DIAGONALLY IMPLICIT RUNGE-KUTTA SCHEMES: DISCRETE ENERGY-BALANCE LAWS AND COMPACTNESS PROPERTIES

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ABSTRACT. We study diagonally implicit Runge-Kutta (DIRK) schemes when applied to abstract evolution problems that fit into the Gelfand-triple framework. We introduce novel stability notions that are well-suited to this setting and provide simple, necessary and sufficient, conditions to verify that a DIRK scheme is stable in our sense and in Bochner-type norms. We use several popular DIRK schemes in order to illustrate cases that satisfy the required structural stability properties and cases that do not. In addition, under some mild structural conditions on the problem we can guarantee compactness of families of discrete solutions with respect to time discretization.

1. INTRODUCTION

The purpose of this work is the study of structure preserving time-marching schemes for a class of evolution problems in Banach spaces; which essentially are used to describe possibly degenerate parabolic and hyperbolic initial boundary value problems. At this stage, it is enough for our purposes to say that, given a Banach space $\mathbb{V}$, a final time $t_F > 0$, and a mapping $\mathcal{F} : (0, t_F)\times\mathbb{V} \to \mathbb{V}^*$, we seek for $u : [0, t_F] \to \mathbb{V}$ that solves

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \mathcal{F}(t, u),\ \ t \in (0, t_F], \qquad u(0) = u_0. \tag{1.1}$$

As usual, $\mathbb{V}^*$ denotes the dual of $\mathbb{V}$, and $\langle\cdot,\cdot\rangle$ is the duality pairing; see Appendix A for a, far from exhaustive, list of example problems of interest. Solutions of problem (1.1) satisfy the following *energy-balance law*:

$$\frac{1}{2}|u(t_F)|^2 - \int_0^{t_F} \langle \mathcal{F}(t, u(t)), u(t)\rangle \,\mathrm{d}t \le \frac{1}{2}|u(0)|^2, \tag{1.2}$$

where the notation is to be specified. Our goal in this work is to find numerical schemes that mimic this law. For instance, given a time partition $0 = t_0 < t_1 < \cdots < t_N = t_F$ with $\tau_n = t_{n+1} - t_n > 0$ being the local timestep size, an approximate solution to (1.1) could be computed by the backward Euler scheme. Ignoring solvability issues, we obtain $\{u_n \approx u(t_n)\}_{n=1}^N$ and it is immediate to see that

$$\frac{1}{2}|u_N|^2 - \sum_{n=1}^{N} \tau_n\langle\mathcal{F}(t_n, u_n), u_n\rangle \le \frac{1}{2}|u_0|^2, \tag{1.3}$$

where, once again, the notation is to be specified.

There are several reasons why discrete energy laws such as (1.3) are important. From the practical point of view, these are a non-perturbative form of stability: they do not rely on any smallness assumption, linearization, asymptotic argument, or proximity to some equilibrium state. For complex PDE problems, where a thorough quantitative and qualitative analysis of the solution, and corresponding numerical

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scheme, are far out of reach, satisfaction of a discrete energy-balance is usually an excellent surrogate to stability.

On the other hand, from a theoretical point of view, it is often the case that with the help of discrete energy-balance laws one can assert compactness of families of numerical solutions. Once again, for complex PDE problems, (weak) convergence of discrete solutions via compactness is all one can hope to achieve without introducing additional assumptions. Examples of a successful application of this approach are numerous. The interested reader is referred to the following references: elliptic problems [28, 23], hyperbolic [57, 43], and parabolic [40]; where one of the main tools is the Aubin-Lions compactness lemma [40], or some refinement of it [53, 17, 11, 4, 27].

The backward Euler scheme is one of the simplest time-stepping schemes, yet it is often possible to prove that it possesses suitable energy-balance laws; see (1.3). Its major drawback, however, is that it is only first order accurate. In order to remedy this issue, higher order generalizations, like Galerkin-in-time schemes, have been developed and analyzed; see for instance [41, 42, 1, 61, 35, 60, 22] and references therein. These schemes can also be shown to possess energy-balance laws, and are of arbitrary high order. However, their practical impact beyond academic examples has been rather limited; see [47, 12] for a few exceptions. This is due to the fact that Galerkin-in-time methods are algebraically equivalent to full-tableau Runge-Kutta (RK) methods [1]. As such, they require the solution of linear algebraic systems where the system matrix is of size $sN \times sN$ for each Newton iteration: here s is the number of stages of the RK method and N is the number of degrees of freedom of the spatial discretization, see for instance [54].

Diagonally implicit Runge-Kutta (DIRK) methods lie between these two extreme possibilities (backward Euler and Galerkin-in-time discretizations). DIRK methods offer significantly added computational benefit, since they only require the solution of linear systems of size $N \times N$ at each stage, as well as higher order accuracy, see [14, 2, 37]. Their popularity is, perhaps, in big part due to the paper [5] which has been extremely influential in the scientific computing community. The rigorous study of the mathematical properties of DIRK schemes, however, seems to be rather underdeveloped. This is particularly the case if we are interested in the numerical approximation of PDEs satisfying a discrete energy-balance law such as (1.2). This brings us to the main motivation for our current work: we wish to present classes of DIRK schemes for which we can prove discrete energy-balance laws, and study under which conditions the solution to these schemes enjoy suitable compactness properties.

To achieve these goals we organize our presentation as follows. Notation and the functional framework we shall operate under are introduced in Section 2. Here we also discuss the minimal set of assumptions we require on the mapping $\mathcal{F}$. Section 3 then begins by introducing the general form of DIRK schemes and making some comments regarding their implementation when applied to PDEs. Two notions of balance laws: discrete energy-balance, and dissipative discrete energy-balance, respectively, are introduced here for DIRK schemes; their importance and meaning is also discussed. This section then presents an exhaustive literature review regarding the existing (algebraic) notions of stability and why we believe these are not suitable for our purposes. A list of some popular two- and three-stage DIRK schemes finalizes this section. The core of our work is Sections 4 and 5 where, for two- and three-stage schemes, respectively, we explore the existence of discrete energy-balance laws. We arrive at a property, which we call *remarkable stability* which immediately implies the existence of a dissipative discrete energy law for a DIRK scheme. We note that, given the Butcher tableau of an s-stage DIRK scheme, verifying remarkable stability only requires some algebraic manipulations using the entries of the tableau, and the solution of an algebraic eigenvalue problem of size s. Each section concludes by verifying remarkable stability for a list of widely used DIRK schemes. Finally, in Section 6, we refine the assumptions on $\mathcal{F}$ to arrive at our strongest notion: discrete Bochner-stability. We show that every remarkably stable scheme is discretely Bochner-stable, and that (families of) solutions to discretely Bochner-stable schemes possess suitable compactness properties.

Finally, we believe that one important feature of our exposition is its simplicity. The main results of this manuscript rely, in essence, on the simple polarization identity

$$a(a-b) = \tfrac{1}{2}|a|^2 - \tfrac{1}{2}|b|^2 + \tfrac{1}{2}|a-b|^2, \tag{1.4}$$

and some algebraic manipulations. At times these manipulations may be long and tedious, and some assistance from a computer algebra software package[1] may be desired. Despite of this, these are nothing but algebraic manipulations. When describing compactness properties, well-known elementary order conditions of RK schemes may be necessary, which are summarized in Appendix C. No high level tools or specialized notions of algebraic stability for ODE solvers are used in our work.

2. Preliminaries

Here we describe the framework and assumptions we shall operate under. If $p \in (1,\infty)$ its Hölder conjugate is $p' = p/(p-1)$. We extend this notation such that $1' = \infty$, $\infty' = 1$, and $1/p + 1/p' = 1$ for all $p \in [1,\infty]$. By $t_F > 0$ we denote a final time.

By $A \lesssim B$ we shall mean $A \le cB$ for a nonessential constant c that may change at each occurrence.

2.1. **Functional framework.**

Throughout our work we shall assume that $\mathbb{H}$ is a separable Hilbert space with inner product $(\cdot,\cdot)$ and norm $|\cdot|$. By $\mathbb{V}$ we denote a Banach space, and its norm is denoted by $\|\cdot\|$. The dual of $\mathbb{V}$ is denoted by $\mathbb{V}^*$, the duality pairing between them is denoted by $\langle\cdot,\cdot\rangle$. The norm in $\mathbb{V}^*$ is denoted by $\|\cdot\|_*$.

We shall assume that $\mathbb{V} \subset \mathbb{H} \subset \mathbb{V}^*$ is a Gelfand triple. We recall that in this setting the duality pairing is an extension of the inner-product. In other words, every $v \in \mathbb{H}$ defines an element of $\mathbb{V}^*$ whose action is defined by

$$\langle v, w\rangle = (v,w), \quad \forall w \in \mathbb{V}. \tag{2.1}$$

This identification will be repeatedly used in our discussion.

Let $\mathbb{W}$ be a separable Banach space with norm $\|\cdot\|_{\mathbb{W}}$ and $p \in [1,\infty]$. For $w : [0,t_F] \to \mathbb{W}$ measurable, we define

$$\|w\|_{L^p(0,t_F;\mathbb{W})} = \begin{cases} \left(\displaystyle\int_0^{t_F} \|w(s)\|_{\mathbb{W}}^p \, \mathrm{d}s \right)^{1/p}, & p < \infty, \\ \operatorname{ess.sup}_{s\in[0,t_F]} \|w(s)\|_{\mathbb{W}}, & p = \infty. \end{cases}$$

Then, we define the Bochner space

$$L^p(0,t_F;\mathbb{W}) = \left\{ w : [0,t_F] \to \mathbb{W} \,\middle|\, \|w(s)\|_{L^p(0,t_F;\mathbb{W})} < \infty \right\},$$

which is Banach for the norm $\|\cdot\|_{L^p(0,t_F;\mathbb{W})}$. The space of functions $w : [0,t_F] \to \mathbb{W}$ that are continuous is denoted by $\mathcal{C}([0,t_F];\mathbb{W})$. We endow this space with the $L^\infty(0,t_F;\mathbb{W})$-norm.

2.2. **Initial value problems.**

With all the previous notation and preparations at hand we can proceed to rigorously describe the class of problems we are interested in approximating. We assume that the initial condition satisfies $u_0 \in \mathbb{H}$, and that the slope function satisfies $\mathcal{F} : [0,t_F] \times \mathbb{V} \to \mathbb{V}^*$. We then seek for $u : [0,t_F] \to \mathbb{H}$ such that $\frac{\mathrm{d}u}{\mathrm{d}t} : [0,t_F] \to \mathbb{V}^*$ and solves (1.1).

We will also assume that $\mathcal{F}$ can be split into an autonomous and purely non-autonomous time-dependent part as

$$\mathcal{F}(t,w) = f(t) - \mathcal{A}(w), \qquad \forall t \in [0,t_F], \quad \forall w \in \mathbb{V},$$

where $f : [0,t_F] \to \mathbb{V}^*$ and $\mathcal{A} : \mathbb{V} \to \mathbb{V}^*$. In the context of PDEs and/or ODEs on graphs, we assume that nonhomogeneous boundary data can always be assimilated into f.

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[1] In this manuscript we used Mathematica©.

The minimal set of assumptions we shall impose on the mapping $\mathcal{A}$ are as follows.

- *Nonnegativity:* The mapping $\mathcal{A}$ is nonnegative, i.e.,

$$\langle \mathcal{A}(w), w \rangle \geq 0, \quad \forall w \in \mathbb{V}. \tag{2.2}$$

- *Local-solvability.* We assume that, for every $F \in \mathbb{V}^*$, there exists $\beta > 0$ such that for every $\gamma \in (0, \beta]$ the problem

$$v + \gamma \mathcal{A}(v) = F, \tag{2.3}$$

  has a unique solution $v \in \mathbb{V}$. This assumption guarantees that nonlinear problems associated to each stage in DIRK schemes have a unique solution, possibly under some timestep size constraint.

As we shall see below, property (2.2) is sufficient in order to derive discrete energy-balance laws for DIRK schemes. While a discrete energy balance law is not, in general, enough to prove a priori bounds in Bochner-type norms for the discrete solution or its time derivative, (2.2) covers a large family of relevant problems; see Appendix A. Stronger assumptions on $\mathcal{A}$ will be imposed in Section 6, and these will allow us to establish a priori bounds in Bochner-type norms.

3. DIRK schemes

In this section we recall some general notions related to RK schemes; and, in particular, present some details regarding DIRK schemes. We will also detail the main stability notion for these schemes that we shall pursue.

We recall that RK schemes are uniquely characterized by their so-called Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^\intercal \end{array} . \tag{3.1}$$

Here $s \in \mathbb{N}$ is the number of stages, $\mathbf{A} = [a_{ij}] \in \mathbb{R}^{s \times s}$ is the matrix of coefficients, $\mathbf{c} = [c_i] \in [0,1]^s$ are the pseudo-collocation times, and $\mathbf{b} = [b_i] \in [0,1]^s$ are the weights. For the sake of completeness, necessary order conditions for (3.1) are summarized in Appendix C. We remind the reader that a DIRK scheme is one where the matrix $\mathbf{A}$ is lower triangular.

Let us now, to make things precise, detail how a DIRK scheme is applied to (1.1). Let $N \in \mathbb{N}$ be the number of steps. We introduce a partition $\mathcal{P}_N = \{t_n\}_{n=0}^N$ of $[0, t_F]$, i.e.,

$$0 = t_0 < \cdots < t_N = t_F,$$

and set $\tau_n = t_{n+1} - t_n$, for $n = 0, \ldots, N-1$ to be the local timestep. Starting from u_0 we will compute the sequence $\{u_n\}_{n=1}^N \subset \mathbb{V}$ such that $u_n \approx u(t_n)$ as follows. For $n \geq 0$ we solve the following equations in $\mathbb{V}^*$

$$\begin{cases} v_{n,i} = u_n + \tau_n \displaystyle\sum_{j=1}^{i} a_{ij} \mathcal{F}_{n,j}, \quad i = 1, \ldots, s, \\ u_{n+1} = u_n + \tau_n \displaystyle\sum_{j=1}^{s} b_j \mathcal{F}_{n,j}, \end{cases} \tag{3.2}$$

where we introduced a shorthand notation $\mathcal{F}_{n,j}$ defined by

$$f_{n,j} = f(t_n + c_j \tau_n), \qquad \mathcal{F}_{n,j} = f_{n,j} - \mathcal{A}(v_{n,j}).$$

For fixed $n \in \{1, \ldots, N\}$, the quantities $\{v_{n,i}\}_{i=1}^s$ are called the stages.

