t\mathbb{L}_{N})^2 + \frac{1}{6}(\Delta t\mathbb{L}_{N})^3 + \frac{1}{24}(\Delta t\mathbb{L}_{N})^4\right)\mathbf{u}_n, \quad n = 0, 1, \ldots. \tag{RK4}$$

The corresponding iterations for a general s-stage *explicit* RK method take the form

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t\mathbb{L}_{N})\mathbf{u}_n, \quad n = 0, 1, 2, \ldots, \qquad \mathcal{P}_s(z) := \sum_{k=0}^{s} a_k z^k, \ \ a_k \in \mathbb{R}, \ a_s \neq 0. \tag{1.3}$$

Different $\{a_k\}_{k=0}^{s}$ dictate different RK methods with emphasize on different aspects of accuracy, efficiency and stability. The resulting s-stage RK methods, (1.3), involve $N \times N$ matrices, denoted $\mathbb{L}_{N}$ to highlight the fact that they are parameterized with respect to N. As already noted above, such large matrices are often encountered in applications, notably in contemporary problems which involve high-dimensional data sets/neural networks, e.g., [HR2017, E2017, CRBD2018, Mis2018]. We therefore pay particular attention to the question of RK stability that is uniform with respect to the increasingly large dimension N.

Following [Tad2002, §2], we consider (1.2) for the class of *semi-bounded* $\mathbb{L}_{N}$'s, namely — $\mathbb{L}_{N}$'s for which there exist constants $\eta, K_{\mathbb{H}} > 0$ independent of N, and *uniformly* positive-definite symmetrizers, $\mathbb{H}_{N}$'s, such that[1],

$$\mathbb{H}_{N}\mathbb{L}_{N}^{\top} + \mathbb{L}_{N}\mathbb{H}_{N} \leqslant 2\eta\mathbb{H}_{N}, \qquad 0 < K_{\mathbb{H}}^{-1} \leqslant \mathbb{H}_{N} \leqslant K_{\mathbb{H}}.$$

It follows that the solutions of the corresponding semi-bounded ODEs (1.2) subject to arbitrary initial data $\mathbf{y}(0) = \mathbf{y}_0$, satisfy

$$|\mathbf{y}(t)|_{\ell^2} \leqslant K_{\mathbb{H}} e^{\eta t}|\mathbf{y}_0|_{\ell^2}.$$

Replacing $\mathbb{L}_{N}$ with $\mathbb{L}_{N} - \eta\mathbb{I}$, allows us to consider without loss of generality the case $\eta = 0$, corresponding to *negative definite* $\mathbb{L}_{N}$'s,

$$\mathbb{H}_{N}\mathbb{L}_{N}^{\top} + \mathbb{L}_{N}\mathbb{H}_{N} \leqslant 0, \qquad 0 < K_{\mathbb{H}}^{-1} \leqslant \mathbb{H}_{N} \leqslant K_{\mathbb{H}}. \tag{1.4}$$

Solutions of ODE governed by such negative[2] $\mathbb{L}_{N}$'s satisfy subject to arbitrary initial data $\mathbf{y}_0$,

$$|\mathbf{y}(t)|_{\ell^2} \leqslant K_{\mathbb{H}}|\mathbf{y}_0|_{\ell^2}. \tag{1.5}$$

Stability of RK scheme. The notion of stability of RK schemes requires the numerical solution to satisfy the bound corresponding to (1.5). To this end, one is focused on a family of negative $\mathbb{L}_{N}$'s parametrized by their dimension N. The s-stage RK scheme (1.3) is *stable*,

[1] Throughout the paper, we use $K_{\square}$ to denote different constants which are independent of N.

[2] Throughout the work, we use the term 'negative' for short of 'negative definite'.

if there exist constants, $K_{\mathbb{L}} > 0$ and $\mathcal{C}_s > 0$ independent of N, such that solutions of (1.3) subject to arbitrary initial data $\mathbf{u}_0$ satisfy, for small enough time step Δt,

$$\text{Stability of RK scheme}: \qquad |\mathbf{u}_n|_{\ell^2} \leqslant K_{\mathbb{L}} |\mathbf{u}_0|_{\ell^2}, \qquad n = 0, 1, 2, \ldots. \tag{1.6}$$

The restriction of having small enough time step is encoded in terms of the bound

$$\Delta t \cdot \|\mathbb{L}_{N}\| \leqslant \mathcal{C}_s; \tag{1.7}$$

in the context of method of lines, the time-step restriction is related to the celebrated Courant-Friedrichs-Levy (CFL) condition, [CFL1928], and we shall therefore often refer to the time-step restriction (1.7) as a CFL condition.
The notion of stability encoded in (1.6) amounts to the question of power-boundedness of $\mathcal{P}_s(\Delta t \mathbb{L}_{N})$,

$$\|\mathcal{P}_s^n(\Delta t \mathbb{L}_{N})\| \leqslant K_{\mathbb{L}}, \qquad n = 0, 1, 2, \ldots. \tag{1.8}$$

Remark 1.1 (**Stability and linearization**). *The general notion of stability for semi-bounded $\mathbb{L}_{N}$'s, limits the exponential stability bound to a finite time interval,*

$$|\mathbf{u}_n|_{\ell^2} \leqslant K_{\mathbb{L}} e^{\eta t} |\mathbf{u}_0|_{\ell^2}, \qquad n \cdot \Delta t \leqslant t.$$

Since we restrict attention to negative $\mathbb{L}_{N}$'s, we may as well let $n \in \mathbb{N}$. This notion of stability is invariant against low-order perturbations, [Kre1962],[Str1964]*, and therefore allows to recover the stability of RK schemes for smooth solutions of fully nonlinear problems, $\dot{\mathbf{y}} = \mathbf{F}(t, \mathbf{y})$. To this end, one can linearize and freeze coefficients at arbitrary $t = t_*$, arriving at the linearized system* (1.2)*,*

$$\dot{\mathbf{y}} = \mathbb{L}_{N} \mathbf{y} \quad \text{with} \quad \mathbb{L}_{N} = \frac{\partial \mathbf{F}\big(t_*, \mathbf{y}(t_*)\big)}{\partial \mathbf{y}}.$$

We shall not dwell on the details, expect for referring to our discussion on stability in presence of variable coefficients in section 5.2 below. This motivates our focus on the question of linearized stability, where $\mathbb{L}_{N}$ is a substitute for the $N \times N$ gradient matrix freezed at arbitrary state.

1.1. **Spectral stability analysis.** The standard approach to address the question of power-boundedness is *spectral analysis*, in which (1.8) requires $\max\limits_{1 \leqslant k \leqslant N} |\lambda_k\big(\mathcal{P}_s(\Delta t \mathbb{L}_{N})\big)| \leqslant 1$. By the spectral mapping theorem,

$$\lambda_k\big(\mathcal{P}_s(\Delta t \mathbb{L}_{N}) = \mathcal{P}_s\big(\Delta t \lambda_k(\mathbb{L}_{N})\big), \tag{1.9}$$

which leads to the necessary stability condition, requiring small enough time-step dictated by the *region of absolute stability* associated with (1.3),

$$\Delta t \cdot \lambda_k(\mathbb{L}_{N}) \in \mathscr{A}_s, \quad k = 1, 2, \ldots, N, \qquad \mathscr{A}_s := \{z \in \mathbb{C} \ : \ |\mathcal{P}_s(z)| \leqslant 1\}. \tag{1.10}$$

Conversely, consider the favorite scenario in which $\mathbb{L}_{N}$ is diagonalizable,

$$\mathbb{T}_N \mathbb{L}_{N} \mathbb{T}_N^{-1} = \Lambda, \qquad \Lambda = \begin{bmatrix} \lambda_1(\mathbb{L}_{N}) & 0 & \ldots & \ldots & 0 \\ 0 & \lambda_2(\mathbb{L}_{N}) & \ddots & & \vdots \\ \vdots & \ddots & & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & \ldots & 0 & \lambda_N(\mathbb{L}_{N}) \end{bmatrix}.$$

Then $\mathcal{P}_s(\Delta t\mathbb{L}_N) = \mathbb{T}_N^{-1}\mathcal{P}_s(\Delta t\Lambda)\mathbb{T}_N$ and (1.10) implies

$$\|\mathcal{P}_s^n(\Delta t\mathbb{L}_N)\| = \|\mathbb{T}_N^{-1}\mathcal{P}_s^n(\Delta t\Lambda)\mathbb{T}_N\| \leqslant \|\mathbb{T}_N^{-1}\|\cdot\|\mathbb{T}_N\|. \tag{1.11}$$

This guarantees the stability of RK schemes for systems of finite *fixed* dimension[3]. However, here we insist that the stability sought in (1.6) will apply uniformly for increasingly large systems, and since the condition number on the right of (1.11), $\|\mathbb{T}_N^{-1}\|\cdot\|\mathbb{T}_N\|$, may grow with N, the spectral condition (1.10) is not enough to secure the desired uniform-in-N stability bound. Indeed, as we elaborate in section 2.1 below, the general question of stability, uniformly in N, cannot be addressed solely in terms of spectral analysis.

1.2. **Resolvent stability.** We now appeal to a stronger notion of stability of RK method. An s-stage RK method $\mathcal{P}_s(\cdot)$ is *stable* if the corresponding RK schemes (1.3) are stable for all negative $\mathbb{L}_N$'s,

$$\text{Stability of RK method}: \qquad \|\mathcal{P}_s^n(\Delta t\mathbb{L}_N)\| \leqslant K_{\mathbb{L}} \quad \text{for all negative } \mathbb{L}_N\text{'s}. \tag{1.12}$$

Observe that we are making a distinction between the stability of RK *scheme* — which examines the boundedness of RK protocol $\mathcal{P}_s^n(\Delta t\mathbb{L}_N)$ for a specific family of negative $\mathbb{L}_N$'s, vs. the stability of RK *method* — which examines the behavior of RK protocol $\mathcal{P}_s^n(\Delta t\ \cdot)$, for *all* negative $\mathbb{L}_N$'s.

This stronger notion of stability restricts the class of stable RK methods. In particular, their stability question should apply to the scalar ODEs, $\dot{y} = \lambda y$, for all negative $Re\,\lambda \leqslant 0$, which in turn implies that (1.10) must hold for purely imaginary $\lambda = i\sigma$, so that $|\mathcal{P}_s(i\Delta t\sigma)| \leqslant 1$, for small enough step-size, Δt. In other words, a stable RK method *must* satisfy the following interval condition.

Definition 1.2 (**Imaginary Interval condition**[4]). A Runge-Kutta method is said to satisfy the *imaginary interval condition* if there exists a constant $R_s > 0$ such that

$$|\mathcal{P}_s(i\sigma)| \leqslant 1, \qquad -R_s \leqslant \sigma \leqslant R_s. \tag{1.13}$$

In other words, the region of absolute stability of a stable RK method must contains a non-trivial interval along the imaginary axis $[-iR_s, iR_s] \subset \mathscr{A}_s$. This secures the stability of RK method for scalar hyperbolic ODEs, $\dot{y} = i\sigma y$, with small enough step-size $\Delta t\sigma < R_s$.

The interval condition excludes the standard 1-stage forward Euler method (for historical perspective of Euler's method which dates back to 1768 see [Wan2010, §1]),

$$\text{Forward Euler}: \qquad \mathbf{u}_{n+1} = (\mathbb{I} + \Delta t\mathbb{L}_N)\,\mathbf{u}_n, \tag{RK1}$$

for which $\mathcal{P}_1(z) = 1 + z \ \rightsquigarrow\ |\mathcal{P}_1(i\sigma)| > 1$ for all $\sigma \neq 0$. The imaginary interval condition (1.13) also excludes the 2-stage Heun's method [DB1974, §8.3.3] (also known as modified Euler method),

$$\text{Heun method}: \quad \mathbf{u}_{n+1} = \left(\mathbb{I} + \Delta t\mathbb{L}_N + \frac{1}{2}(\Delta t\mathbb{L}_N)^2\right)\mathbf{u}_n, \tag{RK2}$$

[3]The precise necessary and sufficient characterization for power-boundedness of a single matrix, $\|\mathcal{P}^n\| \leqslant K$, requires that the eigenvalues $\lambda_k(\mathcal{P})$ are inside the unit disc and those on the unit circle are simple; the constant K may still depend on the dimension of $\mathcal{P}$.

[4]So-called "local stability along the imaginary line" in [KS1992, Definition 2.1].