Notice that a generic step in (3.2) requires, given $F \in \mathbb{V}^*$, to find $v \in \mathbb{V}$ that solves (2.3) with, for some $i \in \{1, \ldots, s\}$, $\gamma = a_{ii} \tau_n$. Thus, owing to the local solvability condition, for this scheme to be well-defined for any partition $\mathcal{P}_N$, it is sufficient to require that $a_{ii} > 0$. For this reason, in what follows we shall assume that this is always the case for a DIRK scheme.

Finally, observe that, although the equations are posed in $\mathbb{V}^*$, it is not difficult to show that, for all $n \geq 0$, $\{v_{n,i}\}_{i=1}^s \cup \{u_{n+1}\} \subset \mathbb{V}$.

Remark 3.1 (smoothness of the right hand side)**.** We comment that usually the theory regarding well-posedness of (1.1), only requires the right hand side f to be such that $f \in L^r(0,t_F;\mathbb{V}^*)$ for some $r > 1$. This makes, in general, the quantities $f_{n,j}$, for $n \geq 0$ and $j = 1,\dots,s$, meaningless, as point evaluations of f are not possible. This usually is circumvented by replacing f by a suitable approximation $f_{\mathcal{P}_N} \in \mathcal{C}([0,t_F];\mathbb{V}^*)$. In order to avoid unnecessary clutter of the notation we will ignore this issue.

Remark 3.2 (interpretation)**.** We note that (3.2) must be understood by its action against suitable "test functions". Owing to (2.1), a generic stage $v_{n,i} \in \mathbb{V}$ for $i = 1,\dots,s$ must be such that, for every $w \in \mathbb{V}$,

$$(v_{n,i}, w) + \tau_n a_{ii} \langle \mathcal{A}(v_{n,i}), w\rangle = (u_n, w) + \tau_n \sum_{j=1}^{i} a_{ij} \langle f(t_n + c_j\tau_n), w\rangle - \tau_n \sum_{j=1}^{i-1} a_{ij} \langle \mathcal{A}(v_{n,j}), w\rangle.$$

3.1. **Discrete energy-balance.** As we described above, s-stage DIRK methods are characterized by its tableau, and are such that the matrix $\mathbf{A}$ is lower triangular and has positive diagonal entries. The following definition will be our main notion of stability for DIRK schemes.

Definition 3.3 (discrete energy-balance)**.** We say that a DIRK scheme with tableau (3.1), where $\mathbf{A}$ is lower triangular and has positive diagonal entries, satisfies a discrete energy-balance if, for any $N \in \mathbb{N}$, every partition $\mathcal{P}_N$, and all $n \in \{0,\dots,N-1\}$, we have that

$$\frac{1}{2}|u_{n+1}|^2 + \sum_{i=1}^{s+1} \delta_i |v_{n,i} - v_{n,i-1}|^2 - \tau_n \sum_{i=1}^{s} \nu_{ii} \langle \mathcal{F}_{n,i}, v_{n,i}\rangle = \frac{1}{2}|u_n|^2 + \tau_n \sum_{i=1}^{s}\sum_{j=i+1}^{s} \nu_{ij} \langle \mathcal{F}_{n,i}, v_{n,j}\rangle, \tag{3.3}$$

where we introduced the notation $v_{n,0} = u_n$ and $v_{n,s+1} = u_{n+1}$. The coefficients $\{\delta_i\}_{i=1}^{s+1} \subset \mathbb{R}$ and $\{\nu_{ij}\}_{i=1,j=i}^{s,s} \subset \mathbb{R}$ depend only on the tableau, and are expected to satisfy the following constraints:

- $\delta_i \geq 0$ for all $i \in \{1,\dots,s+1\}$.
- $\nu_{ii} > 0$ for all $i = \{1,\dots,s\}$.
- The coefficients $\{\nu_{ij}\}_{i=1,j=i}^{s,s}$ must satisfy the constraint

$$\sum_{i=1}^{s} \nu_{ii} + \sum_{i=1}^{s}\sum_{j=i+1}^{s} \nu_{ij} = 1. \tag{3.4}$$

Notice that (3.3) differs from (1.3) in at least two salient terms. First, the presence of the terms $\sum_{i=1}^{s+1} \delta_i |v_{n,i} - v_{n,i-1}|^2$ may seem out of place. However, these terms represent purely numerical artificial damping and are usually quite desirable when dealing with dissipative/parabolic PDEs[2]. However, artificial damping is not desirable when considering the discretization of Hamiltonian, or related, PDEs (e.g., PDEs that preserve quadratic invariants). For this reason, we allow the coefficients δ_i to be all zero if that is suitable for the problem at hand. Second, while the terms $\langle \mathcal{F}_{n,i}, v_{n,i}\rangle$ are expected, the off-diagonal terms, i.e., $\langle \mathcal{F}_{n,i}, v_{n,j}\rangle$ with $i \neq j$, may be problematic and, thus, it is possible that (3.3) will not lead to suitable a priori estimates for discrete solutions. For this reason, we introduce a stronger notion, which we call "dissipative discrete energy-balance".

[2]For instance, in some very specific contexts such as projection methods for incompressible Navier-Stokes equations, artificial damping terms are critical to guarantee numerical stability of the scheme, see for instance [29, 30] and references therein.

Definition 3.4 (dissipative discrete energy-balance)**.** We say that a DIRK scheme with tableau (3.1) satisfies a dissipative discrete energy-balance if there are strictly positive $\{\nu_i\}_{i=1}^s$, and

$$\mathcal{Q} : [\mathbb{H}]^{s+1} \to \mathbb{R}, \qquad \mathcal{Q}(w_1, \ldots, w_{s+1}) = \frac{1}{2}\sum_{i=1}^{s+1}\sum_{j=1}^{s+1} q_{ij}(w_i, w_j), \qquad q_{ij} = q_{ji} \in \mathbb{R},$$

a nonnegative definite quadratic form on $[\mathbb{H}]^{s+1}$ such that, for any $N \in \mathbb{N}$, every partition $\mathcal{P}_N$, and all $n \in \{0, \ldots, N-1\}$, we have

$$\frac{1}{2}|u_{n+1}|^2 + \mathcal{Q}(u_n, v_{n,1}, \ldots, v_{n,s}) - \tau_n \sum_{i=1}^{s} \nu_i \langle \mathcal{F}_{n,i}, v_{n,i}\rangle = \frac{1}{2}|u_n|^2. \tag{3.5}$$

Expression (3.5) states that, beyond the "energy" introduced into the system by the non-autonomous part f, the scheme will not produce any spurious surplus of energy. Moreover, the fact that $\mathcal{Q}$ is nonnegative definite implies that the scheme may even dissipate some energy. The following result makes this intuition rigorous.

Proposition 3.5 (discrete energy dissipation)**.** *Assume that, in* (1.1)*, the mapping $\mathcal{A}$ satisfies* (2.2)*. If the solution to* (1.1) *is approximated with a DIRK scheme that satisfies the dissipative discrete energy-balance of Definition 3.4, then for all $N \in \mathbb{N}$, any partition $\mathcal{P}_N$, and all $n \in \{0, \ldots, N-1\}$, we have*

$$\frac{1}{2}|u_{n+1}|^2 \leq \frac{1}{2}|u_n|^2 + \tau_n \sum_{i=1}^{s} \nu_i \langle f_{n,i}, v_{n,i}\rangle \tag{3.6}$$

Proof. We start by recalling that $\mathcal{F}_{n,i} = f_{n,i} - \mathcal{A}(v_{n,i})$. Since $\mathcal{Q}$ and the diagonal terms $\langle \mathcal{A}(v_{n,i}), v_{n,i}\rangle$ are nonnegative due to the assumption (2.2), they can be dropped from the left hand side of (3.5). $\square$

3.2. **Literature review.** At this point, it is worth making some comments about RK methods, discrete energy laws and the preexisting literature.

There is a significant body of numerical ODE literature attempting to bridge the gap between algebraic notions of stability and nonlinear notions of stability; see for instance: A-stability [16], L-Stability [19, 20], B-Stability [9], AN-Stability [7], BN-stability [7], BS-stability and BSI-stability [25, 26] and G-stability [15] among many others (see also [31, 10]). Similarly, there is a specific body of scientific literature relating algebraic notions of stability and discrete energy laws [7, 8, 36, 48, 56]. However, we find that the classical techniques used in the numerical ODE literature are largely incompatible with our current goals, and the notions of stability that we are trying to advance; see Definitions 3.3–3.4 and Definition 6.4 below. We explain our reasoning in more detail.

- *Functional setting.* A common assumption in the numerical ODE literature is that $\mathcal{A} : \mathbb{H} \to \mathbb{H}$ boundedly; see, for instance [49, 48, 34, 56]. This is a rather stringent assumption that, in general, is not suitable for PDEs. For instance, it does not allow us to capture the linear heat equation, incompressible Navier-Stokes equation, nor large families of advection-reaction-diffusion systems. For this reason we, instead, focus on the Gelfand-triple functional framework and assume that $\mathcal{A} : \mathbb{V} \to \mathbb{V}^*$.
- *Choice of norms.* The numerical ODE literature focuses on the development of $L^\infty(0, t_F; \mathbb{H})$ estimates, i.e., $|u_n| \leq |u_0|$ for all $n \geq 0$; see, for instance [8, 36]. For ODEs in $\mathbb{R}^N$ and some limited cases of linear hyperbolic PDEs, this may suffice. However, for many PDE problems, such as parabolic-like problems, this type of estimate may be insufficient. Without a priori bounds on spatial derivatives in Bochner-type norms, it is not possible to assert stability of such schemes. To assert convergence, usually, one additionally requires an a priori estimate on the time derivative, again in a Bochner-type norm. In other words: discrete energy balances of the form (3.5) are suitable for the analysis of parabolic-like problems, while estimates of the form (3.6), in general cannot yield enough compactness.

We note that estimates in $L^\infty(0,t_F;\mathbb{H})\cap L^p(0,t_F;\mathbb{V})$, for some $p>1$, are standard in the PDE and numerical-PDE literature [40, 44, 59, 60, 27, 24, 39, 51, 50, 3]. On the other hand, to our knowledge, the numerical ODE literature [31, 55, 10, 32] has not focused on a priori bounds in Bochner-type norms, space-time compactness, or convergence without regularity assumptions for problems of growing dimensionality (i.e. discretization of evolutionary PDEs).

- *Finite dimensionality.* We want to develop stability results that are valid for finite dimensional problems as well as their infinite dimensional limits. This is a somewhat delicate issue when dealing with operators of the form $\mathcal{A}:\mathbb{V}\to\mathbb{V}^*$. Let us explain what we mean here. As we detailed above, see (2.3) and Remark 3.2, a generic stage must be interpreted as: find $v\in\mathbb{V}$ such that

$$(v,w)+a\tau_n\langle\mathcal{A}(v),w\rangle=\langle F,w\rangle,\quad \forall w\in\mathbb{V}.$$

At this point one may be tempted to set $w=\mathcal{A}(v)$. However, that is not necessarily well-defined unless additional assumptions are made[3]. Similarly, higher order compositions of the operator, i.e., $\mathcal{A}(\mathcal{A}(v))$, are not meaningful unless $\mathcal{A}$ maps a Banach space to itself. We note that energy identities and a priori bounds in norm using such constructions are common in the numerical ODE literature; see for instance [49, 48, 34, 56] and the review paper [36, p. 1464–1465].

In light of the shortcomings mentioned above, in this manuscript we develop stability results that:

- Target specifically DIRK schemes in the framework of a Gelfand triple and unbounded operators. We limit ourselves to the case of two- and three-stage schemes.
- Energy identities and a priori bounds will solely rely on the inner product in $\mathbb{H}$, the duality pairing $\langle\mathcal{A}(u),v\rangle$, and additive telescopic cancellation arguments. We do not use or invoke higher order compositions of the operator $\mathcal{A}$, higher order products such as $\langle\mathcal{A}(u),\mathcal{A}(v)\rangle$, nor similar “multiplicative” constructions.
- While this may be necessary to show existence of solutions to (1.1), we make no assumption of contractivity/monotonicity of our operator $\mathcal{A}$ to obtain stability. Our primary notion of nonlinear stability revolves around “dissipative discrete energy-balances”, see (3.5), which is, strictly speaking, a property of the scheme, not a property of the operator. This enables the proof of a priori bounds in Bochner-type norms for u and its time derivative $\frac{\mathrm{d}u}{\mathrm{d}t}$ for some families of operators; see Proposition 6.6.
- Our a priori Bochner-type norm estimates make a clear cut distinction between “artificial/numerical damping” and “physical or PDE dissipation” terms. A precise identification of artificial damping terms plays a pivotal role in order to establish stability of the scheme. On the other hand, physical dissipation is fundamental to establish dual norm estimates on the time derivative of the discrete solution.

As a final comment we note that the mathematical theory about Galerkin-in-time and/or full-tableau RK methods developed by the numerical PDE community; see [41, 42, 1, 61, 35, 22] and references therein, rarely ever applies (or even mentions) DIRK schemes. We do however, highlight the preexistence of quite relevant material with specific focus on DIRK schemes that shares a few common points of intersection with the material presented in this manuscript. In particular [52] addresses the issue of gradient flow stability for DIRK schemes, while [33] addresses convergence without regularity assumptions using semi-group methods. However, the material presented in the current paper differs quite significantly in relationship to the mathematical tools used and the degree of generality.

3.3. **Some popular DIRK schemes.** Let us present some popular two- and three-stage DIRK schemes, and briefly mention some of their known properties. These will be our specific examples under consideration used to illustrate the developed theory.

[3] For instance, if $\mathcal{A}=-\Delta$, the product $(\mathcal{A}(v),\mathcal{A}(v))_{L^2(\Omega)}$ is meaningful only if we assume $H^2(\Omega)$-regularity of v.

3.3.1. *Two-stage schemes.* We will consider the following two-stage schemes.

- Alexander's DIRK22 scheme:

$$
\begin{array}{c|cc}
\gamma & \gamma & \\
1 & 1-\gamma & \gamma \\
\hline
 & 1-\gamma & \gamma
\end{array}
\qquad \gamma = 1 - \tfrac{\sqrt{2}}{2}. \tag{3.7}
$$

Tableau (3.7) seems to appear for the first time in [2].

- Butcher-Burrage DIRK22 scheme:

$$
\begin{array}{c|cc}
\gamma & \gamma & \\
1-\gamma & 1-2\gamma & \gamma \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad \gamma = 1 \pm \tfrac{\sqrt{2}}{2}. \tag{3.8}
$$

To the best of our knowledge this tableau appears for the first time in [7, p. 51].

- Kraaijevanger-Spijker DIRK22 scheme

$$
\begin{array}{c|cc}
\frac{1}{2} & \frac{1}{2} & \\
\frac{3}{2} & -\frac{1}{2} & 2 \\
\hline
 & -\frac{1}{2} & \frac{3}{2}
\end{array} \tag{3.9}
$$

see [38, p. 77].

- Crouzeix's DIRK23 scheme:

$$
\begin{array}{c|cc}
\frac{1}{2}+\gamma & \frac{1}{2}+\gamma & \\
\frac{1}{2}-\gamma & -2\gamma & \frac{1}{2}+\gamma \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad \gamma = \tfrac{\sqrt{3}}{6}. \tag{3.10}
$$

This tableau can be found in [13]. This scheme is third order accurate.

3.3.2. *Three-stage schemes.* Regarding three-stage methods we will consider:

- Alexander's DIRK33 scheme

$$
\begin{array}{c|ccc}
\gamma & \gamma & & \\
\frac{1+\gamma}{2} & \frac{1-\gamma}{2} & \gamma & \\
1 & b_1(\gamma) & b_2(\gamma) & \gamma \\
\hline
 & b_1(\gamma) & b_2(\gamma) & \gamma
\end{array} \tag{3.11}
$$

where γ is the root of $6\gamma^3 - 18\gamma^2 + 9\gamma - 1 = 0$ in the interval $(\frac{1}{6}, \frac{1}{2})$. More precisely we have that

$$
\begin{aligned}
\gamma &= 1 - \sqrt{2}\sin\left(\tfrac{2\arctan\frac{\sqrt{2}}{2}}{3}\right) \approx 0.4358665 \\
b_1(\gamma) &= -\tfrac{3}{2}\gamma^2 + 4\gamma - \tfrac{1}{4} \approx 1.2084966 \\
b_2(\gamma) &= \tfrac{3}{2}\gamma^2 - 5\gamma + \tfrac{5}{4} \approx -0.6443631.
\end{aligned}
$$

Tableau (3.11) seems appear for the first time in [2, p. 1012].

- Nørsett DIRK34 order method:

$$
\begin{array}{c|ccc}
\gamma & \gamma & & \\
\frac{1}{2} & \frac{1}{2}-\gamma & \gamma & \\
1-\gamma & 2\gamma & 1-4\gamma & \gamma \\
\hline
 & \delta & 1-2\delta & \delta
\end{array}
\qquad \delta = \tfrac{1}{6(1-2\gamma)^2}, \tag{3.12}
$$

and γ is one of the roots of the equation $\gamma^3 - \frac{3}{2}\gamma^2 + \frac{1}{2}\gamma - \frac{1}{24} = 0$. More precisely these roots are

$$\begin{aligned} \gamma_1 &= \tfrac{\sqrt{3}}{3}\cos(\tfrac{\pi}{18}) + \tfrac{1}{2} \approx 1.068579021, \\ \gamma_2 &= \tfrac{1}{2} - \tfrac{\sqrt{3}}{3}\sin(\tfrac{2\pi}{9}) \approx 0.1288864005, \\ \gamma_3 &= \tfrac{1}{2} - \tfrac{\sqrt{3}}{3}\sin(\tfrac{\pi}{9}) \approx 0.3025345781. \end{aligned} \tag{3.13}$$

The case of γ_1 appears in the literature as the Crouzeix-Raviart scheme [13].

3.4. An alternative representation of DIRK schemes.

Let us finish the general discussion about DIRK schemes with an alternative representation of the solution at the next time step as an extrapolation. This will be useful when deriving discrete energy-balance laws.

Proposition 3.6 (extrapolation). *Assume that the RK scheme with tableau* (3.1) *is such that* $\mathbf{A}$ *is invertible. Then* u_{n+1}*, the solution at the next discrete time, has the following representation*

$$u_{n+1} = \left(1 - \sum_{i=1}^{s} \lambda_i\right) u_n + \sum_{i=1}^{s} \lambda_i v_{n,i},$$

where

$$\lambda_i = \mathbf{b}^\intercal \mathbf{A}^{-1}\mathbf{e}_i,$$

and $\{\mathbf{e}_i\}_{i=1}^s$ *is the canonical basis of* $\mathbb{R}^s$*.*

Proof. For $n \geq 0$ we introduce the notation

$$\mathbf{v}_n = [v_{n,1}, \ldots, v_{n,s}]^\intercal \in \mathbb{R}^s, \qquad \boldsymbol{\mathcal{F}}_n = [\mathcal{F}_{n,1}, \ldots, \mathcal{F}_{n,s}]^\intercal \in \mathbb{R}^s, \qquad \mathbf{1} = [1, \ldots, 1]^\intercal \in \mathbb{R}^s,$$

Therefore, the stages in (3.1) can be rewritten as

$$\mathbf{v}_n = u_n\mathbf{1} + \tau_n \mathbf{A}\boldsymbol{\mathcal{F}}_n \quad \Longleftrightarrow \quad \boldsymbol{\mathcal{F}}_n = \frac{1}{\tau_n}\mathbf{A}^{-1}\left(\mathbf{v}_n - u_n\mathbf{1}\right),$$

where we used that the matrix $\mathbf{A}$ is invertible.

We can then write the solution at the next discrete time as

$$u_{n+1} = u_n + \tau_n \mathbf{b}^\intercal \boldsymbol{\mathcal{F}}_n = \left(1 - \mathbf{b}^\intercal\mathbf{A}^{-1}\mathbf{1}\right) u_n + \mathbf{b}^\intercal \mathbf{A}^{-1}\mathbf{v}_n.$$

Setting

$$\mathbf{b}^\intercal \mathbf{A}^{-1} = [\lambda_1, \ldots, \lambda_s] \in \mathbb{R}_s$$

the result follows. □

4. Discrete energy-balance for two-stage schemes

Here we study discrete energy-balance laws for two-stage schemes. Our main contribution here is to find a class of schemes, which we will call *remarkably stable*, see Definition 4.6, which automatically satisfy a dissipative discrete energy-balance, see Definition 3.4.

4.1. General discrete energy-balance laws.

We begin by specializing Proposition 3.6 for the case of two-stage schemes.

Corollary 4.1 (two-stage extrapolation). *Let the RK scheme* (3.1) *be such that* $s = 2$*,* $\mathbf{A}$ *is lower triangular, and with positive diagonal entries. Then, for all* $n \geq 0$*,*

$$u_{n+1} = (1 - \lambda_1 - \lambda_2)\, u_n + \lambda_1 v_{n,1} + \lambda_2 v_{n,2}, \tag{4.1}$$

with

$$\lambda_1 = \frac{b_1}{a_{11}} - \frac{b_2 a_{21}}{a_{22}a_{11}}, \qquad \lambda_2 = \frac{b_2}{a_{22}}. \tag{4.2}$$

Proof. A direct computation shows that

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{1}{a_{11}} & 0 \\ -\frac{a_{21}}{a_{11}a_{22}} & \frac{1}{a_{22}} \end{bmatrix}, \quad \mathbf{b}^\intercal \mathbf{A}^{-1} = [b_1 \ b_2] \begin{bmatrix} \frac{1}{a_{11}} & 0 \\ -\frac{a_{21}}{a_{11}a_{22}} & \frac{1}{a_{22}} \end{bmatrix} = \begin{bmatrix} \frac{b_1}{a_{11}} - \frac{b_2 a_{21}}{a_{22}a_{11}} \\ \frac{b_2}{a_{22}} \end{bmatrix},$$

as we intended to show. □

Lemma 4.2 (some useful identities)**.** *Let $s = 2$, $N \in \mathbb{N}$, $\mathcal{P}_N$ be any partition of $[0, t_F]$, and $n \in \{0, \dots, N-1\}$. If in* (3.1) *the matrix $\mathbf{A}$ is lower triangular and with positive diagonal entries, then we have*

$$|v_{n,1}|^2 + |v_{n,1} - u_n|^2 - |u_n|^2 = 2a_{11}\tau_n \langle \mathcal{F}_{n,1}, v_{n,1} \rangle, \tag{4.3}$$

$$|v_{n,2}|^2 + |v_{n,2} - v_{n,1}|^2 - |v_{n,1}|^2 = 2\tau_n \left[(a_{21} - a_{11}) \langle \mathcal{F}_{n,1}, v_{n,2} \rangle + a_{22} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle \right], \tag{4.4}$$

$$|v_{n,1}|^2 - (u_n, v_{n,1}) = \tau_n a_{11} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle, \tag{4.5}$$

$$|v_{n,2}|^2 - (u_n, v_{n,2}) = \tau_n \left[a_{21} \langle \mathcal{F}_{n,1}, v_{n,2} \rangle + a_{22} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle \right], \tag{4.6}$$

$$|v_{n,2}|^2 - (v_{n,1}, v_{n,2}) = \tau_n \left[(a_{21} - a_{11}) \langle \mathcal{F}_{n,1}, v_{n,2} \rangle + a_{22} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle \right], \tag{4.7}$$

where $\{u_n, v_{n,1}, v_{n,2}, u_{n+1}\}$ come from (3.2)*.*

Proof. These identities follow from taking duality pairings of each of the stages with suitable functions. Identity (4.3) comes from testing the equation for the first stage with $2v_{n,1}$ and using the well–known polarization identity (1.4). Similarly, identity (4.4) comes from testing the second stage with $2v_{n,2}$. Identity (4.5) comes from testing the first stage with $v_{n,1}$. Similarly, we get (4.6) by testing the second stage with $v_{n,2}$. Finally, we combine the two stages and test the result with $v_{n,2}$ to obtain (4.7). □

We are now in position to prove a precursor to (3.3). Notice that here we are not assuming any order conditions on the entries of the Butcher table.

Theorem 4.3 (discrete energy identity I)**.** *Let $s = 2$, $N \in \mathbb{N}$, $\mathcal{P}_N$ be a partition of $[0, t_F]$, and $n \in \{0, \dots, N-1\}$. If $a_{ii} > 0$ for all $i = \{1, \dots, s\}$, then the solution to* (3.2) *satisfies*

$$\frac{1}{2}|u_{n+1}|^2 + \delta_1 |v_{n,1} - u_n|^2 + \delta_2 |v_{n,2} - v_{n,1}|^2 - \tau_n \left[\nu_{11} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle + \nu_{22} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle \right] = \frac{1}{2}|u_n|^2 + \tau_n \nu_{12} \langle \mathcal{F}_{n,1}, v_{n,2} \rangle, \tag{4.8}$$

where

$$\begin{gathered} \delta_1 = \frac{1}{2}(\lambda_1 + \lambda_2)(2 - \lambda_1 - \lambda_2), \ \delta_2 = \frac{1}{2}\lambda_2(2 - \lambda_2), \ \nu_{11} = a_{11}\left[\lambda_1(1 - \lambda_2) + \lambda_2(2 - \lambda_2) \right], \\ \nu_{22} = a_{22}\lambda_2, \ \nu_{12} = \lambda_2 \left[a_{21} + a_{11}(\lambda_1 + \lambda_2 - 2) \right]. \end{gathered} \tag{4.9}$$

and λ_1, λ_2 where introduced in Corollary 4.1.

Proof. We begin by taking the inner product of the extrapolation identity (4.1) with itself to obtain

$$\begin{aligned} |u_{n+1}|^2 &= (1 - \lambda_1 - \lambda_2)^2 |u_n|^2 + \lambda_1^2 |v_{n,1}|^2 + \lambda_2^2 |v_{n,2}|^2 \\ &\quad + 2\lambda_1 (1 - \lambda_1 - \lambda_2)(u_n, v_{n,1}) + 2\lambda_2 (1 - \lambda_1 - \lambda_2)(u_n, v_{n,2}) + 2\lambda_1\lambda_2 (v_{n,1}, v_{n,2}). \end{aligned}$$

The rest of the proof entails lengthy but trivial computations. One merely has to substitute (4.3)–(4.7) in the previous identity. The reader is encouraged to launch their favorite computer algebra system to verify these computations. □

Remark 4.4 (consistency check)**.** A direct computation shows that $\nu_{11}+\nu_{22}+\nu_{12}=b_1+b_2$. Assuming that the scheme satisfies second order conditions, see Appendix C, we have that $\nu_{11}+\nu_{22}+\nu_{12}=1$.

We now write a precursor to the dissipative energy identity (3.5).

Corollary 4.5 (discrete energy identity II)**.** *The discrete energy-balance law* (4.8) *can be rewritten as*

$$\frac{1}{2}|u_{n+1}|^2+\mathcal{Q}(u_n,v_{n,1},v_{n,2})-\tau_n\nu_1\langle\mathcal{F}_{n,1},v_{n,1}\rangle-\tau_n\nu_2\langle\mathcal{F}_{n,2},v_{n,2}\rangle=\frac{1}{2}|u_n|^2 \tag{4.10}$$

where $\nu_1=\nu_{11}+\nu_{12}$, $\nu_2=\nu_{22}$, *and* $\mathcal{Q}:\mathbb{H}^3\to\mathbb{R}$ *is a quadratic form given by*

$$\mathcal{Q}(u_n,v_{n,1},v_{n,2})=\delta_1|v_{n,1}-u_n|^2+\delta_2|v_{n,2}-v_{n,1}|^2-\frac{\nu_{12}}{a_{11}}(v_{n,1}-u_n,v_{n,2}-v_{n,1}). \tag{4.11}$$

Proof. Exploiting the bilinearity of the duality pairing we have that

$$\nu_{12}\langle\mathcal{F}_{n,1},v_{n,2}\rangle=\nu_{12}\langle\mathcal{F}_{n,1},v_{n,1}\rangle+\nu_{12}\langle\mathcal{F}_{n,1},v_{n,2}-v_{n,1}\rangle.$$

We use this identity to replace the last term on the right hand side of (4.8). After reorganizing the terms we get

$$\begin{aligned}\frac{1}{2}|u_{n+1}|^2+\delta_1|v_{n,1}-u_n|^2+\delta_2|v_{n,2}-v_{n,1}|^2-\tau_n\left[(\nu_{11}+\nu_{12})\langle\mathcal{F}_{n,1},v_{n,1}\rangle+\nu_{22}\langle\mathcal{F}_{n,2},v_{n,2}\rangle\right]&=\\ \frac{1}{2}|u_n|^2+\tau_n\nu_{12}\langle\mathcal{F}_{n,1},v_{n,2}-v_{n,1}\rangle&.\end{aligned} \tag{4.12}$$

Taking the inner product of the first stage of (3.2) with $\nu_{12}(v_{n,2}-v_{n,1})$ we get that

$$\tau_n\nu_{12}\langle\mathcal{F}_{n,1},v_{n,2}-v_{n,1}\rangle=\frac{\nu_{12}}{a_{11}}(v_{n,1}-u_n,v_{n,2}-v_{n,1}).$$

Inserting this identity into the right hand side of (4.12) and reorganizing the terms yields the desired result. ☐

We note that the discrete energy-balance laws (4.8) and (4.10) do not carry much practical value unless the sign of the coefficients is correct, and the quadratic form $\mathcal{Q}$ is nonnegative. However, if this is the case, our schemes will have all requisite stability properties. We encode this in the following definition.