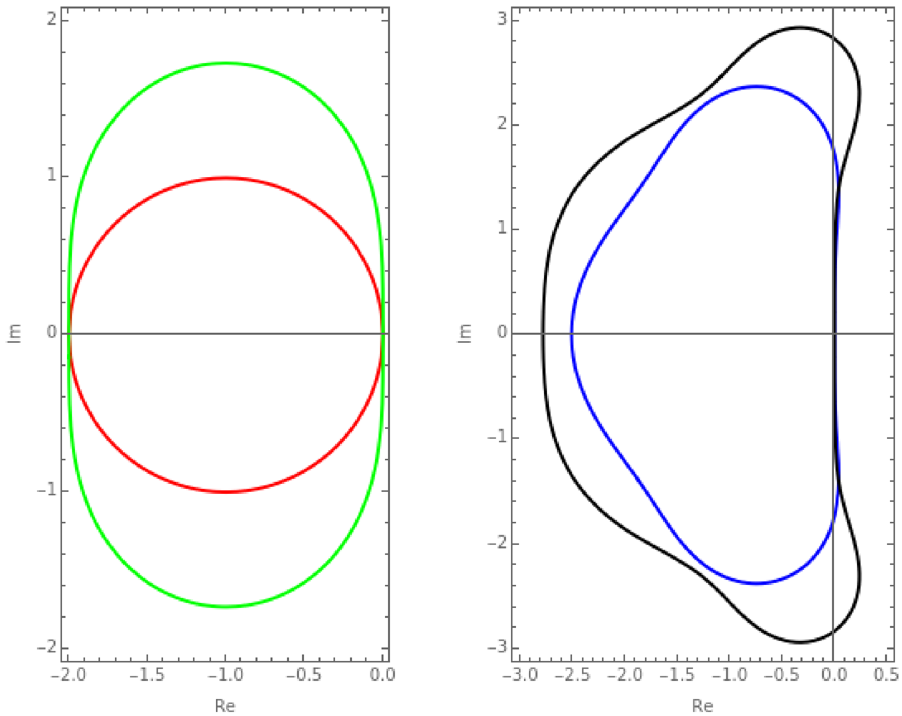

FIGURE 1.1. Regions of absolute stability, $\mathscr{A}_s$, $s = 1, 2$ (left) and $s = 3, 4$ (right)

since $\mathcal{P}_2(z) = 1 + z + \frac{1}{2}z^2 \rightsquigarrow |\mathcal{P}_2(i\sigma)| > 1$ for all $\sigma \neq 0$.
On the other hand, the 3-stage Kutta method,

$$\text{(RK3)} \qquad \text{Kutta method}: \quad \mathbf{u}_{n+1} = \left(\mathbb{I} + \Delta t\mathbb{L}_N + \frac{1}{2}(\Delta t\mathbb{L}_N)^2 + \frac{1}{6}(\Delta t\mathbb{L}_N)^3\right)\mathbf{u}_n,$$

as well as the 4-stage Runge-Kutta method, (RK4), and its higher-order embedded version RK45 of Dormand-Prince method [DP1980, KS1992, HNW1993], do satisfy the interval condition with $R_3 = \sqrt{3}$, and respectively, $R_4 = 2\sqrt{2}$; this is depicted in figure 1.1. A precise characterization of general s-stage RK methods satisfying the interval condition was given in [KS1992, Theorem 3.1] and will be recalled in (4.8b) below.
The interval condition 1.2 is necessary for stability of a RK method. Kreiss & Wu, [KW1993], proved the converse in the sense that the interval condition is sufficient for *resolvent stability*; namely — (1.13) implies that there exists constants $K_R > 0$ and $0 < \mathcal{C}_s < R_s$, independent of N, such that for small step-size,

$$\|\big(z\mathbb{I} - \mathcal{P}_s(\Delta t\mathbb{L}_N)\big)^{-1}\| \leqslant \frac{K_R}{|z| - 1}, \qquad \forall |z| > 1, \qquad \Delta t \cdot \|\mathbb{L}_N\| \leqslant \mathcal{C}_s. \tag{1.14}$$

Resolvent stability guarantees the stability of RK schemes for systems of finite *fixed* dimension, in view of the Kreiss matrix theorem, [Kre1962], [RM1967, §4.9]. Indeed, in [Tad1981] and its improvement [LT1984], it was proved that (1.14) implies

$$\|\mathcal{P}_s^n(\Delta t\mathbb{L}_N)\| \leqslant 2eK_RN, \qquad n = 1, 2, \ldots. \tag{1.15}$$

However, as we shall elaborate in section 2.2 below, the N-dependent bound on the right cannot be completely removed and hence resolvent stability does not secure the desired stability uniformly in growing N.

1.3. **Strong stability.** A Runge-Kutta scheme (1.3) is *strongly stable* if there exists $K_{\mathcal{T}} > 0$ independent of N such that $\mathcal{P}_s(\Delta t \mathbb{L}_N)$ is uniformly similar to a contraction,

$$\|\mathcal{T}_N \mathcal{P}_s(\Delta t \mathbb{L}_N)\mathcal{T}_N^{-1}\| \leqslant 1, \qquad \|\mathcal{T}_N^{-1}\| \cdot \|\mathcal{T}_N\| \leqslant K_{\mathcal{T}}. \tag{1.16}$$

A strongly stable RK scheme is clearly stable, for

$$\|\mathcal{P}_s^n(\Delta t \mathbb{L}_N)\| = \|\mathcal{T}_N^{-1}\big(\mathcal{T}_N \mathcal{P}_s(\Delta t \mathbb{L}_N)\mathcal{T}_N^{-1}\big)^n \mathcal{T}_N\| \leqslant \|\mathcal{T}_N^{-1}\| \cdot \|\mathcal{T}_N\| \leqslant K_{\mathcal{T}} \tag{1.17}$$

The choice $\mathcal{T}_N = \mathbb{T}_N$ recovers (1.11) as a special case of (1.17).
To secure strong stability it remains to construct a uniformly bounded symmetrizer $\mathcal{H}_N := \mathcal{T}_N^* \mathcal{T}_N$ with $0 < K_{\mathcal{T}}^{-1} \leqslant \mathcal{H}_N \leqslant K_{\mathcal{T}}$. We addressed this issue in [Tad2002], proving the strong stability of the 3-stage RK method (RK3) with symmetrizer $\mathcal{H}_N = \mathbb{H}_N$ and $\mathcal{C}_3 = 1$, thus providing the first example of a RK method which is stable uniformly for arbitrarily large system of ODEs. It was later extended to all s-stage RK methods of order $s = 3[\text{mod}4]$, [SS2019]. What about the other s-stage RK methods — does this argument of strong stability can be extended using proper symmetrizers, $\mathcal{H}_N$, for arbitrary s? In [Tad2002] we conjectured that the 4-stage (RK4) fails strong stability in the sense that it is not uniformly similar to a contraction, or equivalently — as outlined in section 2.3 below, that there exist no symmetrizer $\mathcal{H}_N := \mathcal{T}_N^* \mathcal{T}_N$ such that $(1.16)_{s=4}$ holds. This was confirmed in [SS2017, Proposition 1.1] and was later extended in [AAJ2023, Theorem 2], where it was shown that strong stability *fails* for all s-stage RK methods with $s \in 4\mathbb{N}$.

The stability question for RK schemes. We come out from the above discussion, lacking a definitive answer to the question of stability of RK schemes/methods for arbitrarily large systems of ODEs. Thus, for example, the stability question for the widely used RK4 remains open. At this stage, the three different approaches — spectral analysis, resolvent condition and strong stability failed to determine whether RK4 for example, is stable uniformly in N. We therefore raise the question:

Are the Runge-Kutta methods (1.3),(1.12) stable for arbitrarily large systems?

The title of the paper is an affirmative answer to this question. The answer is given in section 4 in terms of the numerical range of $\mathbb{L}_N$.

2. Spectral, resolvent and strong stability analysis are not enough

In this section, we further elaborate with specific counterexamples, on the failure of spectral analysis, resolvent condition and strong stability to capture the uniform-in-N stability of general s-stage RK schemes/methods. Spectral and resolvent analysis are shown to be too weak to secure stability, while strong stability argument is too restrictive.

2.1. **Spectral analysis is not enough.** We recall the spectral analysis led to the necessary stability condition (1.10)

$$\Delta t \cdot \lambda_k(\mathbb{L}_N) \subset \mathscr{A}_s, \qquad k = 1, 2, , \dots, N.$$

As noted above, this spectral condition is not sufficient to secure stability in case of ill-conditioned eigensystems, $\|\mathbb{T}_N^{-1}\| \cdot \|\mathbb{T}_N\|$, which grows with N. An alternative approach, trying to circumvent this difficulty of ill-condtioning is to use a unitary triangulation

$$\mathcal{P}_s(\Delta t \mathbb{L}_N) = \mathbb{U}_N^* \big(\Lambda_{\mathcal{P}} + \mathbb{R}_N\big)\mathbb{U}_N, \qquad \Lambda_{\mathcal{P}} := \mathcal{P}_s(\Delta t \Lambda),$$

where Λ and $\Lambda_{\mathcal{P}}$ are the diagonals made of the eigenvalues of $\mathbb{L}_N$ and, respectively, $\mathcal{P}_s(\Delta t \mathbb{L}_N)$, and $\mathbb{R}_N$ is a nilpotent upper triangular matrix, $(\mathbb{R}_N)_{ij} = 0,\ j \leqslant i$. Since $\|\mathcal{P}_s^n(\Delta t \mathbb{L}_N)\| =$

$\|(\Lambda_{\mathcal{P}}+\mathbb{R}_{N})^n\|$, it remains to study the power-boundedness of the triangular matrix $\Lambda_{\mathcal{P}}+\mathbb{R}_{N}$. But we claim that even a most favorable scenario, in which the spectral stability analysis (1.10) secures the eignevalues *strictly* inside the unit disc,

$$\theta := \max_{1\leqslant k\leqslant N} |\mathcal{P}_s\big(\Delta t\lambda_k(\mathbb{L}_{N})\big)| < 1, \tag{2.1}$$

will not suffice to guarantee the stability of RK method. Indeed, we may assume without restriction that $\mathbb{R}_{N}$ is arbitrarily small by its further re-scaling[5], so that

$$\|S_\delta\mathbb{R}_{N}S_\delta^{-1}\| = \|\{\mathbb{R}_{ij}\delta_\epsilon^{i-j}\}_{j>i}\| \leqslant \epsilon, \qquad S_\delta = \begin{bmatrix} \delta_\epsilon & 0 & \dots & 0 \\ 0 & \delta_\epsilon^2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & \delta_\epsilon^N \end{bmatrix}, \quad \delta_\epsilon := \frac{\epsilon}{\|\mathbb{R}_{N}\|_F}.$$

Here, an arbitrary $\epsilon>0$ is at our disposal to be determined below. It follows that

$$\|\mathcal{P}_s^n(\Delta t\mathbb{L}_{N})\| = \|\mathbb{U}_{N}^* S_\delta^{-1}\big(\Lambda_{\mathcal{P}} + S_\delta\mathbb{R}_{N}S_\delta^{-1}\big)^n S_\delta\mathbb{U}_{N}\| \leqslant \|S_\delta^{-1}\| \times (\|\Lambda_{\mathcal{P}}\|+\epsilon)^n \times \|S_\delta\|.$$

By assumption, $\|\Lambda_{\mathcal{P}}\| = \theta < 1$. Set $\epsilon := 1/2(1-\theta)$, we then end up with the stability bound

$$\|\mathcal{P}_s^n(\Delta t\mathbb{L}_{N})\| \leqslant \delta_\epsilon^{1-N}\left(\frac{1+\theta}{2}\right)^n = \Big(\frac{2\|\mathbb{R}_{N}\|_F}{1-\theta}\Big)^{N-1}\Big(\frac{1+\theta}{2}\Big)^n. \tag{2.2}$$

This bound secures the stability of finite dimensional systems – in fact, it recovers the well-known fact that matrices of finite *fixed* dimension with eigenvalues strictly inside the unit disc have exponentially decreasing iterates. But the argument breaks down when we examine the dependence on N, since the bound (2.2) is *not* uniform in N: for $n=N-1$, for example, we find that unless $\mathbb{R}_{N}$ is sufficiently small[6], then there is an *exponential growth* in N,

$$\|\mathcal{P}_s^n(\Delta t\mathbb{L}_{N})\| \leqslant \Big(\frac{2\|\mathbb{R}_{N}\|_F}{1-\theta}\Big)^{N-1}\Big(\frac{1+\theta}{2}\Big)^n_{\big|n=N-1} = \left(\|\mathbb{R}_{N}\|_F\frac{1+\theta}{1-\theta}\right)^{N-1}. \tag{2.3}$$

This bound is sharp in the sense that the power-growth hinted on the right of (2.3) is realized by the powers of the increasingly large $N\times N$ Jordan blocks

$$\|\mathbb{J}_q^n\| \sim \left(\frac{2}{1-q}\right)^N\left(\frac{1+q}{2}\right)^n, \qquad \mathbb{J}_q := \begin{bmatrix} -q & 1+q & \dots & \dots & 0 \\ 0 & -q & 1+q & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & -q & 1+q \\ 0 & \dots & \dots & \dots & -q \end{bmatrix}. \tag{2.4}$$

Although $|\lambda_k(\mathbb{J}_q)|<1$ for $-1<q<1$, there is a nonuniform growth of $\|\mathbb{J}_q^n\|$ with $0<q<1$, corresponding to $q=\theta$ in (2.3), when $n\sim N\uparrow\infty$. These increasingly large Jordan blocks realize the extreme case of ill-conditioning warned in (1.11).

[5] $\|\cdot\|_F$ refers to Frobenius norm, $\|A\|_F^2 = \text{trace}(A^\top A)$

[6] To avoid an exponential growth of the upper-bound in (2.2) requires $\|\mathbb{R}_{N}\|_F \leqslant \frac{1-\theta}{1+\theta}$; a more delicate tuning of the scaling parameter δ_ϵ shows that uniform bound is achieved for $\|\mathbb{R}_{N}\|_F < 1-\theta$.