Definition 4.6 (remarkable stability I)**.** We say that the DIRK scheme (3.1) with $s=2$, $\mathbf{A}$ lower triangular and with positive diagonal entries is remarkably stable if the following conditions hold

$$\delta_1\geq 0,\quad \delta_2\geq 0,\quad \nu_1=\nu_{11}+\nu_{12}>0,\quad \nu_2=\nu_{22}>0,$$

with δ_1, δ_2, ν_{11}, ν_{22}, and ν_{12} defined in (4.9), and the quadratic form $\mathcal{Q}$, introduced in (4.11), is nonnegative definite.

Remarkable stability defines an exceptional class of schemes for which the off-diagonal term $\langle\mathcal{F}_{n,1},v_{n,2}\rangle$ on the right hand side of (4.8) can always be absorbed into artificial damping terms regardless of the nature of $\mathcal{F}$ (coercive, linear, nonlinear, degenerate, skew symmetric, etc.).

The following result provides sufficient, easy to check, conditions for $\mathcal{Q}$ to be nonnegative.

Proposition 4.7 (nonnegativity)**.** *Assume that, in the setting of Corollary 4.5, we have*

$$\delta_1\geq 0,\qquad \delta_2\geq 0,\qquad \left|\frac{\nu_{12}}{a_{11}}\right|\leq 2\sqrt{\delta_1}\sqrt{\delta_2}.$$

Then, the quadratic from $\mathcal{Q}$, *introduced in* (4.11) *in nonnegative definite.*

Proof. If $\delta_1 \geq 0$ and $\delta_2 \geq 0$ we have that

$$\delta_1|v_{n,1} - u_n|^2 \pm 2\sqrt{\delta_1}\sqrt{\delta_2}(v_{n,1} - u_n, v_{n,2} - v_{n,1}) + \delta_2|v_{n,2} - v_{n,1}|^2 \geq 0.$$

Therefore,

$$\pm 2\sqrt{\delta_1}\sqrt{\delta_2}(v_{n,1} - u_n, v_{n,2} - v_{n,1}) \leq \delta_1|v_{n,1} - u_n|^2 + \delta_2|v_{n,2} - v_{n,1}|^2.$$

This, in particular, implies that

$$\beta(v_{n,1} - u_n, v_{n,2} - v_{n,1}) \leq \delta_1|v_{n,1} - u_n|^2 + \delta_2|v_{n,2} - v_{n,1}|^2,$$

for all $\beta \in \mathbb{R}$ satisfying $|\beta| \leq 2\sqrt{\delta_1}\sqrt{\delta_2}$. □

Remark 4.8 (nonnegativity)**.** We comment that the condition of Proposition 4.7 is only sufficient. Necessary and sufficient conditions are obtained by looking at the spectrum of the coefficient matrix of the quadratic form $\mathcal{Q}$. In this case we have

$$\mathbf{Q} = \begin{bmatrix} \delta_1 & -\delta_1 - \frac{\nu_{12}}{a_{11}} & \frac{\nu_{12}}{a_{11}} \\ -\delta_1 - \frac{\nu_{12}}{a_{11}} & \delta_1 + \delta_2 + \frac{2\nu_{12}}{a_{11}} & -\delta_2 - \frac{\nu_{12}}{a_{11}} \\ \frac{\nu_{12}}{a_{11}} & -\delta_2 - \frac{\nu_{12}}{a_{11}} & \delta_2 \end{bmatrix}.$$

Lengthy and painful, but trivial, computations reveal that

$$\sigma(\mathbf{Q}) = \left\{ 0, \delta_1 + \delta_2 + \frac{\nu_{12}}{2a_{11}} \pm \sqrt{\delta_1^2 - \delta_1\delta_2 + \delta_2^2 + (\delta_1 + \delta_2)\frac{\nu_{12}}{a_{11}} + \left(\frac{\nu_{12}}{a_{11}}\right)^2} \right\}.$$

Remark 4.9 (computational aspects)**.** Two important aspects of computational practice are time-adaptivity and nonlinear solver tolerances. Assume that we are using a remarkably stable scheme and that we are able to solve for the stages $\{v_{n,1}, v_{n,2}\}$ exactly (i.e., to machine accuracy). As a consequence, we obtain

$$\frac{1}{2}\left(|u_{n+1}|^2 - |u_n|^2\right) - \tau_n\nu_1\langle\mathcal{F}_{n,1}, v_{n,1}\rangle - \tau_n\nu_2\langle\mathcal{F}_{n,2}, v_{n,2}\rangle = -\mathcal{Q}(u_n, v_{n,1}, v_{n,2}) \leq 0.$$

We note that the functional $\mathcal{Q}(u_n, v_{n,1}, v_{n,2})$ gives us exactly how much numerical dissipation occurred from time instance t_n to t_{n+1}. In this context, the value of the quadratic form $\mathcal{Q}(u_n, v_{n,1}, v_{n,2})$ may be used as the foundation for the development of an heuristic error indicator in order to drive a time-adaptive process. We note that using numerical dissipation as an a posteriori estimator in order to select the timestep size is not a new idea, see for instance [42, Remark 3.4] and references therein.

However, in the previous paragraph, we made a very strong assumption: we can solve the nonlinear problems at each stage "exactly", which is rarely ever true. In that such context, we may not be able to use $\mathcal{Q}$ in order to quantify numerical dissipation. Let $\{\tilde{v}_{n,1}, \tilde{v}_{n,2}, \tilde{u}_{n+1}\}$ represent our "inexact approximations" of the first stage $v_{n,1}$, second stage $v_{n,2}$ and final solution u_{n+1} respectively, then we can always define the functional

$$\eta(\tilde{v}_{n,1}, \tilde{v}_{n,2}, \tilde{u}_{n+1}) = \frac{1}{2}\left(|\tilde{u}_{n+1}|^2 - |u_n|^2\right) - \tau_n\nu_1\langle\tilde{\mathcal{F}}_{n,1}, \tilde{v}_{n,1}\rangle - \tau_n\nu_2\langle\tilde{\mathcal{F}}_{n,2}, \tilde{v}_{n,2}\rangle,$$

where, for $i = 1, 2$, $\tilde{\mathcal{F}}_{n,i}$ has the expected meaning. Indeed, if η is sufficiently negative, we may argue that the scheme implementation exhibits numerically dissipative behavior. Otherwise, the numerical tolerances and/or the timestep need to be reduced, and the whole time-step should be solved again.

4.2. **Examples of two-stage remarkably stable schemes.** Let us now explore whether the schemes of Section 3.3.1 are remarkably stable.

4.2.1. *The Butcher-Burrage DIRK22 scheme.* We consider the two-stage scheme with tableau given in (3.8). Using formulas (4.2) and (4.9), for the case of γ_1 we get

$$\lambda_1 = -\tfrac{\sqrt{2}}{2}\,,\ \lambda_2 = 1 + \tfrac{\sqrt{2}}{2}\,,\ \delta_1 = \tfrac{1}{2}\,,\ \delta_2 = \tfrac{1}{4}\,,\ \nu_{11} = 1 - \tfrac{\sqrt{2}}{2}\,,\ \nu_{22} = \tfrac{1}{2}\,,\ \nu_{12} = -\tfrac{1}{2} + \tfrac{\sqrt{2}}{2}\,,$$

which leads to the following properties

$$\nu_1 = \tfrac{1}{2}\ ,\quad \nu_2 = \tfrac{1}{2}\ ,\quad \tfrac{\nu_{12}}{a_{11}} = \tfrac{\sqrt{2}}{2}\ ,\quad 2\sqrt{\delta_1}\sqrt{\delta_2} = \tfrac{\sqrt{2}}{2}\,.$$

We conclude that Butcher-Burrage scheme (3.8) is remarkably-stable for the case of γ_1. For the case of γ_2 we obtain:

$$\lambda_1 = \tfrac{\sqrt{2}}{2}\,,\ \lambda_2 = 1 - \tfrac{\sqrt{2}}{2}\,,\ \delta_1 = \tfrac{1}{2}\,,\ \delta_2 = \tfrac{1}{4}\,,\ \nu_{11} = \tfrac{\sqrt{2}}{2} + 1\,,\ \nu_{22} = \tfrac{1}{2}\,,\ \nu_{12} = -\tfrac{\sqrt{2}}{2} - \tfrac{1}{2}\,,$$

leading to:

$$\nu_1 = \tfrac{1}{2}\ ,\quad \nu_2 = \tfrac{1}{2}\ ,\quad \tfrac{\nu_{12}}{a_{11}} = -\tfrac{\sqrt{2}}{2}\ ,\quad 2\sqrt{\delta_1}\sqrt{\delta_2} = \tfrac{\sqrt{2}}{2}\,.$$

We conclude that Butcher-Burrage scheme is remarkably stable for the case of γ_2 as well.

4.2.2. *The Crouzeix DIRK23 scheme.* We consider the two-stage scheme with tableau described in (3.10). Using formulas (4.2) and (4.9) we get

$$\lambda_1 = \tfrac{3\sqrt{3}}{2} - \tfrac{3}{2}\,,\ \lambda_2 = \tfrac{3}{2} - \tfrac{\sqrt{3}}{2}\,,\ \delta_1 = \sqrt{3} - \tfrac{3}{2}\,,\ \delta_2 = \tfrac{\sqrt{3}}{4}\,,\ \nu_{11} = 1\,,\ \nu_{22} = \tfrac{1}{2}\,,\ \nu_{12} = -\tfrac{1}{2}\,,$$

which leads to the following values

$$\nu_1 = \tfrac{1}{2}\,,\quad \nu_2 = \tfrac{1}{2}\,,\quad \tfrac{\nu_{12}}{a_{11}} = \tfrac{\sqrt{3}}{2} - \tfrac{3}{2}\ ,\quad 2\sqrt{\delta_1}\sqrt{\delta_2} = \tfrac{3}{2} - \tfrac{\sqrt{3}}{2}\,,$$

which allows us to conclude that the Crouzeix DIRK23 scheme (3.10) is remarkably stable.

Remark 4.10 (quadrature)**.** We note that the pair of collocation points $\{c_1, c_2\}$ and weights $\{\nu_1, \nu_2\}$ associated to the Crouzeix DIRK23 scheme define a quadrature rule on the interval $[0, 1]$ that is exact for polynomials of degree at most three. This might facilitate the derivation of the "equation satisfied by the error" and the development of an a priori error analysis without the need of defining a quadratic in time piecewise polynomial reconstruction.

4.2.3. *Alexander's DIRK22 scheme.* We consider the two-stage scheme with tableau described in (3.7). Note that in this case $b_1 = a_{21}$ and $b_2 = a_{22}$. Using formulas (4.2) and (4.9) we get

$$\lambda_1 = 0\,,\ \lambda_2 = 1\,,\ \delta_1 = \tfrac{1}{2}\,,\ \delta_2 = \tfrac{1}{2}\,,\ \nu_{11} = 1 - \tfrac{\sqrt{2}}{2}\,,\ \nu_{22} = 1 - \tfrac{\sqrt{2}}{2}\,,\ \nu_{12} = \sqrt{2} - 1\,,$$

which leads to the following properties

$$\nu_1 = \tfrac{\sqrt{2}}{2}\,,\ \nu_2 = 1 - \tfrac{\sqrt{2}}{2}\,,\quad \sigma(\mathbf{Q}) = \left\{0, \frac{1-\sqrt{2}}{2}, \frac{3(1+\sqrt{2})}{2}\right\} \approx \{0., -0.2017107, 3.62132\}.$$

This allows us to conclude that Alexander's DIRK22 scheme (3.7) is **not** remarkably stable.

We comment that, in principle, the fact that a DIRK scheme is not remarkably-stable does not mean that it should not be used. As detailed in Appendix B, if a scheme is not remarkably stable it is, in principle, not possible to guarantee energy-stability if the operator $\mathcal{A}$ is skew-symmetric (i.e. $\langle \mathcal{A}(u), v\rangle = -\langle \mathcal{A}(v), u\rangle$). For this reason, if a scheme is not remarkably stable, its utility may be limited to linear, coercive, self-adjoint problems; see, again, Appendix B.

4.2.4. *Kraaijevanger-Spijker's DIRK22 scheme.* We consider the two-stage scheme with tableau described in (3.9). Using formulas (4.2) and (4.9) we get

$$\lambda_1 = -\tfrac{1}{4}\,,\ \lambda_2 = \tfrac{3}{4}\,,\ \delta_1 = \tfrac{3}{8}\,,\ \delta_2 = \tfrac{15}{32}\,,\ \nu_{11} = \tfrac{7}{16}\,,\ \nu_{22} = \tfrac{3}{2}\,,\ \nu_{12} = \ -\tfrac{15}{16}\,,$$

which leads to the following properties

$$\nu_1 = -\tfrac{1}{2}\,,\ \nu_2 = \tfrac{3}{2}\,.$$

This allows us to conclude DIRK22 scheme (3.9) is **not** remarkably stable. Regardless of the sign of $\mathcal{Q}$, the coefficient ν_1 is negative. For these reasons, the applicability of such scheme to evolutionary PDEs, even in the case of linear, positive, and symmetric operators, is rather limited.

5. Three-stage schemes

The goal of this section is similar to that of the previous one, that is, we will introduce a class of *remarkably stable* DIRK schemes, see Definition 5.6, that satisfy a dissipative discrete energy-balance. Conceptually, this section is no different than the previous one. The logical steps to achieve our goal are exactly the same. The algebraic manipulations, however, are more involved and tedious. We urge the reader to take advantage of a computer algebra system.

5.1. **General discrete energy-balance laws.** We, once again, specialize Proposition 3.6 to the case of a three-stage DIRK.

Corollary 5.1 (three-stage extrapolation)**.** *Let the RK scheme* (3.1) *be such that $s = 3$,* $\mathbf{A}$ *is lower triangular, and with positive diagonal entries. Then, for all $n \geq 0$,*

$$u_{n+1} = (1 - \lambda_1 - \lambda_2 - \lambda_3)\, u_n + \lambda_1 v_{n,1} + \lambda_2 v_{n,2} + \lambda_3 v_{n,3}, \tag{5.1}$$

with

$$\lambda_1 = \frac{b_1}{a_{11}} - \frac{b_2 a_{21}}{a_{11}a_{22}} - \frac{b_3 a_{31}}{a_{11}a_{33}} + \frac{b_3 a_{32} a_{21}}{a_{11}a_{22}a_{33}}, \quad \lambda_2 = \frac{b_2}{a_{22}} - \frac{b_3 a_{32}}{a_{22}a_{33}}, \quad \lambda_3 = \frac{b_3}{a_{33}}. \tag{5.2}$$

Proof. It follows from a direct computation. The fact that $\mathbf{A}$ is lower triangular simplifies these. ☐

Next we obtain some more useful identities.

Lemma 5.2 (more useful identities)**.** *Let $s = 3$. For any $N \in \mathbb{N}$, any partition $\mathcal{P}_N$, and all $n \in \{0, \ldots, N-1\}$ we have that $\{u_n, v_{n,1}, v_{n,2}, v_{n,3}, u_{n+1}\}$, coming from* (3.2) *with $a_{ii} > 0$, satisfy* (4.3)—(4.7)*, and, additionally,*

$$\frac{1}{2}\left(|v_{n,3}|^2 + |v_{n,3} - v_{n,2}|^2 - |v_{n,2}|^2\right) = \tau_n \left[(a_{31} - a_{21})\langle \mathcal{F}_{n,1}, v_{n,3}\rangle + (a_{32} - a_{22})\langle \mathcal{F}_{n,2}, v_{n,3}\rangle + a_{33}\langle \mathcal{F}_{n,3}, v_{n,3}\rangle\right], \tag{5.3}$$

$$|v_{n,3}|^2 - (u_n, v_{n,3}) = \tau_n \left[a_{31}\langle \mathcal{F}_{n,1}, v_{n,3}\rangle + a_{32}\langle \mathcal{F}_{n,2}, v_{n,3}\rangle + a_{33}\langle \mathcal{F}_{n,3}, v_{n,3}\rangle\right], \tag{5.4}$$

$$|v_{n,3}|^2 - (v_{n,2}, v_{n,3}) = \tau_n \left[(a_{31} - a_{21})\langle \mathcal{F}_{n,1}, v_{n,3}\rangle + (a_{32} - a_{22})\langle \mathcal{F}_{n,2}, v_{n,3}\rangle + a_{33}\langle \mathcal{F}_{n,3}, v_{n,3}\rangle\right], \tag{5.5}$$

$$|v_{n,3}|^2 - (v_{n,1}, v_{n,3}) = \tau_n \left[(a_{31} - a_{11})\langle \mathcal{F}_{n,1}, v_{n,3}\rangle + a_{32}\langle \mathcal{F}_{n,2}, v_{n,3}\rangle + a_{33}\langle \mathcal{F}_{n,3}, v_{n,3}\rangle\right], \tag{5.6}$$

Proof. We, first of all, note that owing to the fact that we are dealing with a DIRK scheme we can compute sequentially the states. Therefore, identities (4.3)—(4.7) remain to hold. The new identities can be obtained as before. Identity (5.3) comes from testing the third stage by $v_{n,3}$ and applying the polarization identity (1.4). Identity (5.4) comes from testing the third stage by $v_{n,3}$. Identity (5.5) comes from testing the third stage by $v_{n,2}$. Combining the first and third stage, and testing the result with $v_{n,3}$ gives (5.6). ☐

With these identities at hand we can prove an analogue of (4.8) for the case $s = 3$.

Theorem 5.3 (discrete energy identity I)**.** *Let $s = 3$. For any $N \in \mathbb{N}$, any partition $\mathcal{P}_N$, and any $n \in \{0, \dots, N-1\}$ we have that the solution of* (3.2)*, with $a_{ii} > 0$, satisfies*

$$\frac{1}{2}|u_{n+1}|^2 + \sum_{i=1}^{3} \delta_i |v_{n,i} - v_{n,i-1}|^2 - \tau_n \sum_{i=1}^{3} \nu_{ii} \langle \mathcal{F}_{n,i}, v_{n,i} \rangle = \frac{1}{2}|u_n|^2 + \tau_n \left[\nu_{12} \langle \mathcal{F}_{n,1}, v_{n,2} \rangle + \nu_{13} \langle \mathcal{F}_{n,1}, v_{n,3} \rangle + \nu_{23} \langle \mathcal{F}_{n,2}, v_{n,3} \rangle \right], \tag{5.7}$$

where $v_{n,0} = u_n$,

$$\begin{aligned}
\delta_1 &= \frac{1}{2}(\lambda_1 + \lambda_2 + \lambda_3)(2 - \lambda_1 - \lambda_2 - \lambda_3), \\
\delta_2 &= \frac{1}{2}(\lambda_2 + \lambda_3)(2 - \lambda_2 - \lambda_3), \\
\delta_3 &= \frac{1}{2}\lambda_3(2 - \lambda_3), \\
\nu_{11} &= a_{11}(\lambda_1(1 - \lambda_2 - \lambda_3) + (2 - \lambda_2 - \lambda_3)(\lambda_2 + \lambda_3)), \\
\nu_{22} &= a_{22}(\lambda_2(1 - \lambda_3) + (2 - \lambda_3)\lambda_3), \\
\nu_{33} &= a_{33}\lambda_3, \\
\nu_{12} &= [a_{21}(\lambda_2(1 - \lambda_3) + (2 - \lambda_3)\lambda_3) + a_{11}(\lambda_2(-2 + \lambda_1 + \lambda_2) + 2(-1 + \lambda_2)\lambda_3 + \lambda_3^2)], \\
\nu_{13} &= \lambda_3(a_{31} + a_{11}\lambda_1 + a_{21}(-2 + \lambda_2 + \lambda_3)), \\
\nu_{23} &= \lambda_3(a_{32} + a_{22}(-2 + \lambda_2 + \lambda_3)),
\end{aligned} \tag{5.8}$$

and $\lambda_1, \lambda_2, \lambda_3$ were defined in Corollary 5.1.

Proof. We once again invite the reader to launch their favorite computer algebra software, as the proof of this result merely entails lengthy and tortuous, but trivial, computations. One merely has to take the inner product of the extrapolation identity of Corollary 5.1 with itself, and use in the result identities (4.3)—(4.7) and (5.3)—(5.6). ☐

Remark 5.4 (consistency check)**.** Direct computation shows that $\nu_{11} + \nu_{22} + \nu_{33} + \nu_{12} + \nu_{13} + \nu_{23} = b_1 + b_2 + b_3$. Assuming that the scheme satisfies second-order conditions, see Appendix C, we have that $\nu_{11} + \nu_{22} + \nu_{33} + \nu_{12} + \nu_{13} + \nu_{23} = 1$.

As we did in the previous section for the case of two-stage schemes, we rewrite (5.7) in a form that will resemble a dissipative discrete energy law.

Corollary 5.5 (discrete energy identity II)**.** *The discrete energy identity* (5.7) *can be rewritten as*

$$\frac{1}{2}|u_{n+1}|^2 + \mathcal{Q}(u_n, v_{n,1}, v_{n,2}, v_{n,3}) - \tau_n \sum_{i=1}^{3} \nu_i \langle \mathcal{F}_{n,i}, v_{n,i} \rangle = \frac{1}{2}|u_n|^2, \tag{5.9}$$

where, for $i = 1, \dots, 3$,

$$\nu_i = \nu_{ii} + \sum_{j=i+1}^{3} \nu_{ij}, \tag{5.10}$$

the quadratic form $\mathcal{Q}$ is given by

$$
\begin{aligned}
\mathcal{Q}(u_n, v_{n,1}, v_{n,2}, v_{n,3}) = {} & \delta_1 |v_{n,1} - u_n|^2 + \delta_2 |v_{n,2} - v_{n,1}|^2 + \delta_3 |v_{n,3} - v_{n,2}|^2 \\
& - \frac{\nu_{12}}{a_{11}} (v_{n,1} - u_n, v_{n,2} - v_{n,1}) \\
& - \frac{\nu_{13}}{a_{11}} (v_{n,1} - u_n, v_{n,3} - v_{n,1}) - \frac{\nu_{23}}{a_{22}} (v_{n,2} - u_n, v_{n,3} - v_{n,2}) \\
& + \frac{\nu_{23} a_{21}}{a_{11} a_{22}} (v_{n,1} - u_n, v_{n,3} - v_{n,2}),
\end{aligned} \tag{5.11}
$$

and δ_1, δ_2, δ_3, ν_{11}, ν_{22}, ν_{33}, ν_{12}, ν_{13} and ν_{23} are defined in (5.8).

Proof. We follow the ideas that led to (4.10) in the case of two stage schemes. We exploit the fact that the matrix $\mathbf{A}$ is lower triangular, together with the bilinearity of the duality pairing to get, using the equations of the stages,

$$
\begin{aligned}
\tau_n \nu_{12} \langle \mathcal{F}_{n,1}, v_{n,2} \rangle &= \tau_n \nu_{12} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle + \tau_n \nu_{12} \langle \mathcal{F}_{n,1}, v_{n,2} - v_{n,1} \rangle \\
&= \tau_n \nu_{12} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle + \frac{\nu_{12}}{a_{11}} (v_{n,1} - u_n, v_{n,2} - v_{n,1}), \\
\tau_n \nu_{13} \langle \mathcal{F}_{n,1}, v_{n,3} \rangle &= \tau_n \nu_{13} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle + \tau_n \nu_{13} \langle \mathcal{F}_{n,1}, v_{n,3} - v_{n,1} \rangle \\
&= \tau_n \nu_{13} \langle \mathcal{F}_{n,1}, v_{n,1} \rangle + \frac{\nu_{13}}{a_{11}} (v_{n,1} - u_n, v_{n,3} - v_{n,1}), \\
\tau_n \nu_{23} \langle \mathcal{F}_{n,2}, v_{n,3} \rangle &= \tau_n \nu_{23} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle + \tau_n \nu_{23} \langle \mathcal{F}_{n,2}, v_{n,3} - v_{n,2} \rangle \\
&= \tau_n \nu_{23} \langle \mathcal{F}_{n,2}, v_{n,2} \rangle + \frac{\nu_{23}}{a_{22}} (v_{n,2} - u_n, v_{n,3} - v_{n,2}) - \frac{a_{21} \nu_{23}}{a_{11} a_{22}} (v_{n,1} - u_n, v_{n,3} - v_{n,2}).
\end{aligned}
$$

We use the previous identities in order to rewrite the energy identity (5.7) as follows

$$
\begin{aligned}
\frac{1}{2} |u_{n+1}|^2 + \sum_{i=1}^{3} \left(\delta_i |v_{n,i} - v_{n,i-1}|^2 - \tau_n \left(\nu_{ii} + \sum_{j=i+1}^{3} \nu_{ij} \right) \langle \mathcal{F}_{n,i}, v_{n,i} \rangle \right) &= \frac{1}{2} |u_n|^2 \\
+ \frac{\nu_{12}}{a_{11}} (v_{n,1} - u_n, v_{n,2} - v_{n,1}) + \frac{\nu_{13}}{a_{11}} (v_{n,1} - u_n, v_{n,3} - v_{n,1}) & \\
+ \frac{\nu_{23}}{a_{22}} (v_{n,2} - u_n, v_{n,3} - v_{n,2}) - \frac{a_{21} \nu_{23}}{a_{11} a_{22}} (v_{n,1} - u_n, v_{n,3} - v_{n,2}). &
\end{aligned} \tag{5.12}
$$

Finally, identity (5.9) follows by reorganizing the terms in (5.12). ☐

Once again, the practical value of identity (5.9) rests on the quadratic form $\mathcal{Q}$, and whether or not it is nonnegative definite. As in the case of two-stage schemes, we introduce the notion of remarkably stable three-stage schemes.

Definition 5.6 (remarkable stability)**.** We will say that the DIRK scheme (3.1) with $s = 3$, $\mathbf{A}$ lower triangular, and with positive diagonal entries is remarkably stable if

$$
\delta_1 \geq 0, \quad \delta_2 \geq 0, \quad \delta_3 \geq 0, \quad \nu_1 > 0, \quad \nu_2 > 0, \quad \nu_3 > 0,
$$

where these coefficients were defined in (5.8) and (5.10), and, in addition, the quadratic form $\mathcal{Q}$, defined in (5.11), is nonnegative definite.

Remark 5.7 (nonnegativity)**.** Since $\mathcal{Q}$, as defined in (5.11), can always be expanded in terms of its monomial coefficients, the nonnegativity of the quadratic form $\mathcal{Q}$ can be verified by examining the eigenvalues of the corresponding coefficient matrix $\mathbf{Q} = [q_{ij}]_{i,j=1}^4$, which read

$$q_{11} = \delta_1, \qquad q_{12} = q_{21} = -\delta_1 - \frac{\nu_{12}}{a_{11}} - \frac{\nu_{13}}{a_{11}},$$
$$q_{13} = q_{31} = \frac{\nu_{12}}{a_{11}} - \frac{\nu_{23}}{a_{22}} + \frac{a_{21}\nu_{23}}{a_{11}a_{22}}, \qquad q_{14} = q_{41} = \frac{\nu_{13}}{a_{11}} + \frac{\nu_{23}}{a_{22}} - \frac{a_{21}\nu_{23}}{a_{11}a_{22}},$$
$$q_{22} = \delta_1 + \delta_2 + \frac{2\nu_{12}}{a_{11}} + \frac{2\nu_{13}}{a_{11}}, \qquad q_{23} = q_{32} = -\delta_2 - \frac{\nu_{12}}{a_{11}} - \frac{a_{21}\nu_{23}}{a_{11}a_{22}},$$
$$q_{24} = q_{42} = -\frac{\nu_{13}}{a_{11}} + \frac{a_{21}\nu_{23}}{a_{11}a_{22}}, \qquad q_{33} = \delta_2 + \delta_3 + \frac{2\nu_{23}}{a_{22}},$$
$$q_{34} = q_{43} = -\delta_3 - \frac{\nu_{23}}{a_{22}}, \qquad q_{44} = \delta_2.$$

5.2. **Examples of three-stage remarkably stable schemes.** Let us now investigate the schemes of Section 3.3.2 for remarkable stability.