2.1.1. *Instability of forward Euler scheme.* The extremal example (2.4) is not just of academic interest. The following classical example, [RM1967, §6.6],[KW1993, §3],[Tad2002, §5.1] sheds light on what can go wrong with spectral analysis. Consider the transport equation with fixed speed $a > 0$

$$\left\{\begin{array}{l} y_t(x,t) = a y_x(x,t), \quad (t,x) \in \mathbb{R}_+ \times (0,1) \\ y(1,t) = 0. \end{array}\right. \tag{2.5}$$

Its spatial part is discretized using one-sided spatial differences on equi-spaced grid, $\{x_\nu := \nu\Delta x\}_{\nu=0}^N$, $\Delta x = 1/N$, covering the interval $[0,1]$,

$$\left\{\begin{array}{l} \dfrac{\mathrm{d}}{\mathrm{d}t} y(x_\nu,t) = a\,\dfrac{y(x_{\nu+1},t) - y(x_\nu,t)}{\Delta x}, \qquad \nu = 0,1,\ldots,N-1, \\ y(x_N,t) = 0. \end{array}\right. \tag{2.6}$$

This amounts to method of lines for the N-vector of unknowns, $\mathbf{y}(t) := \big(y(x_0,t),\ldots,y(x_{N-1},t)\big)^\top$, governed by the $N\times N$ semi-discrete system in terms of the forward-difference operator $\mathbb{D}_N^+$,

$$\dot{\mathbf{y}}(t) = a\mathbb{D}_N^+\mathbf{y}, \qquad \mathbb{D}_N^+ := \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & \ldots & \ldots & 0 \\ 0 & -1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & \ddots & -1 & 1 \\ 0 & \ldots & \ldots & \ldots & -1 \end{bmatrix}. \tag{2.7}$$

Observe that $\mathbb{D}_N^+$ is semi-bounded — in fact it is *strictly dissipative* in the sense that

$$(\mathbb{D}_N^+)^\top + \mathbb{D}_N^+ \leqslant -2\Big(1 - \cos\big(\frac{\pi}{N+1}\big)\Big)\mathbb{I}_{N\times N}.$$

This system (2.7) is integrated using one-stage Forward Euler method, (RK1), augmented with boundary condition $u(x_N,t) = 0$,

$$\mathbf{u}_{n+1} = \mathcal{P}_1(\Delta t\cdot a\mathbb{D}_N^+)\mathbf{u}_n, \quad \mathbf{u}_n := \big(u(x_0,t^n),\ldots,u(x_{N-1},t^n)\big)^\top, \qquad n = 0,1,2,\ldots, \tag{2.8}$$

which encodes the fully discrete finite difference scheme

$$\left\{\begin{array}{l} \dfrac{u(x_\nu,t^{n+1}) - u(x_\nu,t^n)}{\Delta t} = a\dfrac{u(x_{\nu+1},t^n) - u(x_\nu,t^n)}{\Delta x}, \qquad \nu = 0,1,\ldots,N-1, \\ u(x_N,t^{n+1}) = 0. \end{array}\right. \tag{2.9}$$

The computation proceeds with hyperbolic scaling of fixed mesh ratio, $\Delta t/\Delta x$. This is precisely the regime $N \sim n$ indicated in (2.3), in which case it is known that the forward Euler scheme (2.9) is *unstable*, if it violates the CFL condition $0 < a\Delta t/\Delta x < 1$. Observe that $\mathcal{P}_1(\Delta t\cdot a\mathbb{D}_N^+)$ amounts to a Jordan block,

$$\mathcal{P}_1(\Delta t\cdot a\mathbb{D}_N^+) = \mathbb{I} + \Delta t\cdot a\mathbb{D}_N^+ = \mathbb{J}_q, \quad q = a\delta - 1, \quad \delta := \frac{\Delta t}{\Delta x}.$$

Therefore, the instability of $\mathbb{J}_q$ with $q \in (0,1]$ follows, corresponding to $1 < a\delta < 2$, which was already claimed by the bound (2.4). In particular, the RK1 scheme (2.8) is unstable, despite having $|\lambda_k(\mathcal{P}_1(\Delta t\cdot a\mathbb{D}_N^+)| = |q| < 1$.

Now consider integration of (2.7) using 4-stage (RK4). Spectral stability analysis

$$|\lambda_k(\mathcal{P}_4(\Delta t\cdot a\mathbb{D}_N^+)| = |\mathcal{P}_4(-a\delta)| \leqslant 1,$$

leads to the CFL condition, $0 < a\delta \leqslant R_4 = 2\sqrt{2}$, which *fails* to guarantee stability, since it does not take capture the power-growth of the increasingly large Jordan block $a\delta\mathbb{D}^+_N$. We conclude that even in the most favorable scenario (2.1), spectral analysis is not enough to secure a uniform-in-N stability of RK methods for increasingly large systems.

2.2. **Resolvent stability is not enough.** Recall that the imaginary interval condition (1.13) is necessary for the stability of RK method. Kreiss and Wu [KW1993, Theorem 3.6] proved that the converse holds in the sense of *resolvent stability*. Here, resolvent stability is interpreted in the sense that there exists a constant $K_R > 0$ independent of N, such that for all negative $\mathbb{L}_{_N}$'s, if the time step is small enough, $\Delta t \cdot \|\mathbb{L}_{_N}\| \leqslant \mathcal{C}_s$, then the corresponding s-stage RK method satisfies

$$\|\big(z\mathbb{I} - \mathcal{P}_s(\Delta t \mathbb{L}_{_N})\big)^{-1}\| \leqslant \frac{K_R}{|z|-1}, \qquad \forall |z| > 1. \tag{2.10}$$

The size of the time step is dictated by region of absolute stability, $\mathscr{A}_s$, specifically — $\mathcal{C}_s \leqslant R_s$ is the radius of largest half disc inscribed inside $\mathscr{A}_s$,

$$B^-_{\mathcal{C}_s}(0) := \{z:\ Re\, z < 0,\ |z| < \mathcal{C}_s\} \subset \mathscr{A}_s, \qquad \mathscr{A}_s = \big\{z \in \mathbb{C}:\ |\mathcal{P}_s(z)| \leqslant 1\big\}.$$

The notion of stability in the sense of power-boundedness, (1.8), implies that the resolvent condition holds with $K_R = K_{\mathbb{L}}$. The Kreiss Matrix Theorem, [Kre1962],[RM1967, §4.9], states that the converse holds for a family of matrices with a *fixed* dimension. Yet this does not enable us to conclude the uniform-in-N power-boundedness stability of RK method sought in (1.12), since the resolvent bound (2.10) may still allow growth $\|\mathcal{P}^n_s(\Delta t \mathbb{L}_{_N})\| \lesssim N K_R$. In [Tad1981] we conjectured that this linear dependence on N is the best possible. This was confirmed in [LT1984] proving that

$$\sup_{A \in M_N(\mathbb{C})} \frac{\sup_{|z|>1}(|z|-1)\|(z\mathbb{I} - A)^{-1}\|}{\sup_{n \geqslant 1}\|A^n\|} \sim eN.$$

The above linear-growth-in-N behavior was exhibited by a sequence of increasingly large $N \times N$ Jordan blocks, $A_N = N\mathbb{J}_0$. We observe that the A_N's in this case are not resolvent bounded uniformly in N ; it is only the ratio on the left that exhibits the sharp linear bound in N. A concrete example of a family of matrices in $M_N(\mathbb{C})$ which are resolvent stable yet their powers admit logarithmic growth in N was constructed in [MS1965].

Remark 2.1 (**Dissipative resolvent condition**). *In* [Tad1986] *we considered a stronger resolvent condition of the form*

$$\|\big(z\mathbb{I} - \mathcal{P}_s(\Delta t \mathbb{L}_{_N})\big)^{-1}\| \leqslant \frac{K_R}{|z-1|}, \quad \forall \{z\ :\ |z| \geqslant 1, z \neq 1\}. \tag{2.11}$$

In [Rit1953] *it was proved that* (2.11) *implies* $n^{-1}\|\mathcal{P}^n_s\| \stackrel{n\to\infty}{\longrightarrow} 0$. *In* [Tad1986] *we stated the improved logarithmic bound* $\|\mathcal{P}^n_s(\Delta t \mathbb{L}_{_N})\| \lesssim \log(n)$*; this was proved in* [Vit2004a]. *More on the dissipative resolvent* (2.11) *and related notions of stability can be found in* [Vit2004b, Vit2005, Sch2016]. *The dissipative resolvent bound* (2.11) *reflects a flavour of coercivity condition which will be visited in section 3.3 below; however, it does* <u>*not*</u> *secure uniform-in-N power-boundedness. A more precise notion of a dissipative resolvent condition of order* $2r > 0$ *requires the existence of* $\eta_r > 0$ *such that*

$$\|(z\mathbb{I} - \mathcal{P}_s(\Delta t \mathbb{L}_{_N}))^{-1}\| \leqslant \frac{K_R}{\text{dist}\{z, \Omega_r\}}, \quad \forall z \notin \Omega_r := \{w\ :\ |w| + \eta_r|w-1|^{2r} \leqslant 1\}. \tag{2.12}$$

The resolvent bound (2.12) *reflects the classical notion of "dissipativity of order $2r$" due to Kreiss* [Kre1964]*. It remains an open question whether* (2.12) *implies uniform-in-N power-boundedness.*

2.3. **Strong stability is not enough.** The contractivity stated in (1.16), $\|\mathcal{T}_N\mathcal{P}_s(\Delta t\mathbb{L}_N)\mathcal{T}_N^{-1}\| \leqslant 1$ with uniformly bounded $\|\mathcal{T}_N^{-1}\|\cdot\|\mathcal{T}_N\| \leqslant K_{\mathcal{T}}$, is equivalent to strong stability in the sense that there exist uniformly positive definite symmetrizer $\mathcal{H}_N$ and $K_{\mathcal{H}} > 0$, such that

$$\mathcal{P}_s^\top(\Delta t\mathbb{L}_N)\mathcal{H}_N\mathcal{P}_s(\Delta t\mathbb{L}_N) \leqslant \mathcal{H}_N, \qquad 0 < \frac{1}{K_{\mathcal{H}}} \leqslant \mathcal{H}_N \leqslant K_{\mathcal{H}}. \tag{2.13}$$

Just set $\mathcal{H}_N = \mathcal{T}_N^*\mathcal{T}_N$ with uniformly bounded $K_{\mathcal{H}} = K_{\mathcal{T}}$. In other words, (2.13) tells us that[7]

$$\|\mathcal{P}_s(\Delta t\mathbb{L}_N)\|_{\mathcal{H}_N} \leqslant 1, \qquad \Delta t\cdot\|\mathbb{L}_N\| \leqslant \mathcal{C}_s. \tag{2.14}$$

This coincides with the usual notion of strong stability,[8] e.g., [Tad2002, Ran2021]. It follows that a strongly stable RK scheme, $\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t\mathbb{L}_N)\mathbf{u}_n$, satisfies

$$|\mathbf{u}_{n+1}|_{\mathcal{H}_N} = |\mathcal{P}_s(\Delta t\mathbb{L}_N)\mathbf{u}_n|_{\mathcal{H}_N} \leqslant |\mathbf{u}_n|_{\mathcal{H}_N} \leqslant \ldots \leqslant |\mathbf{u}_0|_{\mathcal{H}_N},$$

and hence the RK iterations satisfy the uniform-in-N stability bound, $|\mathbf{u}(t_n)|_{\ell^2} \leqslant K_{\mathcal{H}}|\mathbf{u}_0|_{\ell^2}$. The strong stability of the 3-stage RK method (RK3) with symmetrizer $\mathcal{H}_N = \mathbb{H}_N$ and $\mathcal{C}_3 = 1$, was proved in [Tad2002] and was later extended in [SS2019, Theorem 4.2] to all s-stage RK methods of order $s = 3[\text{mod}4]$, namely — for small enough time step, $\Delta t\cdot\|\mathbb{L}_N\| \leqslant \mathcal{C}_s$, there holds,

$$\|\mathcal{P}_s(\Delta t\mathbb{L}_N)\|_{\mathbb{H}_N} \leqslant 1, \qquad \mathcal{P}_s(z) = \sum_{k=0}^{s}\frac{z^k}{k!}, \quad s = 3[\text{mod}4]. \tag{2.15}$$

As mentioned above, this line of arguing stability by construction of the strong stability symmetrizer, fails to extend to s-stage RK methods with $s \in 4\mathbb{N}$, [SS2017, RO2018, AAJ2023]. But this does not mean that the latter RK methods are necessarily unstable. Indeed, the general question whether stable methods are necessarily strongly stable was addressed in [Fog1964] — they are not. It leaves open the possibility that the question stability can be pursued by other approaches — other than strong stability. This will be addressed in the next section.

3. Numerical range and stability of coercive Runge-Kutta schemes

3.1. **Numerical range.** We let $\ell^2_H(\mathbb{C}^N)$ denote the weighted Euclidean space associated with a given positive definite matrix $H > 0$, and equipped with

$$\langle\mathbf{x},\mathbf{y}\rangle_H := \mathbf{x}^*H\mathbf{y}, \quad |\mathbf{x}|^2_H := \langle\mathbf{x}, H\mathbf{x}\rangle, \quad H > 0.$$

Let $A \in M_N(\mathbb{C})$ be an $N\times N$ matrix with possibly complex-valued entries. The H-weighted *numerical range*, $W_H(A)$, is the set in the complex plane

$$W_H(A) := \big\{\langle A\mathbf{x},\mathbf{x}\rangle_H \ : \ \mathbf{x}\in\mathbb{C}^N,\ |\mathbf{x}|_H = 1\big\}.$$

In the case of the standard Euclidean framework corresponding to $H = \mathbb{I}$, we drop the subscript $\mathbb{H} = \mathbb{I}$ and remain with the usual $|\cdot|^2_{\ell^2} = \langle\cdot,\cdot\rangle$, and the corresponding numerical

[7] We let $|\cdot|_{\mathcal{H}}$ denote the weighted norm, $|\mathbf{w}|^2_{\mathcal{H}} = \langle\mathbf{w},\mathcal{H}\mathbf{w}\rangle$, and $\|\cdot\|_{\mathcal{H}}$ denote the corresponding induced matrix norm, $\|\mathcal{P}\|_{\mathcal{H}} := \max_{\mathbf{w}\neq 0}|\mathcal{P}\mathbf{w}|_{\mathcal{H}}/|\mathbf{w}|_{\mathcal{H}}$.