5.2.1. *Crouzeix-Raviart DIRK34 scheme.* We consider the scheme described by tableau (3.12) with γ_1 as defined in (3.13), also known as the Crouzeix-Raviart scheme. In this case we have that (with 20 digits of accuracy for the sake of computational utility):

$$[\lambda_1, \lambda_2, \lambda_3] \approx [0.44562240728771388189, 1.0641777724759121408, 0.12061475842818323189]$$
$$[\delta_1, \delta_2, \delta_3] \approx [0.30128850285230865863, 0.48292586026102947830, 0.11334079845283873290]$$
$$[\nu_{11}, \nu_{22}, \nu_{33}] \approx [0.94409386961162504966, 1.2422271989685591552, 0.12888640051572042236]$$
$$[\nu_{12}, \nu_{13}, \nu_{23}] \approx [-1.1863210685801842049, 0.37111359948427957763, -0.5]$$

which leads to:

$$\nu_1 \approx 0.12888, \quad \nu_2 \approx 0.74222, \quad \nu_3 \approx 0.12888.$$

Up to 20 digits of accuracy we find that the eigenvalues of the matrix $\mathbf{Q}$ are approximately

$$\{0.564309, 0, 0, 0\},$$

hinting at the fact that $\mathcal{Q}$ is nonnegative definite. A reduction to row echelon form of this matrix gives us that it has exactly three rows that consist only of zeros. This means this matrix has three zero eigenvalues, and the scheme is remarkably stable.

To conclude with this example, we mention that neither the case of γ_2 nor γ_3, defined in (3.13), lead to remarkably stable schemes. In particular, they lead to $\delta_1, \delta_2, \delta_3 < 0$.

5.2.2. *Alexander's DIRK33 scheme.* We consider the scheme described by tableau (3.11). In this context we have:

$$[\lambda_1, \lambda_2, \lambda_3] \approx [0, 0, 1]$$
$$[\delta_1, \delta_2, \delta_3] \approx [0.5, 0.5, 0.5]$$
$$[\nu_{11}, \nu_{22}, \nu_{33}] \approx [0.435866, 0.435866, 0.435866]$$
$$[\nu_{12}, \nu_{13}, \nu_{23}] \approx [-0.153799, 0.926429, -1.080229]$$

leading to

$$\nu_1 \approx 1.2084966\ ,\ \nu_2 \approx -0.644363 \text{ and } \nu_3 \approx 0.43586652\,.$$

We conclude that, regardless of the spectrum of $\mathbf{Q}$, Alexander's DIRK33 scheme is **not** remarkably stable. Just like Alexander's DIRK22 scheme, defined in tableau (3.7) and considered in section 4.2.3, Alexander's DIRK33 scheme is not unconditionally stable for skew-symmetric problems. We delve into these details in Appendix B.

6. Bochner-type norm estimates

In this section we introduce a more stringent set of assumptions on the mapping $\mathcal{A}$. These will be invoked if we wish to prove a priori bounds in the Bochner-type norm $L^p(0,t_F;\mathbb{V})$, for some $p>1$, on the solution of (1.1). These assumptions, in addition, will allow us to obtain a priori bounds for the time derivative of the solution in the Bochner-type norm $L^{q'}(0,t_F;\mathbb{V}^*)$ for some $q>1$. These two estimates are enough to establish compactness of the family of approximate solutions via the well-celebrated Aubin-Lions compactness lemma.

Lemma 6.1 (Aubin-Lions)**.** *Let $\mathbb{X}$, $\mathbb{Y}$ and $\mathbb{Z}$ be three Banach spaces such that $\mathbb{X}\subseteq\mathbb{Y}\subseteq\mathbb{Z}$. Assume that $\mathbb{X}$ is compactly embedded in $\mathbb{Y}$, and $\mathbb{Y}$ is continuously embedded in $\mathbb{Z}$. Then, for $1\le p,q\le+\infty$ we define*

$$\mathbb{U}=\left\{u\in L^p(0,t_F;\mathbb{X})\ \middle|\ \frac{\mathrm{d}u}{\mathrm{d}t}\in L^{q'}(0,t_F;\mathbb{Z})\right\}.$$

Then

- *If $p<+\infty$ the embedding of $\mathbb{U}$ into $L^p(0,t_F;\mathbb{Y})$ is compact.*
- *If $p=+\infty$ and $q<\infty$ the embedding of $\mathbb{U}$ into $\mathcal{C}([0,t_F];\mathbb{Y})$ is compact.*

Remark 6.2 (references)**.** The origins of Lemma 6.1 go back to [6, 40]. This result has been extended, improved, and reviewed several times; see [53, 4, 17, 27, 11, 3] and references therein. In particular, we note that in practice it is very difficult to obtain estimates for the discrete time derivative. Therefore, there have been major efforts in order to replace bounds on the derivative by some form of equicontinuity, or uniform modulus continuity in Bochner-type norms.

Let us now state the additional set of assumptions we shall impose on $\mathcal{A}$. These are lower bounds and growth conditions for $\langle\mathcal{A}(w),w\rangle$. More precisely, we will assume that:

- p–coercivity: There exist $p>1$ and $C_1>0$ such that[4]

$$\langle\mathcal{A}(w),w\rangle\ge C_1\|w\|^p,\quad\forall w\in\mathbb{V}. \tag{6.1}$$

- q–growth: There exist $q\ge p$ and an increasing function $C_3:\mathbb{R}\to\mathbb{R}$ for which[5]

$$\|\mathcal{A}(w)\|_*\le C_3(|w|)\|w\|^{p/q'},\quad\forall w\in\mathbb{V}. \tag{6.2}$$

We highlight that conditions (6.1) and (6.2) indeed do appear in a large class of problems of mathematical and technical interest; see Appendix A.

Notice that our assumptions allow us to obtain a priori estimates on the solution and its derivative.

Proposition 6.3 (a priori estimates)**.** *Assume that $f\in L^{p'}(0,t_F;\mathbb{V}^*)$. If $\mathcal{A}$ satisfies* (6.1)*, then we have that the solution to* (1.1) *satisfies*

$$\frac{1}{2}\|u\|^2_{L^\infty(0,t_F;\mathbb{H})}+\frac{C_1}{p'}\|u\|^p_{L^p(0,t_F;\mathbb{V})}\le\frac{1}{2}|u_0|^2+\frac{1}{p'C_1^{1/(p-1)}}\|f\|^{p'}_{L^{p'}(0,t_F;\mathbb{V}')}. \tag{6.3}$$

If, in addition, $\mathcal{A}$ satisfies (6.2) *we also have*

$$\left\|\frac{\mathrm{d}u}{\mathrm{d}t}\right\|^{q'}_{L^{q'}(0,t_F;\mathbb{V}^*)}\lesssim|u_0|^2+\|f\|^{p'}_{L^{p'}(0,t_F;\mathbb{V}')}. \tag{6.4}$$

[4]This can be generalized, with $C_2>0$, to the case

$$\langle\mathcal{A}(w),w\rangle\ge C_1\|w\|^p-C_2|w|^2,$$

but this will inevitably lead to conditional stability in our schemes, or to the need of Grönwall inequalities.

[5]This can also be generalized to have lower order terms.

Proof. We recall that, in this setting, equation (1.1) must be understood in $\mathbb{V}^*$ for *a.e.* $t \in (0,T)$. We apply said functional to $u(t)$ and obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|u(t)|^2 + C_1\|u(t)\|^p \leq \left\langle \frac{\mathrm{d}u(t)}{\mathrm{d}t}, u(t) \right\rangle + \langle \mathcal{A}(u(t)), u(t)\rangle = \langle f(t), u(t)\rangle \leq \frac{1}{p'\varepsilon^{p'}}\|f(t)\|_*^{p'} + \frac{\varepsilon^p}{p}\|u(t)\|^p,$$

where the lower bound is obtained using the coercivity condition (6.1), and the upper bound is obtained using Young's inequality. Integrating we can conclude that

$$\frac{1}{2}\|u\|^2_{L^\infty(0,t_F;\mathbb{H})} + \left(C_1 - \frac{\varepsilon^p}{p}\right)\|u\|^p_{L^p(0,t_F;\mathbb{V})} \leq \frac{1}{2}|u_0|^2 + \frac{1}{p'\varepsilon^{p'}}\|f\|^{p'}_{L^{p'}(0,t_F;\mathbb{V}^*)}.$$

A suitable choice of $\varepsilon > 0$ then shows (6.3).

On the other hand, by definition, we have

$$\begin{aligned}\left\|\frac{\mathrm{d}u(t)}{\mathrm{d}t}\right\|_* &= \sup_{0\neq w\in\mathbb{V}} \frac{\langle \frac{\mathrm{d}u(t)}{\mathrm{d}t}, w\rangle}{\|w\|} = \sup_{0\neq w\in\mathbb{V}} \frac{\langle f(t) - \mathcal{A}(u(t)), w\rangle}{\|w\|} \\ &\leq \|f(t)\|_* + \|\mathcal{A}(u(t))\|_* \leq \|f(t)\|_* + C_3(|u(t)|)\|u(t)\|^{p/q'}.\end{aligned}$$

where in the last step we used the q–growth condition. Notice now that, the uniform $L^\infty(0,t_F;\mathbb{H})$ estimate on u, and the fact that C_3 is increasing, imply that

$$\sup_{t\in[0,t_F]} C_3(|u(t)|) \leq \bar{C}_3 < \infty.$$

Thus, raising to power q' the previous estimate and integrating we get

$$\left\|\frac{\mathrm{d}u}{\mathrm{d}t}\right\|^{q'}_{L^{q'}(0,t_F;\mathbb{V}^*)} \lesssim \|f\|^{q'}_{L^{q'}(0,t_F;\mathbb{V}^*)} + \|u(t)\|^p_{L^p(0,t_F;\mathbb{V})}.$$

Since $q' \leq p'$ we have that $L^{p'} \hookrightarrow L^{q'}$, and the desired derivative estimate follows from (6.3). □

Let us now turn to DIRK schemes. In light of the a priori estimates presented above we now introduce our strongest notion of stability, namely, discrete Bochner stability.

Definition 6.4 (discrete Bochner stability)**.** We will say that the s-stage DIRK scheme with tableau (3.1) is Bochner stable when applied to the problem (1.1) if there are strictly positive C_A, C_f, $\{\omega_i\}_{i=1}^s$, $\{\gamma_i\}_{i=1}^s$, $p > 1$, and $q \geq p$ such that, for all $N \in \mathbb{N}$, any partition $\mathcal{P}_N$, and all $n \in \{0,\ldots,N-1\}$, we have

$$\frac{1}{2}|u_{n+1}|^2 + C_A\tau_n\sum_{i=1}^s \omega_i\|v_{n,i}\|^p \leq \frac{1}{2}|u_n|^2 + C_f\tau_n\sum_{i=1}^s\gamma_i\|f_{n,i}\|_*^{q'}. \tag{6.5}$$

Remark 6.5 (notation)**.** Notice that, since $\gamma_i > 0$ for all $i = 1,\ldots,s$, the linear functional

$$\varphi \mapsto \frac{1}{\sum_{i=1}^s \gamma_i}\sum_{i=1}^s \gamma_i\varphi(c_i), \qquad \forall\varphi \in \mathcal{C}([0,1])$$

defines a quadrature formula that is exact for at least constant functions. For this reason, and to alleviate notation, we shall define, for $r \in (1,\infty)$,

$$\|f\|_{L^r_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)} = \left(\sum_{n=1}^N \tau_n\sum_{i=1}^s\gamma_i\|f(t_n + c_i\tau_n)\|_*^r\right)^{1/r}.$$

It turns out that satisfaction of a dissipative discrete energy-balance such as (3.5) is a rather strong foundation for stability in the context of practical applications. In fact, under our additional assumptions on $\mathcal{A}$, Definition 3.4 implies (6.5).

Proposition 6.6 (discrete Bochner stability). *Assume that the mapping $\mathcal{A}$ satisfies the coercivity assumption* (6.1)*. If a DIRK scheme satisfies the dissipative discrete energy balance* (3.5)*, then it is discretely Bochner stable in the sense of Definition 6.4.*

Proof. We note that (3.5) can be rewritten as

$$\frac{1}{2}|u_{n+1}|^2 + \tau_n \sum_{i=1}^{s} \nu_i \langle \mathcal{A}(v_{n,i}), v_{n,i}\rangle \leq \frac{1}{2}|u_n|^2 + \tau_n \sum_{i=1}^{s} \nu_i \|f_{n,i}\|_* \|v_{n,i}\|.$$

Using the p–coercivity condition on $\mathcal{A}$ the left hand side of this inequality can be bounded from below. An application of Young's inequality on the right hand side, and the fact that $q' \geq p'$, then leads to (6.5). ☐

The following result is further evidence of the relevance of remarkably stable schemes.

Corollary 6.7 (remarkable stability). *If a DIRK scheme is remarkably stable in the sense of Definitions 4.6 or 5.6, then it is discretely Bochner stable in the sense of Definition 6.4.*

Proof. Owing to Proposition 6.6 it suffices to recall that remarkably stable schemes have a dissipative discrete energy law of the form (3.5). ☐

Examples of two- and three-stage schemes that are remarkably stable are presented in Sections 4.2 and 5.2. In the remainder of this section we further explore properties of discretely Bochner stable schemes.

Notice, first of all, that (6.5) can be thought of as a discrete and local, in time, version of (6.3), as the following result shows.

Proposition 6.8 (global stability). *Assume that* (3.2) *satisfies* (6.5)*. Then, for all $N \in \mathbb{N}$, and any partition $\mathcal{P}_N$ we have*

$$\frac{1}{2}\max_{n=0}^{N} |u_n|^2 + C_A \sum_{n=1}^{N} \tau_n \sum_{i=1}^{s} \omega_i \|v_{n,i}\|^p \leq \frac{1}{2}|u_0|^2 + C_f \|f\|^{q'}_{L^{q'}_{\mathcal{P}_N}(0,t_F,\mathbb{V}^*)}.$$

Proof. It suffices to add (6.5) over n. ☐

As a final, important, property of discrete Bochner stable schemes we now show that, under the assumption that (6.5) holds, an estimate on the discrete time derivative of the solution, in the spirit of (6.4), can be obtained. We begin with a uniform bound on the stages of the form

$$\mathfrak{C}_3 = \sup_{N\in\mathbb{N}} \sup_{\mathcal{P}_N} \sup_{n\in\{0,\dots,N-1\}} \max_{i=1}^{s} C_3\left(|v_{n,i}|\right) < \infty. \tag{6.6}$$

Lemma 6.9 (bound on stages). *Assume that the scheme* (3.2) *satisfies* (6.5)*. Then, there is a constant $C > 0$ such that for every $N \in \mathbb{N}$, and every partition $\mathcal{P}_N$ we have.*

$$\max_{n=0}^{N-1} \max_{i=1}^{s} |v_{n,i}| \leq C.$$

The constant C may depend on s, the entries of the tableau (3.1)*, and natural norms on the data, i.e., $|u_0|$ and $\|f\|_{L^{p'}(0,t_F;\mathbb{V}^*)}$. As a consequence, we have that* (6.6) *holds.*

Proof. The idea of the proof is to exploit the fact that $\mathbf{A}$ is lower triangular and with positive diagonal entries. For simplicity we present the proof for the case $s = 2$, but the reader may easily verify that the procedure extends to arbitrary s.