[8] also called monotonicity in the literature on Runge-Kutta methods.

range denoted $W(A)$. If A is real symmetric then $W(A)$ is an interval on the real line (and conversely — if $W(A)$ is a real interval then A is symmetric, [Kat1995, Problem 3.9]); if A is skew-symmetric then $W(A)$ is an interval on the imaginary line. For general A's, the Hausdorff-Toeplitz theorem asserts that $W(A)$ is convex set in $\mathbb{C}$. As an example, we compute the numerical range of the $N\times N$ translation matrix, J_0,

$$\mathbb{J}_0 := \begin{bmatrix} 0 & 1 & \dots & \dots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & 0 & 1 \\ 0 & \dots & \dots & \dots & 0 \end{bmatrix}_{N\times N}. \tag{3.1}$$

For any unit vector $\mathbf{x} = (x_1, x_2, \dots, x_N)^\top$ we set a new unit vector $x_j(\xi) := e^{ij\xi}x_j$ to find

$$\langle \mathbb{J}_0\mathbf{x}(\xi), \mathbf{x}(\xi)\rangle = \sum_{j=1}^{N-1} x_{j+1}(\xi)\overline{x_j(\xi)} = e^{i\xi}\langle \mathbb{J}_0\mathbf{x}, \mathbf{x}\rangle, \qquad x_j(\xi) := e^{ij\xi}x_j,$$

which proves that $W(\mathbb{J}_0)$ is a disc centered at the origin, $B_\rho(0)$; its radius, $\rho = \rho_{_N}$, is found by considering the eigenvalues $\lambda_k(Re\,\mathbb{J}_0) = \cos(\frac{k\pi}{N+1})$, $k = 1, 2, \dots, N$: since for any A, $Re\,W(A) = W(Re\,A)$, we find $\rho_{_N} = \lambda_1(Re\,\mathbb{J}_0) = \cos(\frac{\pi}{N+1})$, and we conclude that $W(\mathbb{J})$ is the disc $B_{\rho_N}(0)$,

$$W(\mathbb{J}_0) = \{z \,:\, |z| \leqslant \rho_{_N}\}, \qquad \rho_{_N} = \cos\big(\frac{\pi}{N+1}\big). \tag{3.2}$$

3.2. **The nuemrical radius.** The numerical radius of $A \in M_N(\mathbb{C})$ is given by

$$r_{_H}(A) := \max_{|\mathbf{x}|_H=1} |\langle A\mathbf{x}, \mathbf{x}\rangle_H|.$$

The role of the numerical radius in addressing the question of stability was pioneered in the celebrated work of Lax & Wendroff, [LW1964], in which they proved the stability of their 2D Lax-Wendroff scheme, i.e., power-boundedness of a family amplification matrices, $\|G^n\| \leqslant Const.$, by securing $r(G) \leqslant 1$. The original proof, by induction on N (!), was later replaced by Halmos inequality, [Hal1967],[Pea1966]

$$r(G^n) \leqslant r^n(G). \tag{3.3}$$

Note that although the numerical radius is not sub-multiplicative, that is — although $r(AB) \leqslant r(A)r(B)$ may fail for general $A, B \in M_N(\mathbb{R})$, [GT1982], Halmos' inequality states that it holds whenever $A = B$.
Since for all A's there holds $\|A\| \leqslant 2r(A)$, (3.3) immediately yields the stability asserted by Lax & Wendroff

$$r(G) \leqslant 1 \ \rightsquigarrow\ \|G^n\| \leqslant 2, \tag{3.4}$$

and more important for our purpose — power-boundedness is secured uniformly in N. It is straightforward to extend these arguments to the weighted framework, [Tad1981, §3]

$$r_{_\mathbb{H}}(G^n) \leqslant r^n_{_\mathbb{H}}(G), \text{ and therefore } r_{_\mathbb{H}}(G) \leqslant 1 \ \rightsquigarrow\ \|G^n\| \leqslant 2K_\mathbb{H}, \quad 0 < K_\mathbb{H}^{-1} \leqslant \mathbb{H} \leqslant K_\mathbb{H}. \tag{3.5}$$

Remark 3.1. *H.-O. Kreiss proved the LW stability (3.4) by linking it to a (strict) resolvent condition*

$$r(A) \leqslant 1 \ \rightsquigarrow \|(z\mathbb{I}-A)^{-1}\| \leqslant \frac{1}{|z|-1}, \qquad \forall |z|>1$$

and conversely, [Spi1993], the numerical range is the smallest set $S = W(A)$, which induces the strict resolvent condition

$$\|(z\mathbb{I}-A)^{-1}\| \leqslant \frac{1}{\mathrm{dist}(z,S)}, \quad \forall z \in S^c.$$

3.3. **Coercivity and RK stability.** We turn to verify the stability of the 1-stage forward Euler scheme (RK1),

$$\mathbf{u}_{n+1} = (\mathbb{I} + \Delta t \mathbb{L}_{N})\mathbf{u}_n.$$

There are two regions of interest in the complex plane that we need to consider: the weighted numerical range, $W_{\mathbb{H}_N}(\mathbb{L}_N)$, and the region of absolute stability associated with forward Euler, $\mathscr{A}_1 = \{z \,:\, |1+z| \leqslant 1\}$. We make the assumption that the time step Δt is small enough so that

$$\Delta t\, W_{\mathbb{H}_N}(\mathbb{L}_N) \subset \mathscr{A}_1, \qquad \mathscr{A}_1 = \{z : |1+z| \leqslant 1\}, \tag{3.6}$$

then

$$r_{\mathbb{H}_N}(\mathcal{P}_1(\Delta t \mathbb{L}_N)) = \max_{|\mathbf{x}|_{\mathbb{H}_N}=1} |1 + \langle \Delta t \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N}| = \max_{z \in \Delta t W_{\mathbb{H}_N}(\mathbb{L}_N)} |1+z| \leqslant \max_{z\in\mathscr{A}_1} |\mathcal{P}_1(z)| = 1. \tag{3.7}$$

We summarize by stating the following.

Theorem 3.2 (**Numerical range stability of** RK1)**.** *Consider the forward Euler scheme associated with 1-stage forward Euler method (RK1),*

$$\mathbf{u}_{n+1} = (\mathbb{I} + \Delta t \mathbb{L}_N)\mathbf{u}_n, \quad n = 0, 1, 2, \ldots,$$

with assume the CFL condition (3.6) holds. Then the scheme is stable, and the following stability bound holds

$$|\mathbf{u}_n|_{\ell^2} \leqslant 2K_{\mathbb{H}} |\mathbf{u}_0|_{\ell^2}, \qquad \forall n \geqslant 1.$$

Example 3.3. *As an example for theorem 3.2 we consider the one-sided differences (2.7),*

$$\Delta t \cdot a\mathbb{D}_N^+ = a\frac{\Delta t}{\Delta x}\begin{bmatrix} -1 & 1 & \ldots & \ldots & 0 \\ 0 & -1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & \ddots & -1 & 1 \\ 0 & \ldots & \ldots & \ldots & -1 \end{bmatrix} = a\delta\big(-\mathbb{I} + \mathbb{J}_0\big), \quad a>0, \quad \delta = \frac{\Delta t}{\Delta x}. \tag{3.8}$$

By translation and dilation, $W(\Delta t \cdot a\mathbb{D}_N^+) = a\delta\big(-1 \oplus W(\mathbb{J}_0)\big)$, where (3.2) tells us that $W(\mathbb{J}_0)$ is the ball $B_{\rho_N}(0)$. Hence $W(\Delta t \cdot a\mathbb{D}_N^+)$ is given by the shifted ball,

$$W(\Delta t \cdot a\mathbb{D}_N^+) = \Big\{z \,:\, |z + a\delta| \leqslant a\delta\rho_N\Big\}, \qquad \delta = \frac{\Delta t}{\Delta x}, \quad \rho_N = \cos\big(\frac{\pi}{N+1}\big). \tag{3.9}$$

In particular, $W(\Delta t \cdot a\mathbb{D}_N^+) \subset B_1(-1)$ uniformly in N if and only if the CFL condition $a\delta \leqslant 1$ holds, which in turn secures the stability of the 1-stage forward Euler method, (RK1), for one-sided the transport equation(2.7), $\mathbf{u}_{n+1} = (\mathbb{I} + \Delta t \cdot a\mathbb{D}_N^+)\mathbf{u}_n$.

Corollary 3.4 (Stability of forward Euler scheme). *Consider the forward Euler scheme* (2.9) *associated with 1-stage RK method* (RK1)*,*

$$\mathbf{u}_{n+1} = \mathcal{P}_1(\Delta t \cdot a\mathbb{D}_N^+)\mathbf{u}_n, \quad n = 0, 1, 2, \ldots.$$

The scheme is stable under the CFL condition, $0 < a\delta \leqslant 1$*, and the following stability bound holds* $|\mathbf{u}_n|_{\ell^2} \leqslant 2|\mathbf{u}_0|_{\ell^2}$*,* $\forall n \geqslant 1$*.*

The last corollary can be recast in terms of a stability statement for $\mathbb{J}_q = \mathcal{P}_1(\Delta t \cdot a\mathbb{D}_N^+)$,

$$\|\mathbb{J}_q^n\| \leqslant 2, \qquad q \in (-1, 0).$$

This complements the statement of instability of $\mathbb{J}_q$ in the range $q \in (0, 1]$, discussed in section 2.1.1.
We note that the stability of $\mathbb{J}_q$, $q \in [-1, 0)$ can be independently verified by its induced ℓ^1-norm ,

$$\|\mathbb{J}_q\|_{\ell^1} = |-q| + |1+q| = 1 \ \rightsquigarrow \ \|\mathbb{J}_q^n\|_{\ell^1} \leqslant 1, \qquad q \in [-1, 0). \tag{3.10}$$

However, the ℓ^2-stability $\|\mathbb{J}_q\|_{\ell^2} \leqslant 2$ stated in corollary 3.4 and the ℓ^1-stability (3.10) are *not* equivalent uniformly in N. Also, $\mathbb{J}_q$ is subject to ℓ^2 von-Neumann stability analysis, [RM1967, §4.7]

$$\max_{\varphi} \left| -q + (1+q)e^{i\varphi} \right| = 1, \qquad q \in [-1, 0).$$

However, since the underlying problem (2.9) is not periodic, von Neumann stability analysis may not suffice: it requires the normal mode analysis [Kre1968] to prove ℓ^2-stability. Thus, the numerical range argument summarized in corollary 3.4 offers a genuinely different approach of addressing the question of stability, at least for 1-stage RK1.

Remark 3.5 (Coercivity). *The CFL restriction encoded in* (3.6)*,* $|\langle \Delta t\mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N} + 1| \leqslant 1$*, leads to the sub-class of negative* $\mathbb{L}_N$*'s which satisfy the* coercivity bound

$$2\mathrm{Re}\,\langle \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N} \leqslant -\beta|\langle \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N}|^2, \qquad \forall \mathbf{x} \in \{\mathbb{C}^N : |\mathbf{x}|_{\mathbb{H}_N} = 1\}. \tag{3.11}$$

Indeed, if $\mathbb{L}_N$ *is* β*-coercive in the sense that* (3.11) *holds with* $\beta > 0$*, then* (3.6) *is satisfied under the CFL condition* $\Delta t \leqslant \beta$*, and stability follows,* $r_{\mathbb{H}_N}(\mathbb{I} + \Delta t\mathbb{L}_N) \leqslant 1$*. We note that* (3.11) *places a weaker coercivity condition than the stronger notion of coercivity introduced in* [LT1998]

$$\mathbb{L}_N^\top \mathbb{H}_N + \mathbb{H}_N \mathbb{L}_N \leqslant -\beta \mathbb{L}_N^\top \mathbb{H}_N \mathbb{L}_N, \qquad \beta > 0. \tag{3.12}$$

Indeed, the latter implies (3.11)*, for*

$$2\mathrm{Re}\,\langle \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N} \leqslant -\beta\langle \mathbb{L}_N^\top \mathbb{H}_N \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle = -\beta|\mathbb{L}_N \mathbf{x}|^2_{\mathbb{H}_N} \leqslant -\beta|\langle \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N}|^2, \qquad |\mathbf{x}|_{\mathbb{H}_N} = 1.$$

One can then revisit the coercivity-based examples for stable RK methods in [LT1998] *using the relaxed coercivity* (3.11)*. The notion of* β*-coercivity is related to the dissipative resolvent condition* (2.11) *but we shall not dwell on this point in this work.*

3.4. **Numerical range stability of SSP RKs.** We extend theorem 3.2 to multi-stage RK methods using their Strong Stability Preserving (SSP) format[GST2001, §3]. We demonstrate the first three cases of RKs, $s = 2, 3, 4$.
Assume that the numerical range stability (3.7) holds. For example, the CFL condition $\Delta t \leqslant \beta$ for β-coercive $\mathbb{L}_{N}$'s, (3.11), implies $r_{\mathbb{H}_N}(\mathbb{I} + \Delta t\mathbb{L}_{N}) \leqslant 1$. Then, for the 2-stage RK method, (RK2), we have by Halmos inequality (3.3)

$$r_{\mathbb{H}_N}\big(\mathcal{P}_2(\Delta t\mathbb{L}_{N})\big) \leqslant {}^1\!/_2 + {}^1\!/_2\, r^2_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) \leqslant {}^1\!/_2+{}^1\!/_2 = 1, \quad \mathcal{P}_2(\Delta t\mathbb{L}_{N}) \equiv {}^1\!/_2\,\mathbb{I} + {}^1\!/_2\,(\mathbb{I}+\Delta t\mathbb{L}_{N})^2.$$

Similarly, the 3-stage RK method (RK3) can be expressed as

$$\mathcal{P}_3(\Delta t\mathbb{L}_{N}) \equiv {}^1\!/_3\,\mathbb{I} + {}^1\!/_2\,(\mathbb{I}+\Delta t\mathbb{L}_{N}) + {}^1\!/_6\,(\mathbb{I}+\Delta t\mathbb{L}_{N})^3,$$

and hence if (3.7) holds, then the stability of (RK3) follows from Halmos inequality,

$$r_{\mathbb{H}_N}\big(\mathcal{P}_3(\Delta t\mathbb{L}_{N})\big) \leqslant {}^1\!/_3 + {}^1\!/_2\, r_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) + {}^1\!/_6\, r^3_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) \leqslant {}^1\!/_3 + {}^1\!/_2 + {}^1\!/_6 = 1.$$

A similar argument applies to the 4-stage RK (RK4),

$$\mathcal{P}_4(\Delta t\mathbb{L}_{N}) \equiv {}^3\!/_8\,\mathbb{I} + {}^1\!/_3\,(\mathbb{I}+\Delta t\mathbb{L}_{N}) + {}^1\!/_4\,(\mathbb{I}+\Delta t\mathbb{L}_{N})^2 + {}^1\!/_{24}\,(\mathbb{I}+\Delta t\mathbb{L}_{N})^4;$$

the numerical stability (3.7), $r_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) \leqslant 1$ implies the stability of RK4,

$$\begin{aligned} r_{\mathbb{H}_N}\big(\mathcal{P}_4(\Delta t\mathbb{L}_{N})\big) &\leqslant {}^3\!/_8 + {}^1\!/_3\, r_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) + {}^1\!/_4\, r^2_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N})^2 + {}^1\!/_{24}\, r^4_{\mathbb{H}_N}(\mathbb{I}+\Delta t\mathbb{L}_{N}) \\ &\leqslant {}^3\!/_8 + {}^1\!/_3 + {}^1\!/_4 + {}^1\!/_{24} = 1. \end{aligned}$$

We summarize by stating

Corollary 3.6 (**Coercivity implies stability of RKs, $s = 2, 3, 4$**)**.** *Consider the RK schemes*

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t\mathbb{L}_{N})\mathbf{u}_n, \ n = 0, 1, 2, \ldots, \quad s = 2, 3, 4.$$

Assume the numerical range stability (3.7) *holds. In particular if $\mathbb{L}_{N}$ is β-coercive in the sense of* (3.11)*, and that the CFL condition, $\Delta t \leqslant \beta$, is satisfied. Then these s-stage RK schemes are stable,*

$$|\mathbf{u}(t_n)|_{\mathbb{H}_N} \leqslant 2|\mathbf{u}(0)|_{\mathbb{H}_N} \ \rightsquigarrow \ |\mathbf{u}(t_n)|_{\ell^2} \leqslant 2K_{\mathbb{H}}|\mathbf{u}(0)|_{\ell^2}.$$

The building block of corollary 3.6 is the condition of numerical range stability (3.7) originated with (RK1). While this argument is sharp for the 1-stage forward Euler, this SSP-based argument is too restrictive for multi-stage RKs. In particular, corollary 3.6 rules out the large sub-class of negative yet non-coercive $\mathbb{L}_{N}$'s, due to a numerical range which has non-trivial intersection with the imaginary axes. In particular, this includes the important sub-class of skew-symmetric (hyperbolic) $\mathbb{L}_{N}$'s with purely imaginary numerical range. For example, if the one-sided differences in (2.7) are replaced by centered-differences

$$\mathbf{u}_{n+1} = (\mathbb{I} + \Delta t \cdot a\mathbb{D}^0_N)\mathbf{u}_n, \qquad \mathbb{D}^0_N := \frac{1}{\Delta x}\begin{bmatrix} 0 & 1 & \ldots & \ldots & 0 \\ -1 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & -1 & 0 & 1 \\ 0 & \ldots & \ldots & -1 & 0 \end{bmatrix}_{N\times N}. \tag{3.13}$$

The numerical range lies on the imaginary interval, $W(\Delta t \cdot a\mathbb{D}^0_N) = [-iR, iR]$ with $R = R_N = a\delta\cos(\frac{\pi}{N+1})$. The 1-stage forward Euler (3.13) fails to satisfy the imaginary interval condition, and therefore, corollary 3.6 fails to capture the stability of the corresponding RKs, $\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t \cdot a\mathbb{D}^0_N)\mathbf{u}_n$ for $s = 3, 4$.

4. Spectral sets and stability of Runge-Kutta methods

We now turn our attention to the stability of multi-stage RK methods, $\mathcal{P}_s(\Delta t\mathbb{L}_N)$. Clearly, spectral analysis is not enough. On the other hand, direct computation based on ℓ^1 or ℓ^2-von Neumann analysis is not accessible: even the entries in the example of one-sided differences, $\mathcal{P}_s(\Delta t{\cdot}a\mathbb{D}^+_N)$, for $s = 3, 4$, become excessively complicated to write down. Instead, we suggest to pursue a stability argument based on numerical radius along the lines of (3.7), starting with

$$r(\mathcal{P}_s(\Delta t\mathbb{L}_N)) = \max_{\substack{|\mathbf{x}|=1\\ \mathbf{x}\in\mathbb{C}^N}} \Big|\sum_{k=0}^{s} a_k\langle(\Delta t\mathbb{L}_N)^k\mathbf{x},\mathbf{x}\rangle\Big|.$$

This requires a proper functional calculus of numerical range, relating the sets $W(\mathcal{P}_s(\Delta t\mathbb{L}_N))$ and $\{|\mathcal{P}_s(z)|\,,\colon\ z \in W(\Delta t\mathbb{L}_N)\}$, similar to the role of the spectral mapping theorem (1.9) as the centerpiece of spectral stability analysis. To this end we recall the notion of a K-*spectral set* developed in [Del1999, CG2019], which dates back to von Neumann [vN1951]; we refer to [SdV2023] for a most recent overview.

Definition 4.1 (**K-spectral sets).** Given $A \in M_N(\mathbb{C})$, we say that $\Omega \subset \mathbb{C}$ is a K-*spectral set* of A if there exists a finite $K > 0$ such that for all analytic f's bounded on Ω, there holds

$$\|f(A)\|_H \leqslant K \max_{z\in\Omega} |f(z)|. \tag{4.1}$$

In a remarkable work, [Cro2007], Crouzeix proved that for every matrix A, the numerical range $W_H(A)$ is a K-spectral set of A with $K \leqslant 11.08$; this was later improved to $K = 1+\sqrt{2}$, [CP2017]. An elegant proof of Crouzeix & Palencia $(1+\sqrt{2})$-bound, [RS2018] is included in an appendix. It follows, in particular, that for all polynomials p,

$$\|p(A)\|_H \leqslant (1+\sqrt{2}) \max_{z\in W_H(A)} |p(z)|. \tag{4.2}$$

Theorem 4.2 (**Stability of Runge-Kutta schemes).** *Consider the s-stage explicit RK method* $\mathcal{P}_s(z) = \sum_{k=0}^{s} a_k z^k$, *associated with region of absolute stability* $\mathscr{A}_s = \{z : |\mathcal{P}_s(z)| \leqslant 1\}$. *Then, the RK scheme*

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t\mathbb{L}_N)\mathbf{u}_n, \qquad n = 0, 1, 2, \dots.$$

is stable under the CFL condition $\Delta t W_{\mathbb{H}_N}(\mathbb{L}_N) \subset \mathscr{A}_s$,

$$\Delta t\, W_{\mathbb{H}_N}(\mathbb{L}_N) \subset \mathscr{A}_s \quad\leadsto\quad |\mathbf{u}_n|_{\ell^2} \leqslant (1+\sqrt{2})K_{\mathbb{H}}|\mathbf{u}_0|_{\ell^2}, \qquad n = 1, 2, \dots. \tag{4.3}$$

For proof we apply (4.2) with $p = \mathcal{P}^n_s$:

$$\|\mathcal{P}^n_s(\Delta t\mathbb{L}_N)\|_{\mathbb{H}_N} \leqslant (1+\sqrt{2}) \max_{z\in\Delta t W_{\mathbb{H}_N}(\mathbb{L}_N)} |\mathcal{P}^n_s(z)| \leqslant (1+\sqrt{2}) \max_{z\in\mathscr{A}_s} |\mathcal{P}^n_s(z)| \leqslant 1+\sqrt{2},$$

and hence $\|\mathcal{P}^n_s(\Delta t\mathbb{L}_N)\| \leqslant (1+\sqrt{2})K_{\mathbb{H}}$.

Remark 4.3 (**Implicit RK methods).** *The argument above makes a critical use of the striking fact that the spectral set bound,* $K = 1+\sqrt{2}$, *is independent of neither the increasing degree,* $\deg(\mathcal{P}^n_s) = sn$, *nor of the increasingly large dimension,* $\dim(\mathbb{L}_N) = N$. *In fact, since* (4.2) *applies to the larger algebra of* rational functions *bounded on* $W_H(A)$, *theorem 4.2 can be equally well formulated to general* __*implicit*__ *RK methods,* [HNW1993, II.7].

We recall the spectral stability analysis (1.10) which is quantified in terms of the the spectrum $\sigma(\mathbb{L}_N)$

$$\Delta t\, \sigma(\mathbb{L}_N) \subset \mathscr{A}_s, \qquad \sigma(A) := \{\lambda_k(A) \,:\, k = 1, 2, \ldots, N\}.$$

In the terminology of (4.1), the spectrum $\sigma(\mathbb{L}_N)$ is not a spectral set for $\mathbb{L}_N$. Theorem 4.2 tells us that replacing the spectrum with the larger set of H-weighted numerical range, $W_{\mathbb{H}_N}(\mathbb{L}_N) \supset \sigma(\mathbb{L}_N)$, provides a very general framework for the stability of any Runge-Kutta scheme, in conjunction with any $\mathbb{L}_N$. For example, the forward Euler (RK1) applies to the one-sided difference (3.8) which was covered in Corollary 3.4. Observe that for *normal* matrices[9], $\mathbb{L}_N$, there holds $\text{conv}\{\sigma(\mathbb{L}_N)\} = W(\mathbb{L}_N)$, e.g., [Hen1962]. Thus, the gap $W_{\mathbb{H}_N}(\mathbb{L}_N)\backslash\text{conv}\{\sigma(\mathbb{L}_N)\}$ comes into play in the stability statement (4.3) when normality uniform-in-N fails — precisely the scenario described in section 2.1 for failure of spectral analysis to secure stability. Remark that since $\cap_{H>0} W_H(\mathbb{L}_N) = \text{conv}(\{\sigma(\mathbb{L}_N)\}$, it is essential to restrict attention to uniformly bounded symmetrizers $\mathbb{H}_N$, (1.4), serving as spectral set of general $\mathbb{L}_N$'s.

A main drawback of the CFL condition (4.3) is its formulation in terms of a weighted numerical range which is not always easily accessible. Here comes the imaginary interval condition, (1.13), which provides an accessible sufficient condition for stability of multi-stage RK methods.

Theorem 4.4 (**Stability of Runge-Kutta methods**). *Consider the s-stage explicit RK method and assume it satisfies the imaginary interval condition* (1.13)*, namely — there exists $R_s > 0$ such that*

$$\max_{-R_s \leqslant \sigma \leqslant R_s} |\mathcal{P}_s(i\sigma)| \leqslant 1, \qquad \mathcal{P}_s(z) = 1 + z + a_2 z^2 + \ldots + a_s z^s. \tag{4.4}$$

Then, there exists a consonant $0 < \mathcal{C}_s < R_s$ such that for all negative $\mathbb{L}_N$'s, (1.4)*, the RK method*

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t \mathbb{L}_N)\mathbf{u}_n, \qquad n = 0, 1, 2, \ldots,$$

is stable under the CFL condition $\Delta t \cdot r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \mathcal{C}_s$,

$$\Delta t \cdot r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \mathcal{C}_s \quad \rightsquigarrow \quad |\mathbf{u}_n|_{\ell^2} \leqslant (1 + \sqrt{2}) K_{\mathbb{H}} |\mathbf{u}_0|_{\ell^2}, \qquad n = 1, 2, \ldots. \tag{4.5}$$

Proof. Recall B^-_α denotes the semi-disc, $B^-_\alpha := \{z \,:\, \text{Re}\, z \leqslant 0, \quad |z| \leqslant \alpha\}$. Consider an arbitrary negative $\mathbb{L}_N$,

$$2\text{Re}\, \langle \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle_{\mathbb{H}_N} = \langle \mathbb{L}_N^\top \mathbb{H}_N + \mathbb{H}_N \mathbb{L}_N \mathbf{x}, \mathbf{x}\rangle \leqslant 0$$

The negativity of $\mathbb{L}_N$ states that the weighted numerical range $W_{\mathbb{H}_N}(\mathbb{L}_N)$ lies on the left side of complex plane, and in fact, inside the left semi-disc

$$W_{\mathbb{H}_N}(\mathbb{L}_N) \subset B^-_{r_{\mathbb{H}_N}(\mathbb{L}_N)} := \{z \,:\, \text{Re}\, z \leqslant 0, \quad |z| \leqslant r_{\mathbb{H}_N}(\mathbb{L}_N)\}.$$

Next, we make use of [KS1992, Theorem 3.2] which asserts[10] that for an s-stage RK method satisfying the imaginary interval condition, its region of absolute stability contains a non-trivial semi-disc $B^-_{\mathcal{C}_s}$ with $\mathcal{C}_s \leqslant R_s$, so that

$$\mathscr{A}_s \supset B^-_{\mathcal{C}_s} := \{z \,:\, \text{Re}\, z \leqslant 0, \quad |z| \leqslant \mathcal{C}_s\}, \qquad \mathcal{C}_s \leqslant R_s. \tag{4.6}$$

[9] $\mathbb{L}_N^* \mathbb{L}_N = \mathbb{L}_N \mathbb{L}_N^*$ where $\mathbb{L}_N^*$ is the ℓ^2-adjoint of $\mathbb{L}_N$.

[10] Note that this requires $\mathcal{P}_s(0) = \mathcal{P}_s'(0) = 1$ in (4.4).

We conclude that for small step-size (4.5)

$$\Delta t\, W_{\mathbb{H}_N}(\mathbb{L}_N) \subset \Delta t\, B^-_{r_{\mathbb{H}_N}(\mathbb{L}_N)} = B^-_{\Delta t \cdot r_{\mathbb{H}_N}(\mathbb{L}_N)} \subset B^-_{\mathcal{C}_s} \subset \mathscr{A}_s.$$

Theorem 4.2 implies stability (1.6) with $K_{\mathbb{L}} = (1+\sqrt{2})K_{\mathbb{H}}$. □

Remark 4.5. *We note that theorem 4.4 makes use of the semi-disc $B^-_{\mathcal{C}_s}$ as a spectral set for $\mathcal{P}_s(\Delta t \mathbb{L}_N)$. In this case, one expects a sharper bound, compared with (4.2), [SdV2023, §3.2], $\|p(A)\|_H \leqslant 2 \max_{z\in W_H(A)} |p(z)|$. The constant 2 — corresponding to (3.4) with $p(z) = z^n$, agrees with Crouzeix's conjecture [Cro2007] regarding the optimality of the numerical range as 2-spectral set.*

4.1. **Optimality of the numerical radius-based CFL condition.** We observe that the CFL condition quoted in (4.5),

$$\Delta t \cdot r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \mathcal{C}_s, \tag{4.7}$$

offers a refinement of the CFL condition (1.7). Indeed, since $\mathbb{H}_N$ is uniformly bounded $0 < K_{\mathbb{H}}^{-1} \leqslant \mathbb{H}_N \leqslant K_{\mathbb{H}}$, we have

$$r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \|\mathbb{L}_N\|_{\mathbb{H}_N} \leqslant K_{\mathbb{H}}\|\mathbb{L}_N\|,$$

and hence, the CFL condition — compare with (1.7), $\Delta t \cdot \|\mathbb{L}_N\| \leqslant \mathcal{C}'_s$ with $\mathcal{C}'_s := \mathcal{C}_s/K_{\mathbb{H}}$, implies that (4.5) holds, and stability follows.
In fact, we claim that (4.7) offers an optimal CFL condition in the following sense. The proof of theorem 4.4 compares two semi-discs: on one hand we identified $B^-_{\mathcal{C}_s}$ as the largest semi-disc inscribed inside $\mathscr{A}_s$ (this is a property of the RK method under consideration); on the other hand, we identified $B^-_{r_{\mathbb{H}_N}(\mathbb{L}_N)}$ as the smallest semi-disc which contains $W_{\mathbb{H}_N}(\mathbb{L}_N)$. The CFL condition (4.7) secures the dilation of the latter semi-disc inside the former, and there, we seek the smallest semi-disc associated with $\mathbb{L}_N$ which satisfies a set of desired requirements. We claim that we cannot find a smaller semi-disc which will secure this line of argument. Indeed, let $[\![\cdot]\!]$ denote an arbitrary (vector) norm on $M_N(\mathbb{C})$, with a semi-disc $B^-_{[\![\mathbb{L}_N]\!]}$ which would be a candidate for a better CFL condition, i.e., an even smaller semi-disc $B^-_{[\![\mathbb{L}_N]\!]} \subset B^-_{r_{\mathbb{H}_N}(\mathbb{L}_N)}$. Clearly, by the necessity encoded in (1.10), the CFL condition requires that $[\![A]\!]$ is *spectrally dominant* in the sense that $[\![A]\!] \geqslant |\lambda_{\max}(A)|$ for all $A \in M_N(\mathbb{C})$. Moreover, since power-boundedness is invarainat under unitary transformations, $\|(UAU^*)^n\|_{\mathbb{H}_N} = \|A^n\|_{\mathbb{H}_N}$, we ask that the semi-disc associated with $[\![\cdot]\!]$ be unitarily invariant,

$$UB^-_{[\![\mathbb{L}_N]\!]}U^* = B^-_{[\![\mathbb{L}_N]\!]} \ \text{ for all } \ U'\text{s} \ \text{ such that } \ |U\mathbf{x}|_{\mathbb{H}_N} = |\mathbf{x}|_{\mathbb{H}_N}.$$

It follows from the main theorem of [FT1984] that the semi-disc $B^-_{[\![\mathbb{L}_N]\!]}$ must contains $B^-_{r_{\mathbb{H}_N}(\mathbb{L}_N)}$. That is, the corresponding CFL condition (4.7) is optimal in the sense that it is the smallest, spectrally dominant, unitarily invariant semi-disc which makes the argument of theorem 4.4 work.