Let $n \in \{0, \dots, N-1\}$ and consider the first stage,

$$v_{n,1} - u_n + a_{11}\tau_n \mathcal{A}(v_{n,1}) = a_{11}\tau_n f_{n,1}.$$

Testing this identity with $v_{n,1}$ we arrive at

$$\frac{1}{2}\left(|v_{n,1}|^2 + |v_{n,1}-u_n|^2 - |u_n|^2\right) + C_1 a_{11}\tau_n \|v_{n,1}\|^p \le a_{11}\tau_n \left(\frac{\|f_{n,1}\|_*^{p'}}{p' C_1^{1/(p-1)}} + \frac{C_1\|v_{n,1}\|^p}{p} \right),$$

where we used the p–coercivity condition (6.1) and Young's inequality. Rearranging we have obtained that

$$\begin{aligned}\frac{1}{2}|v_{n,1}|^2 + \frac{1}{2}|v_{n,1}-u_n|^2 + \frac{C_1 a_{11}\tau_n}{p'}\|v_{n,1}\|^p &\le \frac{1}{2}|u_n|^2 + \frac{a_{11}\tau_n}{p' C_1^{1/(p-1)}}\|f_{n,1}\|_*^{p'} \\ &\le \frac{1}{2}\max_{n=0}^{N}|u_n|^2 + \kappa_1 \|f\|^{p'}_{L^{p'}_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)}\end{aligned} \tag{6.7}$$

where the constant κ_1 depends only on a_{11}, p, and C_1. In conclusion, for every n, $|v_{n,1}|$ is uniformly bounded only in terms of data.

With the bound on the first stage at hand we proceed to bound the second stage, which we write as

$$v_{n,2} - u_n + a_{22}\tau_n \mathcal{A}(v_{n,2}) = a_{22}\tau_n f_{n,2} + a_{21}\tau_n \mathcal{F}_{n,1}.$$

Testing with $v_{n,2}$ yields

$$\frac{1}{2}\left[|v_{n,2}|^2 + |v_{n,2}-u_n|^2 - |u_n|^2\right] + C_1 a_{22}\tau_n\|v_{n,2}\|^p \le a_{22}\tau_n\left(\frac{\|f_{n,2}\|_*^{p'}}{p' C_1^{1/(p-1)}} + \frac{C_1\|v_{n,2}\|^p}{p}\right) + a_{21}\tau_n\langle \mathcal{F}_{n,1}, v_{n,2}\rangle.$$

We now multiply the equation that defines the first stage by $v_{n,2}$ to get

$$\frac{a_{21}}{a_{11}}(v_{n,1}-u_n, v_{n,2}) = a_{21}\tau_n \langle \mathcal{F}_{n,1}, v_{n,2}\rangle.$$

In summary, we have obtained that

$$\begin{aligned}\frac{1}{2}\left[|v_{n,2}|^2 + |v_{n,2}-u_n|^2\right] + \frac{a_{22}C_1\tau_n}{p'}\|v_{n,2}\|^p &\le \frac{1}{2}|u_n|^2 + \frac{a_{22}\tau_n}{p' C_1^{1/(p-1)}}\|f_{n,2}\|_*^{p'} + \frac{a_{21}}{a_{11}}(v_{n,1}-u_n, v_{n,2}) \\ &\le \frac{1}{2}\max_{n=0}^{N}|u_n|^2 + \kappa_2\|f\|^{p'}_{L^{p'}_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)} + \frac{1}{4}|v_{n,2}|^2 \\ &+ \left(\frac{a_{21}}{a_{11}}\right)^2 |v_{n,1}-u_n|^2,\end{aligned}$$

where κ_2 is a constant that depends only on $\mathbf{A}$, p, and C_1. The previously obtained bound (6.7) then shows that

$$\begin{aligned}\frac{1}{4}\left[|v_{n,2}|^2 + |v_{n,2}-u_n|^2\right] + \frac{a_{22}C_1\tau_n}{p'}\|v_{n,2}\|^p &\le \left[\frac{1}{2} + \left(\frac{a_{21}}{a_{11}}\right)^2\right]\max_{n=0}^{N}|u_n|^2 \\ &+ \left[\kappa_2 + 2\left(\frac{a_{21}}{a_{11}}\right)^2\kappa_1\right]\|f\|^{p'}_{L^{p'}_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)},\end{aligned}$$

so that, for all n, $|v_{n,2}|$ is also uniformly bounded in terms of data. □

Proposition 6.10 (derivative estimate)**.** *Assume that the scheme* (3.2) *is at least first order accurate, and that it satisfies* (6.5) *and* (6.6). *Then, for any $N \in \mathbb{N}$, and any partition $\mathcal{P}_N$, the solution to* (3.2) *satisfies*

$$\left[\mu\sum_{n=0}^{N-1}\tau_n\left\|\frac{u_{n+1}-u_n}{\tau_n}\right\|_*^{q'}\right]^{1/q'} \le (\mu t_F)^{\frac{p'-q'}{p'q'}}\|f\|_{L^{p'}_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)} + \mathfrak{C}_3\left[\sum_{n=1}^{N}\tau_n\sum_{i=1}^{s}\omega_i\|v_{n,i}\|^p\right]^{1/q'},$$

where

$$\mu = \min\left\{ \min_{i=1}^{s} \gamma_i, \min_{i=1}^{s} \omega_i \right\},$$

and $\mathfrak{C}_3 > 0$ *is defined in* (6.6).

Proof. We begin by recalling that $b_i \geq 0$. Moreover, since the scheme is at least first order accurate, (C.1) holds and, consequently, for all $r \in [1, \infty)$

$$\left(\sum_{i=1}^{s} b_i^r \right)^{1/r} \leq \sum_{i=1}^{s} b_i = 1. \tag{6.8}$$

Notice now that the last equation in (3.2) implies

$$\left\| \frac{u_{n+1} - u_n}{\tau_n} \right\|_* \leq \sum_{i=1}^{s} b_i \|f(t_n + c_i \tau_n)\|_* + \mathfrak{C}_3 \sum_{i=1}^{s} b_i \|v_{n,i}\|^{p/q'},$$

where we used the q–growth condition (6.2). Raise this inequality to power q', multiply the result by $\mu\tau_n$, and add over n to obtain

$$\left[\mu \sum_{n=0}^{N-1} \tau_n \left\| \frac{u_{n+1} - u_n}{\tau_n} \right\|_*^{q'} \right]^{1/q'} \leq \left[\sum_{n=0}^{N-1} |A_n + B_n|^{q'} \right]^{1/q'} \leq \left[\sum_{n=0}^{N-1} |A_n|^{q'} \right]^{1/q'} + \left[\sum_{n=0}^{N-1} |B_n|^{q'} \right]^{1/q'}, \tag{6.9}$$

where we denoted

$$A_n = \mu^{1/q'} \tau_n^{1/q'} \sum_{i=1}^{s} b_i \|f(t_n + c_i \tau_n)\|_*, \qquad B_n = \mathfrak{C}_3^{1/q'} \mu^{1/q'} \tau_n^{1/q'} \sum_{i=1}^{s} b_i \|v_{n,i}\|^{p/q'}.$$

We now estimate each term on the right hand side of (6.9) separately. Using repeatedly Hölder's inequality we observe that

$$\begin{aligned}
\left[\sum_{n=0}^{N-1} |A_n|^{q'} \right]^{1/q'} &= \left[\sum_{n=0}^{N-1} \mu\tau_n \left| \sum_{i=1}^{s} b_i \|f(t_n + c_i \tau_n)\|_* \right|^{q'} \right]^{1/q'} \\
&\leq \left[\sum_{n=0}^{N-1} \mu\tau_n \right]^{\frac{1}{q'} \frac{1}{(p'/q')'}} \left[\sum_{n=0}^{N-1} \mu\tau_n \left| \sum_{i=1}^{s} b_i \|f(t_n + c_i \tau_n)\|_* \right|^{p'} \right]^{\frac{1}{q'} \frac{1}{p'/q'}} \\
&\leq (\mu t_F)^{\frac{p'-q'}{p'q'}} \left[\sum_{n=0}^{N-1} \tau_n \sum_{i=1}^{s} \gamma_i \|f(t_n + c_i \tau_n)\|_*^{p'} \right]^{1/p'} = (\mu t_F)^{\frac{p'-q'}{p'q'}} \|f\|_{L^{p'}_{\mathcal{P}_N}(0,t_F;\mathbb{V}^*)},
\end{aligned}$$

where we used (6.8), and that $\mu \leq \gamma_i$. Similarly,

$$\begin{aligned}
\left[\sum_{n=0}^{N-1} |B_n|^{q'} \right]^{1/q'} &= \mathfrak{C}_3 \left[\sum_{n=0}^{N-1} \mu\tau_n \left| \sum_{i=1}^{s} b_i \|v_{n,i}\|^{p/q'} \right|^{q'} \right]^{1/q'} \\
&\leq \mathfrak{C}_3 \left[\sum_{n=0}^{N-1} \tau_n \sum_{i=1}^{s} \omega_i \|v_{n,i}\|^{p} \right]^{1/q'},
\end{aligned}$$

where we again used (6.8) and $\mu \leq \omega_i$. The result follows. ∎

Under further structural assumptions on $\mathcal{A}$, like hemicontinuity [50, Definition 2.3], the previous results together with a standard exercise in compactness (cf. Lemma 6.1) allow us to assert convergence of discretely Bochner stable DIRK schemes under minimal regularity assumptions. We shall not dwell on this.

Appendix A. Example problems accommodating our assumptions

Let us present several examples of problems that our framework can manage. We will indicate when such problems satisfy our minimal set of assumptions, i.e., (2.2), and when they do satisfy the more stringent assumptions of Section 6. For a more comprehensive list and insight we refer the reader to [50, Chapter 8]. In all of the descriptions below $d \geq 1$, and $\Omega \subset \mathbb{R}^d$ is a bounded domain with, at least, Lipschitz boundary.

A.1. **Nonlinear diffusion equations.**

Let $K : \Omega \times \mathbb{R} \to \mathbb{R}^{d\times d}$ be bounded, measurable, and nonnegative definite, i.e.,

$$\boldsymbol{\xi}^\intercal K(x,s)\boldsymbol{\xi} \geq 0, \quad \forall x \in \Omega, \quad \forall s \in \mathbb{R}, \quad \forall \boldsymbol{\xi} \in \mathbb{R}^d.$$

The problem

$$\begin{cases} \partial_t u(x,t) - \operatorname{div}\, (K(x,u(x,t))\nabla u(x,t)) = f(x,t), & (x,t) \in \Omega \times (0,T), \\ u(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T), \\ u(x,0) = u_0(x), & x \in \Omega, \end{cases}$$

can be cast into (1.1) by setting $\mathbb{V} = H_0^1(\Omega)$, $\mathbb{H} = L^2(\Omega)$ and

$$\langle \mathcal{A}(v), w\rangle = \int_\Omega \nabla w(x)^\intercal K(x, v(x))\nabla v(x)\,\mathrm{d}x.$$

Clearly this operator satisfies (2.2).

If, in addition, we assume that K is uniformly bounded, and uniformly positive definite, that is, there is $K_0 > 0$ such that

$$K_0^{-1}|\boldsymbol{\xi}|^2 \leq \boldsymbol{\xi}^\intercal K(x,s)\boldsymbol{\xi} \leq K_0|\boldsymbol{\xi}|^2, \quad \forall x \in \bar{\Omega}, \quad \forall s \in \mathbb{R}, \quad \forall \boldsymbol{\xi} \in \mathbb{R}^d,$$

then with $p = q = 2$, $C_1 = K_0^{-1}$ and $C_3 = K_0$ this problem satisfies (6.1) and (6.2).

A.2. **Nonlinear diffusion reaction problems.**

The previous example can be slightly generalized to

$$\partial_t u(x,t) - \operatorname{div}\, (K(x,u(x,t))\nabla u(x,t)) + \gamma(x,u(x,t)) = f(x,t),$$

where $\gamma : \Omega \times \mathbb{R} \to \mathbb{R}$ is nonnegative for a nonnegative second argument, and it has sufficiently mild growth. For instance, if $\gamma = |w|^2 w$, we see that

$$\gamma(w)w = |w|^4 \geq 0,$$

so we get positivity, i.e., (2.2). If, in addition, $d = 2$ we recall that for $v, w \in H_0^1(\Omega)$

$$\int_\Omega |w|^3 v\,\mathrm{d}x \leq \|w\|^3_{L^6(\Omega)}\|v\|_{L^2(\Omega)} \leq C\|w\|^3_{L^6(\Omega)}\|\nabla v\|_{L^2(\Omega;\mathbb{R}^2)},$$

where we used Poincaré inequality. Now, the Gagliardo–Nirenberg interpolation inequality [50, Theorem 1.24] implies that

$$\|w\|^3_{L^6(\Omega)} \leq C\left[\|w\|^{5/9}_{L^2(\Omega)}\|\nabla w\|^{4/9}_{L^2(\Omega;\mathbb{R}^2)}\right]^3 = C\|w\|^{5/3}_{L^2(\Omega)}\|\nabla w\|^{4/3}_{L^2(\Omega;\mathbb{R}^2)}.$$

Consequently, our problem fits into the framework of Section 6 with $p = 2$, $q = 3$, $C_1 = K_0^{-1}$, and $C_3 = 1 + \|u\|_{L^2(\Omega)}^{5/3}$. To see this, it suffices to realize that, since $q' = \frac{3}{2}$

$$\frac{4}{3} = \frac{2}{3/2}.$$

A.3. **Parabolic quasilinear equations.** One further generalization that nonlinear diffusions allow is the following. Let $G : \Omega \times \mathbb{R}^d \to \mathbb{R}$ be convex in its second argument and $\mathbf{F} = D_2 G$ its derivative with respect to its second argument. Assume that these functions satisfy classical conditions of the form

$$G(x, \boldsymbol{\xi}) \geq \alpha_1 |\boldsymbol{\xi}|^p, \qquad |\mathbf{F}(x, \boldsymbol{\xi})| \leq \alpha_3 |\boldsymbol{\xi}|^{p-1}, \quad \forall x \in \Omega, \ \boldsymbol{\xi} \in \mathbb{R}^d,$$

with $p > \max\{1, \frac{2d}{d+2}\}$. The equation

$$\partial_t u(x,t) - \operatorname{div} \mathbf{F}(x, \nabla u(x,t)) = f(x,t),$$

supplemented with suitable initial and boundary conditions, can be cast into the framework of Section 6 with $p = q$, $\mathbb{H} = L^2(\Omega)$, and $\mathbb{V} = W_0^{1,p}(\Omega)$. Clearly, $C_1 = \alpha_1$ and $C_3 = \alpha_3$.