A main aspect of theorem 4.4 is going beyond any specific coercivity requirement which was sought in the SSP-based arguments in section 3.4. It applies to *all* negative $\mathbb{L}_N$'s, thus addressing the question sought in [LT1998, §3.5]. A precise characterization for RK methods

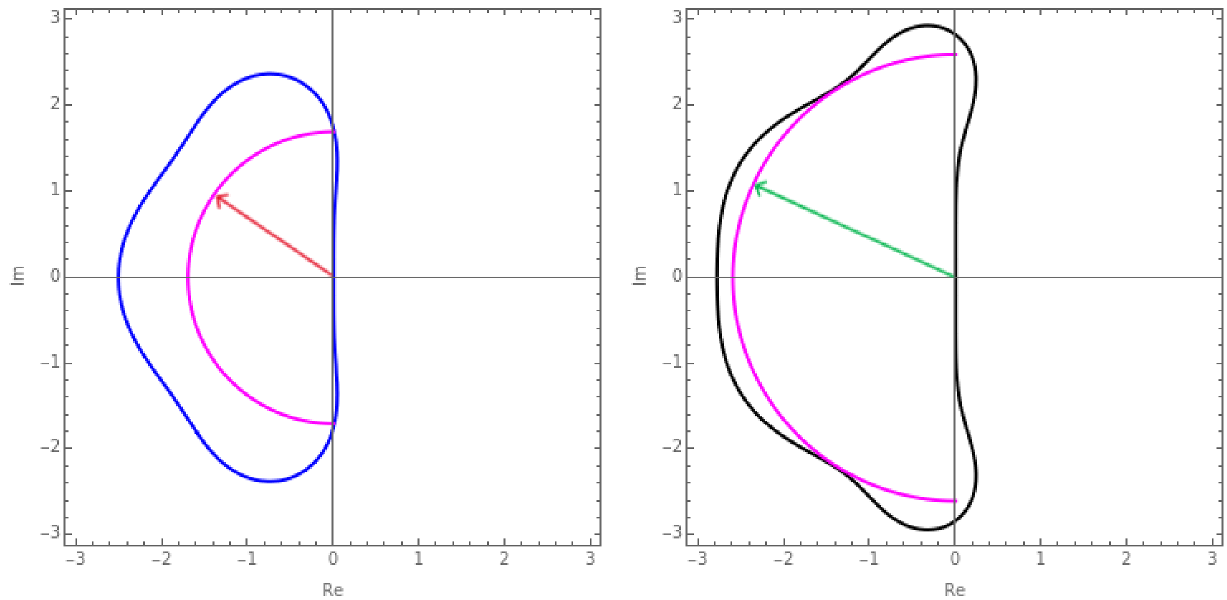

FIGURE 4.1. The semi-circles $B^-_{\mathcal{C}_s}(0)$ inscribed inside $\mathscr{A}_3$ (left) and $\mathscr{A}_4$ (right),

satisfying the imaginary interval condition was given in [KS1992, Theorem 3.1]. Consider an explicit s stage RK method, accurate of order $r \geqslant 1$,

$$\mathcal{P}_s(z) = \sum_{k=0}^{r} \frac{z^k}{k!} + \sum_{k=r+1}^{s} a_k z^k, \qquad r \geqslant 1. \tag{4.8a}$$

It satisfies the imaginary interval condition (1.13) if and only if

$$\begin{cases} (-1)^{\frac{r+1}{2}}(a_{r+1}-1) < 0, & r \text{ is odd}, \\ (-1)^{\frac{r+2}{2}}(a_{r+2}-(r+2)a_{r+1}+r+1) < 0, & r \text{ is even}. \end{cases} \tag{4.8b}$$

In the particular case of $s = r = 3, 4$ we find that the 3-stage RK method (RK3) and 4-stage RK method RK4 satisfy the imaginary interval condition and hence the existence of semi-discs with radii $\mathcal{C}_3 = \sqrt{3}$ and $\mathcal{C}_4 = 2.61$, shown in figure 4.1 which imply stability under the respective CFL conditions,

$$\Delta t \cdot \|\mathbb{L}_N\| \leqslant \mathcal{C}'_s, \qquad \mathcal{C}'_s = \mathcal{C}_s/K_{\mathbb{H}}.$$

In particular, this extends the strong stability statement of 3-stage (RK3) in [Tad2002, Theorem 2] and provides the first stability proof for the 4-stage RK (RK4) for arbitrarily large systems.

Condition (4.8b) becomes more restrictive for higher order methods; instead, one can increase r and use s-stage protocol, $s > r$ to form a dissipative term $\sum_{k=r+1}^{s} a_k z^k$ which enforces the imaginary interval condition. In particular, the 7-stage Dormand-Prince method [DP1980], with embedded fourth- and fifth-order accurate RK45, $(r, s) = (5, 7)$ which is used in MATLAB, does satisfy the imaginary interval condition (4.8b), [SR1997]. See the example of the 10-stage explicit RK method SSPRK(10,4) in [RO2018, Fig. 2].

5. Stability of time-dependent methods of lines

We demonstrate application of the new stability results for arbitrarily large systems in the context of methods of lines for difference approximation of the scalar hyperbolic equation

$$y_t = a(x)y_x, \quad (t,x) \in \mathbb{R}_+ \times [0,1],$$

augmented with proper boundary conditions. The stability results extend, mutatis mutandis[11], to multi-dimensional hyperbolic problems, $\mathbf{y}_t = \sum_{j=1}^{d} A_j(x)\mathbf{y}_{x_j}$. Stability theories for such difference approximations were developed in the classical works in the 50s–70s, e.g., [LR1956, LW1964, LN1964, Kre1964, RM1967, Kre1968, GKS1972] and can be found in the more recent texts of [Lev2007, GKO2013, Hes2017]. Our aim here is to revisit the question of stability for RK time-discretizations of such difference approximations, from a perspective of the stability theory developed in section 4. A central part of this approach requires computation of the (weighted) numerical range of the large matrices that arise in the context of such difference approximations. The development of full stability theory along these lines is beyond the scope of this paper, and is left for future work.

5.1. **Periodic problems. Constant coefficients.** We consider the 1-periodic problem

$$\begin{cases} y_t(x,t) = a y_x(x,t), & (t,x) \in \mathbb{R}_+ \times [0,1] \\ y(0,t) = y(1,t). \end{cases}$$

It spatial part is discretized using finite-difference method with constant coefficients (depending on a), $\{q_\alpha\}$, and acting on a discrete grid, $x_\nu = \nu\Delta x$, $\Delta x = {}^1/_N$,

$$\frac{\mathrm{d}}{\mathrm{d}t} y(x_\nu,t) = Q(E)y(x_\nu,t), \quad \nu = 0,1,\ldots,N-1, \qquad Q(E) := \frac{1}{\Delta x}\sum_{\alpha=-\ell}^{r} q_\alpha E^\alpha.$$

Here E is the 1-periodic translation operator, $Ey_\nu = y_{(\nu+1)[modN]}$. The resulting scheme amounts to a system of ODEs for the N-vector of unknowns, $\mathbf{y}(t) = \big(y(x_0,t),\ldots,y(x_{N-1},t)\big)^\top$, which admits the *circulant* matrix representation

$$\dot{\mathbf{y}}(t) = Q(\mathbb{E}_N)\mathbf{y}, \quad Q(\mathbb{E}_N) = \frac{1}{\Delta x}\sum_{\alpha=-\ell}^{r} q_\alpha \mathbb{E}^\alpha, \qquad \mathbb{E}_N := \begin{bmatrix} 0 & 1 & \ldots & \ldots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & \ddots & 0 & 1 \\ 1 & \ldots & \ldots & 0 & 0 \end{bmatrix}_{N\times N}. \tag{5.1}$$

[11] In particular, ℓ^2-stability needs to be adjusted to weighted H-stability, weighted by the smooth symmetrizer $H = H(x,\xi)$ so that $H(x,\xi)\sum_j A_j(x)e^{ij\xi}$ is symmetric.

The numerical range of circulant matrices is given by convex polytopes. Indeed, let $\mathbb{F}$ denote the unitary Fourier matrix, $\mathbb{F}_{jk} = \Big\{\dfrac{1}{\sqrt{N}} e^{2\pi ijk/N}\Big\}_{j,k=1}^{N}$. Then $\mathbb{F}$ diagonalizes $\mathbb{E}_{N}$,

$$\langle \mathbb{E}_{N}\mathbf{x},\mathbf{x}\rangle = \langle \widehat{\mathbb{E}}_N\widehat{\mathbf{x}},\widehat{\mathbf{x}}\rangle, \quad \widehat{\mathbb{E}}_N := \mathbb{F}^*\mathbb{E}_{N}\mathbb{F} = \begin{bmatrix} e^{\frac{2\pi i}{N}} & 0 & \dots & \dots & 0 \\ 0 & e^{2\frac{2\pi i}{N}} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \ddots & e^{(N-1)\frac{2\pi i}{N}} & 0 \\ 0 & \dots & \dots & \dots & 1 \end{bmatrix}, \quad \widehat{\mathbf{x}} := \mathbb{F}^*\mathbf{x}.$$

and hence $W(\mathbb{E}_{N}) = \Big\{\sum_{j=1}^{N} |\widehat{x}_j|^2 e^{2\pi ij/N} \ : \ \sum_j |\widehat{x}_j|^2 = 1\Big\}$ is the regular N-polytope with vertices at $\{e^{2\pi ij/N}\}_{j=1}^{N}$. This should be compared with the numerical range of the Jordan block (3.2).

It follows that $\widehat{Q(\mathbb{E}_{N})} = Q(\widehat{\mathbb{E}}_N)$ and hence the action of the $N\times N$ circulant $Q(\mathbb{E}_{N})$ is encoded it terms of its *symbol*, $\widehat{q}(\xi) := \dfrac{1}{\Delta x}\sum_\alpha q_\alpha e^{i\alpha\xi}$,

$$\langle Q(\mathbb{E}_{N})\mathbf{x},\mathbf{x}\rangle = \langle \widehat{Q(\mathbb{E}_{N})}\widehat{\mathbf{x}},\widehat{\mathbf{x}}\rangle, \qquad \widehat{Q(\mathbb{E}_{N})} = \begin{bmatrix} \widehat{q}(\frac{2\pi}{N}) & 0 & \dots & \dots & 0 \\ 0 & \widehat{q}(2\frac{2\pi}{N}) & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \widehat{q}((N-1)\frac{2\pi}{N}) & 0 \\ 0 & \dots & \dots & 0 & \widehat{q}(2\pi) \end{bmatrix}.$$

Lemma 5.1 (**Numerical range of circulant matrices).** *The numerical range of the circulant matrix $Q(\mathbb{E}_{N})$ is given by the convex polytope with vertices at $\{\widehat{q}(2\pi j/N)\}_{j=1}^{N}$,*

$$W(Q(\mathbb{E}_{N})) = \Big\{\sum_j |\widehat{x}_j|^2\, \widehat{q}\big(2\pi j/N\big) \ : \ |\widehat{\mathbf{x}}| = 1\Big\}.$$

We now appeal to theorem 3.2 which secures the stability of forward Euler time discretization for $\mathbb{L}_{N} = Q(\mathbb{E}_{N})$, provided the CFL condition $\Delta t W(Q(\mathbb{E}_{N})) \subset B_1(-1)$ holds.

Proposition 5.2 (**Stability — difference schemes with constant coefficients. I).** *Consider the fully-discrete finite difference scheme*

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{\Delta t}{\Delta x}\sum_\alpha q_\alpha \mathbb{E}_{N}^\alpha \mathbf{u}_n, \quad n = 0,1,2,\dots.$$

The scheme is stable under the CFL condition,

$$\max_{1\leqslant j\leqslant N}\Big|1 + \Delta t\cdot\widehat{q}(2\pi j/N)\Big| \leqslant 1, \qquad \widehat{q}(\xi) := \frac{1}{\Delta x}\sum_\alpha q_\alpha e^{i\alpha\xi}, \tag{5.2}$$

and the following stability bound holds $|\mathbf{u}_n|_{\ell^2} \leqslant 2|\mathbf{u}_0|_{\ell^2}$, $\forall n \geqslant 1$.

Since the CFL condition (5.2) guarantees that $\mathbb{L}_{N} = \mathbb{I} + \Delta t\cdot Q(\mathbb{E}_{N})$ is coercive, the result goes over to SSP-based multi-stage RK time differencing. In fact, theorem 4.4 applies for multi-stage RK time differencing and for <u>all</u> negative $Q(\mathbb{E}_{N})$'s.

Proposition 5.3 (**Stability — difference schemes with constant coefficients. II**). *Consider the fully-discrete finite difference scheme*

$$\mathbf{u}_{n+1} = \mathcal{P}_s\big(\Delta t \cdot Q(\mathbb{E}_{\scriptscriptstyle N})\big)\mathbf{u}_n, \quad n = 0,1,2,\ldots, \tag{5.3}$$
$$\mathcal{P}_s(z) = \sum_{k=0}^{s} a_k z^k, \quad Q(\mathbb{E}_{\scriptscriptstyle N}) = \frac{1}{\Delta x}\sum_{\alpha} q_\alpha \mathbb{E}_{\scriptscriptstyle N}^\alpha.$$

Here, $\mathcal{P}_s$ is an s-stage RK stencil satisfying the imaginary interval condition, so that (4.6) holds with $\mathcal{C}_s > 0$. If the spatial discretization is neagtive, Re $\widehat{q}(2\pi j/N) \leqslant 0$, then the scheme (5.3) is stable under the CFL condition

$$\max_{1\leqslant j\leqslant N} |\Delta t \cdot \widehat{q}(2\pi j/N)| \leqslant \mathcal{C}_s, \qquad \widehat{q}(\xi) = Q(e^{i\xi}), \tag{5.4}$$

and the following stability bound holds,

$$|\mathbf{u}_n|_{\ell^2} \leqslant (1+\sqrt{2})|\mathbf{u}_0|_{\ell^2}, \qquad n = 1,2,\ldots.$$

Propositions 5.2 and 5.3 recover von-Neumann stability analysis for difference schemes with constant coefficients, [GKO2013, §4.2]. We shall consider three examples.

Example 5.4 (**One-sided differences**). *Consider the periodic setup of the one-sided difference (2.7),*

$$\mathbf{u}_{n+1} = \big(\mathbb{I} + \Delta t \cdot Q(\mathbb{E}_{\scriptscriptstyle N}))\big)\mathbf{u}_n, \qquad Q(\mathbb{E}_{\scriptscriptstyle N}) = \frac{a}{\Delta x}(\mathbb{E}_{\scriptscriptstyle N} - \mathbb{I}),$$

with spatial symbol $\widehat{q}(\xi) = \dfrac{a}{\Delta x}(e^{i\xi} - 1)$. This amounts to the $N \times N$ system

$$\mathbf{u}_{n+1} = \mathbb{L}_{\scriptscriptstyle N}\mathbf{u}_n, \qquad \mathbb{L}_{\scriptscriptstyle N} = \begin{bmatrix} 1-\delta a & \delta a & 0 & \ldots & 0 \\ 0 & 1-\delta a & \delta a & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 1-\delta a & \delta a \\ \delta a & 0 & \ldots & 0 & 1-\delta a \end{bmatrix}_{N\times N}, \quad \delta = \frac{\Delta t}{\Delta x}.$$

Using proposition 5.2 we secure stability under the usual CFL condition $\delta a \leqslant 1$,

$$\delta a \leqslant 1 \ \rightsquigarrow \ \max_{1\leqslant j\leqslant N} \big|1 + \delta a(e^{2\pi ij/N} - 1)\big|^2 = |1-\delta a|^2 + 2|1-\delta a|\delta a + (\delta a)^2 \leqslant 1.$$

This extends to multi-stage time differencing, RKs, $s, 3, 4$

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t \cdot Q(\mathbb{E}_{\scriptscriptstyle N}))\mathbf{u}_n, \qquad \mathcal{P}_s(z) = \sum_{k=0}^{s}\frac{z^k}{k!}, \ \ s = 3,4.$$

Clearly, Re $\widehat{q} \leqslant 0$, and we can appeal to proposition 5.3 which secures stability under CFL condition $\delta a \leqslant \mathcal{C}_s$; indeed,

$$\delta a \leqslant \mathcal{C}_s \quad \rightsquigarrow \quad \delta a(e^{2\pi ij/N} - 1) \in B^-_{\mathcal{C}_s}, \quad j = 1,2,\ldots,N.$$

Example 5.5 (**Centered differences**). *Consider the periodic setup of the centered spatial difference scheme, (3.13), combined with multi-stage RK time differencing, RKs, $s = 3,4$,*

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t \cdot Q(\mathbb{E}_{\scriptscriptstyle N}))\mathbf{u}_n, \qquad Q(\mathbb{E}_{\scriptscriptstyle N}) = \frac{a}{2\Delta x}(\mathbb{E}_{\scriptscriptstyle N} - \mathbb{E}_{\scriptscriptstyle N}^{-1}).$$

Spatial differencing has purely imaginary symbol $\widehat{q}(\xi)=\dfrac{a}{\Delta x}i\sin(\xi)$*, and we invoke proposition 5.3 which secures stability under the CFL condition (5.4),*

$$\delta a=\max_{1\leqslant j\leqslant N}\left|\delta a i\sin({}^{2\pi ij}/_{N}\right|\leqslant \mathcal{C}_s, \qquad \delta=\frac{\Delta t}{\Delta x}.$$

This line of argument extends to higher order centered differences, [Tad2002, §5.2]*, e.g., the fourth-order difference*

$$Q(\mathbb{E}_{N})=\frac{a}{12\Delta x}(-\mathbb{E}_{N}^2+8\mathbb{E}_{N}-8\mathbb{E}_{N}^{-1}+\mathbb{E}_{N}^{-2}) \tag{5.5}$$

or the fourth-order finite-element difference

$$Q(\mathbb{E}_{N})=\begin{bmatrix} {}^4/_6 & {}^1/_6 & 0 & \dots & {}^1/_6\\ {}^1/_6 & {}^4/_6 & {}^1/_6 & \ddots & 0\\ 0 & \ddots & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & {}^4/_6 & {}^1/_6\\ {}^1/_6 & 0 & \dots & {}^1/_6 & {}^4/_6\end{bmatrix}^{-1}\times\frac{1}{2\Delta x}\begin{bmatrix} 0 & 1 & \dots & \dots & -1\\ -1 & 0 & 1 & \ddots & \vdots\\ 0 & \ddots & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & 0 & 1\\ 1 & 0 & \dots & -1 & 0\end{bmatrix}_{N\times N}.$$

Example 5.6 (**Lax-Wendroff differencing**). *We use the Lax-Wendroff protocol for second-order spatial difference* [LW1964] *(observe that the mesh ratio,* $\delta={}^{\Delta t}/_{\Delta x}$*, is kept fixed),*

$$Q_{\text{LW}}(\mathbb{E}_{N})=\frac{a}{2\Delta x}(\mathbb{E}_{N}-\mathbb{E}_{N}^{-1})+\frac{\delta a^2}{2\Delta x}(\mathbb{E}_{N}-2\mathbb{I}+\mathbb{E}_{N}^{-1}),$$

with symbol

$$\widehat{q}_{\text{LW}}(\xi)=\frac{a}{\Delta x}i\sin(\xi)+\frac{\delta a^2}{\Delta x}(\cos(\xi)-1).$$

Stability of the Lax-Wendroff (LW) scheme

$$\mathbf{u}_{n+1}=\big(\mathbb{I}+\Delta t Q_{\text{LW}}(\mathbb{E}_{N})\big)\mathbf{u}_n \tag{5.6}$$

follows provided CFL condition (5.2) holds, namely $|1+\Delta t\widehat{q}_{\text{LW}}({}^{2\pi j}/_{N})|\leqslant 1$*. Noting that*

$$\widehat{q}_{\text{LW}}(\xi)=\frac{2a}{\Delta x}i\sin({}^{\xi}/_2)\cos({}^{\xi}/_2)-\frac{2\delta a^2}{\Delta x}\sin^2({}^{\xi}/_2),$$

it is a standard argument, e.g., [GKO2013, §1.2] *to conclude that* $\delta a\leqslant 1$ *secures the desired CFL condition,*

$$\delta a\leqslant 1 \ \rightsquigarrow \ \max_{1\leqslant j\leqslant N}|1+\Delta t\widehat{q}_{\text{LW}}({}^{2\pi j}/_{N})|^2\leqslant 1.$$

We note that LW differencing has a negative symbol $Re\,\widehat{q}_{\text{LW}}(\xi)\leqslant 0$*, and therefore theorem 4.4 secures the stability of higher-order time discretizations of LW scheme*

$$\mathbf{u}_{n+1}=\mathcal{P}_s\big(\Delta t Q_{\text{LW}}(\mathbb{E}_{N})\big)\mathbf{u}_n, \quad s=3,4,$$

under the relaxed CFL condition, $2\delta a\leqslant\mathcal{C}_s$*. Indeed,*

$$2\delta a\leqslant\mathcal{C}_s \ \rightsquigarrow \ \max_{1\leqslant j\leqslant N}\big|\Delta t\,\widehat{q}_{\text{LW}}({}^{2\pi j}/_{N})\big|^2\leqslant\max_{\xi}\big\{4\big(\delta a\sin({}^{\xi}/_2)\cos({}^{\xi}/_2)\big)^2+4\big(\delta a\sin({}^{\xi}/_2)\big)^4\big\}\leqslant\mathcal{C}_s^2.$$

The constant coefficient case in the period setup involves the algebra of circulant matrices, all of which are uniformly diagonlizable by the Fourier matrix $\mathbb{F}$. This is a rather special case, in which von Neumann spectral stability analysis prevails for arbitrarily large systems. Clearly, the numerical range-based stability results of sections 3 and 4 offer a more general framework for studying stability of general non-periodic cases. Examples are outlined below.

5.2. **Periodic problems. Variable coefficients.** We consider the 1-periodic problem with C^2-variable coefficient $a(\cdot)$

$$\begin{cases} y_t(x,t) = a(x)y_x(x,t), & (t,x) \in \mathbb{R}_+ \times [0,1] \\ y(0,t) = y(1,t). \end{cases} \tag{5.7}$$

The spatial part is discretized using finite-difference method with $a(x)$-dependent variable coefficients, $\{q_\alpha(x)\}$, and acting on a discrete grid, $x_\nu = \nu\Delta x$, $\Delta x = {}^1\!/_N$,

$$\frac{\mathrm{d}}{\mathrm{d}t} y(x_\nu,t) = Q(E)y(x_\nu,t), \quad \nu = 0,1,\ldots,N-1, \qquad Q(E) := \frac{1}{\Delta x}\sum_{\alpha=-\ell}^{r} q_\alpha(x)E^\alpha. \tag{5.8}$$

The accuracy requirement places the restriction $\sum_\alpha q_\alpha(x) = 0$, $\sum_\alpha \alpha q_\alpha(x) = a(x)$ and so on. The difference scheme (5.8) amounts to an $N \times N$ system of ODEs with 'slowly varying' circulancy, that is $Q(x,\mathbb{E}_{_N})_{ij}$ changes smoothly in the sense that $|Q(x,\mathbb{E}_{_N})_{i+1,j+1} - Q(x,\mathbb{E}_{_N})_{ij}|$ is bounded independent of $1/\Delta x$.

$$\Delta x \sum_\alpha \alpha^2 |q_\alpha(x)|_{C^2} \leqslant K_q. \tag{5.9}$$

Let $\widehat{Q}$ denote the formal symbol associated with (5.8)

$$\widehat{Q}(x,\xi) := \frac{1}{\Delta x}\sum_{\alpha=-\ell}^{r} q_\alpha(x)e^{i\alpha\xi}.$$

Assume that the symbol is negative $Re\, \widehat{Q}(x,\xi) \leqslant 0$. Then by the sharp Gårding inequality, [LN1964, Theorem 1.1], see also [LW1962], the corresponding difference operator is semi-bounded[12], namely — there exists a constant $\eta > 0$ depending of K_q but otherwise independent of N, such that

$$Re\, Q(x,\mathbb{E}_{_N}) \leqslant 2\eta \mathbb{I}_{N\times N}. \tag{5.10}$$

Theorem 4.4 applies to $Q(x,\mathbb{E}_{_N}) - \eta\mathbb{I}$, implying its power-boundedness under the CFL condition (1.7),

$$\|\mathcal{P}_s^n\big(\Delta t(Q(x,\mathbb{E}_{_N}) - \eta\mathbb{I})\big)\| \leqslant 1+\sqrt{2}, \qquad \Delta t \cdot r\big(Q(x,\mathbb{E}_{_N})\big) \leqslant \mathcal{C}_s.$$

Next, we note that the shift $-\eta\mathbb{I}$ produces only a finite bounded perturbation B, namely

$$\begin{aligned}\mathcal{P}_s\big(\Delta t \cdot Q(x,\mathbb{E}_{_N})\big) &= \mathcal{P}_s\big(\Delta t \cdot (Q(x,\mathbb{E}_{_N}) - \eta\mathbb{I}) + \Delta t\cdot\eta\mathbb{I}\big) \\ &= \mathcal{P}_s\big(\Delta t \cdot (Q(x,\mathbb{E}_{_N}) - \eta\mathbb{I})\big) + B, \quad B = \Delta t\cdot\eta\sum_{k=1}^{s} a_k k\big(\Delta t \cdot Q(x,\mathbb{E}_{_N})\big)^{k-1},\end{aligned}$$

with $\|B\| \leqslant 2\Delta t\cdot \eta K$, $K := \displaystyle\sum_{k=1}^{s} |a_k| k \mathcal{C}_s^{k-1}$, which in turn implies the stability bound

$$|\mathbf{u}(t_n)| \leqslant \|\mathcal{P}_s^n\big(\Delta t\cdot Q(x,\mathbb{E}_{_N})\big)\||\mathbf{u}_0| \leqslant (1+\sqrt{2})e^{\eta K t_n}.$$

We summarize by stating

[12] Note that $Q(x,\mathbb{E}_{_N})$ is unbounded, $\|Q(x,\mathbb{E}_{_N})\| = \mathcal{O}({}^1\!/_{\Delta x})$.

Proposition 5.7 (**Stability — finite difference schemes with variable coefficients).** *Consider the fully-discrete finite difference scheme*

$$\mathbf{u}_{n+1} = \mathcal{P}_s\big(Q(x,\mathbb{E}_{\scriptscriptstyle N})\big)\mathbf{u}_n, \quad n=0,1,2,\ldots, \tag{5.11}$$

where $Q(x,\mathbb{E}_{\scriptscriptstyle N}) = \dfrac{1}{\Delta x}\displaystyle\sum_\alpha q_\alpha(x)\mathbb{E}^\alpha_{\scriptscriptstyle N}$ *is a local difference operator,* (5.9)*, and* $\mathcal{P}_s$ *is an s-stage RK stencil satisfying the imaginary interval condition,* (4.6)*. If the spatial symbol is negative,*

$$Re\,\widehat{Q}(x,\xi) \leqslant 0, \qquad \widehat{Q}(x,\xi) := \frac{1}{\Delta x}\sum_\alpha q_\alpha(x)e^{i\alpha\xi}, \tag{5.12}$$

then the scheme (5.11) *is stable under the CFL condition*

$$\max_\xi |\Delta t\cdot \widehat{Q}(x,\xi)| \leqslant \mathcal{C}_s, \tag{5.13}$$

and the following stability bound holds with $K=\sum_{k=1}^s |a_k|k\mathcal{C}_s^{k-1}$,

$$|\mathbf{u}_n|_{\ell^2} \leqslant (1+\sqrt{2})e^{\eta K t_n}|\mathbf{u}_0|_{\ell^2}, \quad n=1,2,\ldots, \quad \Delta t\cdot r\big(Q(x,\mathbb{E}_{\scriptscriptstyle N})\big) \leqslant \mathcal{C}_s.$$

Stability of Fourier method. There are two approaches to handle the stability of difference approximations of problems with variable coefficients: the von-Neumann spectral analysis based on sharp Gårding inequality (5.10), or the energy method e.g., [Tad1987, §2]; both approaches requires *local* stencils (5.9). An alternative approach for stability with variable coefficients in based on *numerical dissipation*, [Kre1964]. As an extreme example for using our RK stability result, we consider the *Fourier method*, [KO1972, §4],[GO1977], which is neither local nor dissipative. Set $\Delta x = {}^1\!/_{(2N+1)}$ with an odd number of $(2N+1)$ gridpoints. The Fourier method for (5.7) amounts to $(2N+1)\times(2N+1)$ system of ODEs

$$\dot{\mathbf{y}}(t) = Q(\mathbb{D}^{\mathbb{F}}_N)\mathbf{y}(t), \qquad Q(\mathbb{D}^{\mathbb{F}}_N) = A\mathbb{D}^{\mathbb{F}}_N, \quad A = \begin{bmatrix} a(x_0) & & & \\ & a(x_1) & & \\ & & \ddots & \\ & & & a(x_{2N}) \end{bmatrix}, \tag{5.14}$$

where the diagonal matrix A encodes $a(x)$ and $\mathbb{D}^{\mathbb{F}}_N$ is the $(2N+1)\times(2N+1)$ Fourier differencing matrix

$$\mathbb{D}^{\mathbb{F}}_N = \mathbb{F}\begin{bmatrix} -iN & 0 & \ldots & & 0 \\ 0 & -i(N-1) & 0 & \ddots & \\ \vdots & & \ddots & \ddots & \vdots \\ \vdots & & \ddots & i(N-1) & 0 \\ 0 & \ldots & \ldots & 0 & iN \end{bmatrix}\mathbb{F}^*, \qquad \mathbb{F}_{jk} = \left\{\frac{e^{ijk\Delta x}}{\sqrt{2N+1}}\right\}_{j,k=1}^{2N+1}.$$

The Fourier difference method is neither local, $(\mathbb{D}^{\mathbb{F}}_N)_{jk} = \dfrac{(-1)^{j-k}}{2\sin({}^{(k-j)\Delta x}\!/_2)}$ fails (5.9), nor dissipative, and the method is <u>unstable</u> in presence of variable coefficients, [GHT1994]. However, there is a different weighted-stability. Specifically — for the prototypical case $a(x)=\sin(x)$, there exists a symmetrizer $\mathbb{H}_{\scriptscriptstyle N}$ such that [GHT1994, Theorem 2.1]

$$Q(\mathbb{D}^{\mathbb{F}}_N)^\top\mathbb{H}_{\scriptscriptstyle N} + \mathbb{H}_{\scriptscriptstyle N}Q(\mathbb{D}^{\mathbb{F}}_N) \leqslant \mathbb{H}_{\scriptscriptstyle N},$$

where the $\mathbb{H}_N$-norm corresponds to the H^1-norm

$$|\mathbf{u}|^2_{\mathbb{H}_N} = |\mathbf{u}|^2_{H^1}, \qquad |\mathbf{u}|^2_{H^s} := \sum_{k=-N}^{N} |(1+k^2)^{\frac{s}{2}}|\widehat{u}_k|^2.$$

Proposition 5.8 (Stability — Fourier method). *Consider the time discretization of the Fourier method,*

$$\dot{\mathbf{y}}(t) = Q(\mathbb{D}_N^{\mathbb{F}})\mathbf{y}(t), \qquad Q(\mathbb{D}_N^{\mathbb{F}}) = A\mathbb{D}_N^{\mathbb{F}}, \quad A = \begin{bmatrix} \sin(x_0) & & & \\ & \sin(x_1) & & \\ & & \ddots & \\ & & & \sin(x_{2N}) \end{bmatrix},$$

using RK methods which satisfy the imaginary interval condition,

$$\mathbf{u}_{n+1} = \mathcal{P}_s\big(\Delta t \cdot Q(\mathbb{D}_N^{\mathbb{F}})\big)\mathbf{u}_n, \quad n = 1, 2, \ldots, \qquad \Delta t \cdot N \leqslant \mathcal{C}_s.$$

The Fourier method is H^1-stable

$$|\mathbf{u}_n|_{\mathbb{H}_N} \leqslant (1+\sqrt{2})e^{t_n/2}|\mathbf{u}_0|_{\mathbb{H}_N}. \tag{5.15}$$

We note that the symmetrizer $\mathbb{H}_N$ is not uniformly bounded from below, $N^{-2}\mathbb{I} \leqslant \mathbb{H}_N \leqslant 4\mathbb{I}$, so ℓ^2-stability fails. Converted to ℓ^2-framework, (5.15) yields

$$|\mathbf{u}_n|_{\ell^2} \leqslant N|\mathbf{u}_n|_{\mathbb{H}_N} \leqslant N(1+\sqrt{2})|e^{t_n/2}|\mathbf{u}_0|_{\mathbb{H}_N} = 2N(1+\sqrt{2})|e^{t_n/2}|\mathbf{u}_0|_{\ell^2}.$$

5.3. **Initial-boundary value problems.** We consider the problem (2.5) in the the strip

$$\begin{cases} y_t(x,t) = a y_x(x,t), \quad a > 0, \qquad (t,x) \in \mathbb{R}_+ \times [0,1] \\ y(1,t) = 0. \end{cases}$$

A general stability theory for difference approximations of initial-boundary value problems was developed in [Kre1968, GKS1972]. It is based on normal mode analysis and secures the resolvent-type stability of such approximations. The following example shows how to utilize the framework offered in theorem 4.2, to study the stability of difference approximations of initial-boundary value problems.

Example 5.9 (One-sided difference). *Consider an interior centered differencing augmented with one-sided difference at the outflow boundary $x = 0$,*

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} y(x_0,t) = a\,\dfrac{y(x_1,t) - y(x_0,t)}{\Delta x} \\ \dfrac{\mathrm{d}}{\mathrm{d}t} y(x_\nu,t) = a\,\dfrac{y(x_{\nu+1},t) - y(x_{\nu-1},t)}{2\Delta x}, \qquad \nu = 1, 2, \ldots, N-1 \\ y(x_N,t) = 0. \end{cases} \tag{5.16}$$

We emphasize that we treat the semi-infinite problem, which amounts to method of lines for the N-vector of unknowns, $\mathbf{y}(t) := \big(y(x_0,t), y(x_1,t), \ldots, y(x_{N-1},t)\big)^\top$, governed by the *semi-discrete system ("method of lines")*

$$\dot{\mathbf{y}}(t) = \mathbb{L}_N \mathbf{y}(t), \qquad \mathbb{L}_N = \frac{a}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & \dots & \dots & \dots \\ -1/2 & 0 & 1/2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & -1/2 & \ddots & \ddots & 0 \\ \vdots & \dots & \ddots & -1/2 & 0 & 1/2 \\ \dots & \dots & \dots & 0 & -1/2 & 0 \end{bmatrix}. \tag{5.17}$$

Although the matrix $\mathbb{L}_N$ is not negative, $\mathbb{L}_N^\top + \mathbb{L}_N = \frac{a}{\Delta x}\begin{bmatrix} -2 & 1/2 \\ 1/2 & 0 \end{bmatrix} \oplus \mathit{0}_{(N-2)\times(N-2)}$, it is weighted negative with the simple symmetrizer $\mathbb{H}_N$:

$$\mathbb{L}_N^\top \mathbb{H}_N + \mathbb{H}_N \mathbb{L}_N = \frac{a}{\Delta x}\begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix} \oplus \mathit{0}_{(N-2)\times(N-2)} \leqslant 0, \qquad \mathbb{H}_N := \begin{bmatrix} 1/2 & 0 \\ 0 & 1 \end{bmatrix} \oplus \mathbb{I}_{(N-2)\times(N-2)}.$$

Using theorem 4.4, we conclude the stability of time discretization of (5.17) using any RK method satisfying the imaginary interval condition, (4.8). In particular, the fully-discrete schemes based on the s-stage RK time discretization

$$\mathbf{u}_{n+1} = \mathcal{P}_s(\Delta t \mathbb{L})\mathbf{u}_n, \quad s = 3, 4, \qquad n = 1, 2, \dots,$$

are stable under the CFL condition $\Delta t \cdot r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \mathcal{C}_s$,

$$|\mathbf{u}(t_n)| \leqslant 4(1+\sqrt{2})|\mathbf{u}_0|.$$

Observing the simple bound, $r_{\mathbb{H}_N}(\mathbb{L}_N) \leqslant \dfrac{a}{\Delta x} K_{\mathbb{H}}$ with $K_{\mathbb{H}} = 2$, we end with CFL condition sufficient for stability, $\delta a \leqslant \mathcal{C}_s/2$.

The last example depends on verifying weighted negativity, $\mathbb{L}_N^\top \mathbb{H}_N + \mathbb{H}_N \mathbb{L}_N \leqslant 0$, which requires the construction of a proper symmetrizer on a case by case basis. A systematic approach for studying the weighted negativity for properly designed boundary treatment augmenting centered difference schemes was developed in [KS1974, Str1994, Gus1998, BEF2010]. To extend our RK stability framework to larger classes of difference approximations of initial-boundary values problems requires a more precise characterization of the *weighted* numerical range of Teoplitz-like spatial discretizations. This is left for future study.

Appendix A. The numerical range is $(1+\sqrt{2})$-spectral set

In his remarkable work [Cro2007], Crouzeix proved that $W_H(A)$ is a K-numerical set with $K = 11.08$ which was later improved by Crouzeix & Palencia to $K = 1+\sqrt{2}$. We quote here the elegant proof of Ransford & Schwenninger [RS2018] for Crouzeix & Palencia $(1+\sqrt{2})$-bound, based on the following lemma. In particular, we refer to the recent review [SdV2023].

Lemma A.1 (Ransford & Schwenninger $(1+\sqrt{2})$-spectral set)**.** *Let T be a Hilbert space bounded operator $\|T\| < \infty$, and let Ω be a bounded open set containing the spectrum of T. Suppose that for each f analytic on Ω, there exists an analytic g on Ω such that the following holds (here and below, $\|f\|_\Omega := \sup_\Omega |f|$):*

$$\|g\|_\Omega \leqslant \|f\|_\Omega \quad \text{and} \quad \|f(T) + g(T)^*\| \leqslant 2\|f\|_\Omega. \tag{A.1}$$

Then

$$\|f(T)\| \leqslant (1+\sqrt{2})\|f\|_\Omega$$

Proof. Let $K := \sup_{\|f\|_\Omega=1} \|f(T)\|$. By assumption, for each f, $\|f\|_\Omega \leqslant 1$, there exists g such that (A.1) holds. Ransford & Schwenninger invoked the identity

$$f(T)f(T)^*f(T)f(T)^* \equiv f(T)\big(f(T)+g(T)^*\big)^* f(T)f(T)^* - (fgf)(T)f(T)^*.$$

A simple exercise shows that the norm of the quantity on the left equals $\|f(T)\|^4$. Since by $(\text{A.1})_1$, $\|(fgf)\|_\Omega \leqslant 1$ hence $\|fgf(T)\| \leqslant K$, and since by $(\text{A.1})_2$, $\|f(T)+g(T)^*\| \leqslant 2$, then the expression on the right does not exceed

$$\begin{aligned}\|f(T)\|^4 &= \|f(T)f(T)^*f(T)f(T)^*\| \\ &\leqslant \|f(T)\|\|f(T)+g(T)^*\|\|f(T)\|\|f(T)^*\| + \|(fgf)(T)\|\|f(T)^*\| \leqslant 2K^3+K^2.\end{aligned}$$

Hence, $K^4 = \sup_{\|f\|_\Omega=1} \|f(T)\|^4 \leqslant 2K^3+K^2$ which implies $K \leqslant 1+\sqrt{2}$. ☐

Note that the lemma does not involve the numerical range of T — this comes into play in the construction of $g = g_\Omega$ satisfying (A.1), in terms of Cauchy transform,

$$g_\Omega(z) := \frac{1}{2\pi i}\int_{\partial\Omega} \frac{\overline{f(\zeta)}}{\zeta - z}\mathrm{d}\zeta, \quad z \in \Omega.$$

The main thrust of the work, originated in [vN1951] and then developed in [Del1999] [Cro2007] and finally [CP2017], is to show that such g_Ω with $\Omega = W_H(T)$ satisfies (A.1).

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Department of Mathematics and Institute for Physical Science & Technology
University of Maryland, College Park
Email address: tadmor@umd.edu