A classical example of this scenario is the parabolic p–Laplacian problem

$$\partial_t u(x,t) - \operatorname{div} \left(|\nabla u(x,t)|^{p-2} \nabla u(x,t) \right) = f(x,t).$$

To see this, it suffices to set $G(x, \boldsymbol{\xi}) = \frac{1}{p} |\boldsymbol{\xi}|^p$.

A.4. **The Navier-Stokes equations.** The well known Navier-Stokes equations read

$$\partial_t \mathbf{u}(x,t) + \operatorname{div} \left[\mathbf{u}(x,t) \otimes \mathbf{u}(x,t) \right] - \nu \Delta \mathbf{u}(x,t) + \nabla \pi(x,t) = \mathbf{f}(x,t), \quad \operatorname{div} \mathbf{u}(x,t) = 0,$$

and are supplemented with suitable initial and boundary conditions. Here $\nu > 0$ is the viscosity. To see how this problem fits the framework of Section 6 we set, for definiteness, $d = 3$ and

$$\begin{aligned} \mathbb{H} &= \left\{ \mathbf{v} \in L^2(\Omega; \mathbb{R}^3) : \operatorname{div} \mathbf{v} = 0, \mathbf{v} \cdot \mathbf{n}_{|\partial\Omega} = 0 \right\}, \\ \mathbb{V} &= H_0^1(\Omega; \mathbb{R}^3) \cap \mathbb{H}. \end{aligned}$$

The operator $\mathcal{A}$ is defined as

$$\langle \mathcal{A}(\mathbf{v}), \mathbf{w} \rangle = \nu \int_\Omega \nabla \mathbf{v} : \nabla \mathbf{w} \, \mathrm{d}x - \int_\Omega (\mathbf{v} \otimes \mathbf{v}) : \nabla \mathbf{w} \, \mathrm{d}x.$$

Owing to the skew symmetry of the convective term (over divergence free fields) we have

$$\nu \|\nabla \mathbf{w}\|_{L^2(\Omega; \mathbb{R}^{3\times 3})}^2 \leq \langle \mathcal{A}(\mathbf{w}), \mathbf{w} \rangle,$$

so that, clearly, $C_1 = \nu$ and $p = 2$.

Consider now

$$\left| \int_\Omega (\mathbf{v} \otimes \mathbf{v}) : \nabla \mathbf{w} \, \mathrm{d}x \right| \leq \|\mathbf{v}\|_{L^4(\Omega;\mathbb{R}^3)}^2 \|\nabla \mathbf{w}\|_{L^2(\Omega;\mathbb{R}^{3\times 3})} \leq \left[\|\mathbf{v}\|_{L^2(\Omega;\mathbb{R}^3)}^{1/4} \|\nabla \mathbf{v}\|_{L^2(\Omega;\mathbb{R}^{3\times 3})}^{3/4} \right]^2 \|\nabla \mathbf{w}\|_{L^2(\Omega;\mathbb{R}^{3\times 3})},$$

where we, again, used the Gagliardo–Nirenberg interpolation inequality. This shows that

$$C_3 = 1 + \|\mathbf{v}\|_{L^2(\Omega;\mathbb{R}^3)}^{1/2}, \qquad \frac{3}{2} = \frac{p}{q'} \implies q' = \frac{4}{3}.$$

A.5. **Hamiltonian problems.** The operator $\mathcal{A}$ is linear and induces a skew symmetric bilinear form on $\mathbb{V}$, i.e.,

$$\langle \mathcal{A}(u), v \rangle = -\langle \mathcal{A}(v), u \rangle, \quad \forall u, v \in \mathbb{V}. \tag{A.1}$$

This is the prototypical case of Hamiltonian problems such as Maxwell's equations in free space.

A.6. **GENERIC systems.** The operator $\mathcal{A}$ is a combination of the cases in Sections A.1 and A.5, that is, a combination of a dissipative and a Hamiltonian parts. For instance we could consider, for $\epsilon \geq 0$, an operator of the form $\mathcal{A}(w) = \mathcal{S}(w) + \epsilon\mathcal{D}(w)$ where, for all $v, w \in \mathbb{V}$, we have

$$\langle \mathcal{S}(w), v \rangle = -\langle w, \mathcal{S}(v) \rangle, \qquad \langle \mathcal{D}w, w \rangle \geq 0.$$

This type of PDE problems are usually called GENERIC [46, 45, 18, 21]. For instance, the linear wave equation with damping is a GENERIC system. Similarly, incompressible Navier-Stokes equations could be understood as the sum of a dissipative system (i.e., the bilinear form associated to viscous effects) and a nonlinear Hamiltonian system (the skew symmetric trilinear form associated to convective terms), see for instance [58, 44].

Appendix B. Some properties of non-remarkable schemes

We start with a rather trivial observation.

Remark B.1 (non-remarkable schemes and skew-symmetric problems)**.** Consider (1.1) with $f \equiv 0$ and $\mathcal{A}$ a skew-symmetric operator, i.e.,

$$\langle \mathcal{A}(u), v \rangle = -\langle \mathcal{A}(v), u \rangle, \quad \forall u, v \in \mathbb{V}.$$

In other words, we consider purely autonomous dynamics. A non-remarkable two-stage DIRK scheme, meaning a scheme that does not satisfy the properties described in Definition 4.6, will satisfy the following discrete energy-balance

$$\frac{1}{2}|u_{n+1}|^2 + \mathcal{Q}(u_n, v_{n,1}, v_{n,2}) = \frac{1}{2}|u_n|^2 \,, \tag{B.1}$$

where the quadratic form $\mathcal{Q}$, introduced in (4.11), is unsigned. Similarly, a non-remarkable three-stage DIRK scheme, meaning a scheme that does not satisfy the properties described in Definition 5.6, will satisfy the discrete energy-balance

$$\frac{1}{2}|u_{n+1}|^2 + \mathcal{Q}(u_n, v_{n,1}, v_{n,2}, v_{n,3}) = \frac{1}{2}|u_n|^2 \,, \tag{B.2}$$

where $\mathcal{Q}$, defined in (5.11), is unsigned.

Identities (B.1) and (B.2) are an immediate consequence of (4.10) and (5.9) respectively. They follow from the fact that if $\mathcal{A}$ is skew-symmetric, then we have that $\langle \mathcal{A}(v_{n,i}), v_{n,i} \rangle = 0$ for each stage $i \in \{1, \ldots, s\}$. Remark B.1 tells us that non-remarkable schemes cannot be guaranteed to be stable when applied to problems of skew-symmetric nature. The same holds true for GENERIC-like PDEs, see Section A.6, with $\epsilon > 0$ sufficiently small.

While simple, this is an important observation. Most nonlinear problems, either locally in time, or through linearization, can be thought as having a symmetric and skew-symmetric parts. The symmetric part is usually positive and related to dissipative behavior. The skew-symmetric part describes conserved quantities and/or wave-like nature of the problem. In this regard, Remark B.1 tells us that unconditional stability cannot be expected when using non-remarkable schemes for PDEs strongly dominated by their skew-symmetric part. In this very specific context of non-remarkably stable schemes and problems with skew-symmetric operator it is pointless to attempt to develop any theory regarding convergence or error estimates; or to engage in any discussion related to order-reduction; or to compare its performance to other schemes. This is because, to begin with, the scheme cannot be proven to be stable. For many problems, say for instance the linear acoustic wave equations in first-order form, Remark B.1 should be the final argument against the use of non-remarkably stable schemes.

We notice, in particular, that the very popular Alexander's DIRK22 and DIRK33 L-stable schemes, described by tableaus (3.7) and (3.11) respectively, are not remarkably stable. This severely limits their applicability to the solution of evolutionary PDEs. For the sake of completeness we present an optimal proof of stability for Alexander's DIRK22 scheme in the context of linear, self-adjoint, and positive operators.

Proposition B.2 (energy identity I)**.** *Consider* (1.1) *with* $f \equiv 0$. *Assume that the operator* $\mathcal{A}$ *is linear; coercive/positive-definite, i.e.,* (6.1) *holds with* $p = 2$*; and symmetric, that is,*

$$\langle \mathcal{A}(v), w\rangle = \langle \mathcal{A}(w), v\rangle, \quad \forall v, w \in \mathbb{V}.$$

Identity (4.8) *for Alexander's DIRK22 scheme takes the following specific form*

$$\begin{aligned} &\tfrac{1}{2}|u_{n+1}|^2 - \tfrac{1}{2}|u_n|^2 + \tfrac{1}{2}|v_{n,1} - u_n|^2 + \tfrac{1}{2}|u_{n+1} - v_{n,1}|^2 \\ &\quad + \tau_n\gamma\langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle + \tau_n\gamma\langle \mathcal{A}(u_{n+1}), u_{n+1}\rangle = -\tau_n(1-2\gamma)\langle \mathcal{A}(v_{n,1}), u_{n+1}\rangle \end{aligned} \tag{B.3}$$

with γ *as defined in* (3.7).

Proof. One only needs to use the values of the tableau, which are given in (3.7). ☐

As usual the problem lies with the unsigned off-diagonal term $\langle \mathcal{A}(v_{n,1}), u_{n+1}\rangle$ in the right-hand side of (B.3). We may consider absorbing part of it into the artificial damping terms as described in the following result.

Proposition B.3 (partial damping)**.** *Let* $\kappa \in \mathbb{R}$ *be any real number. In the setting of Proposition B.2, the energy balance* (B.3) *can be rewritten as*

$$\begin{aligned} &\tfrac{1}{2}|u_{n+1}|^2 - \tfrac{1}{2}|u_n|^2 + \mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1}) + \tau_n(\gamma+\kappa)\langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle \\ &\quad + \tau_n\gamma\langle \mathcal{A}(u_{n+1}), u_{n+1}\rangle = -\tau_n(1-2\gamma-\kappa)\langle \mathcal{A}(v_{n,1}), u_{n+1}\rangle\,, \end{aligned} \tag{B.4}$$

where $\mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1})$ *is a quadratic form, depending on the free parameter* κ*, defined as*

$$\mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1}) = \tfrac{1}{2}|v_{n,1} - u_n|^2 + \tfrac{1}{2}|u_{n+1} - v_{n,1}|^2 - \tfrac{\kappa}{\gamma}(v_{n,1} - u_n, u_{n+1} - v_{n,1})\,. \tag{B.5}$$

Proof. One needs to use techniques similar to those advanced in the proof of Lemma (4.5). ☐

Given the structure of (B.4)–(B.5) we may want to determine what is the optimal value of κ in order to preserve stability, at the very least when $\mathcal{A}$ is a linear, positive-definite, symmetric operator.

- Finding the optimal value of κ has two primary restrictions: we need $\mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1})$ to remain non-negative; in addition, we also need to satisfy the property $\gamma + \kappa > 0$ in order to preserve the a priori bound on $\langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle$.
- Setting $\kappa = 1 - 2\gamma$ allows us absorb the off-diagonal term $\tau_n(1-2\gamma-\kappa)\langle \mathcal{A}(v_{n,1}), u_{n+1}\rangle$, in its entirety, into the quadratic form $\mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1})$. However, we already know from Section 4.2.3 that is not feasible. Since Alexander's DIRK22 scheme is not remarkably-stable, the choice $\kappa = 1 - 2\gamma$ will lead to $\mathcal{Q}_\kappa(u_n, v_{n,1}, u_{n+1})$ being unsigned.
- Some inspection reveals that the largest value of κ we can use, while also retaining non-negativity of $\mathcal{Q}(u_n, v_{n,1}, u_{n+1})$ and positivity of $\gamma + \kappa$, is $\kappa = \gamma$.

These observations lead to the following result.

Lemma B.4 (a priori energy-estimate)**.** *Consider* (1.1) *with* $f \equiv 0$. *Assume that the operator* $\mathcal{A}$ *is linear; coercive/positive-definite, i.e.,* (6.1) *holds with* $p = 2$*; and symmetric, that is,*

$$\langle \mathcal{A}(v), w\rangle = \langle \mathcal{A}(w), v\rangle, \quad \forall v, w \in \mathbb{V}.$$

Then, the numerical solution using Alexander's DIRK22 scheme satisfies the following optimal a priori energy estimate:

$$\tfrac{1}{2}|u_{n+1}|^2 + \mathcal{Q}_\gamma(u_n, v_{n,1}, u_{n+1}) + \tau_n\big(\tfrac{7\gamma-1}{2}\big)\langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle + \tau_n\big(\tfrac{5\gamma-1}{2}\big)\langle \mathcal{A}(u_{n+1}), u_{n+1}\rangle \leq \tfrac{1}{2}|u_n|^2 \tag{B.6}$$

with $\mathcal{Q}_\gamma(u_n, v_{n,1}, u_{n+1})$ *is defined in* (B.5).

Proof. Estimate (B.6) is just a consequence of setting $\kappa = \gamma$ in (B.4) and using Cauchy-Schwarz and Young's inequality

$$\langle \mathcal{A}(v_{n,1}), u_{n+1}\rangle \leq \langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle^{1/2} \langle \mathcal{A}(u_{n+1}), u_{n+1}\rangle^{1/2} \leq \tfrac{1}{2}\langle \mathcal{A}(v_{n,1}), v_{n,1}\rangle + \tfrac{1}{2}\langle \mathcal{A}(u_{n+1}), u_{n+1}\rangle\,,$$

for the unsigned off-diagonal term. We claim that (B.6) is optimal, in the sense that it maximizes the use of artificial damping terms while also preserving stability of the scheme. □

In conclusion, our assessment is that non-remarkably stable schemes may only be used either for positive linear problems, or positive nonlinear problems with very mild growth conditions. They may fail to be stable for problems strongly dominated by their skew-symmetric component. We assume that the arguments used in Propositions B.2 and B.3, and Lemma B.4, can be extended to the analysis of the Alexander's DIRK33 scheme, but given the observations developed Remark B.1, we find very little motivations to do so.

Appendix C. Order conditions

It is well known [31, 10] that the entries of the Butcher table (3.1) are bound by the following, necessary, consistency order conditions:

- Order one:

$$\mathbf{b}^{\mathsf{T}}\mathbf{1} = 1, \qquad \mathbf{A}\mathbf{1} = \mathbf{c}, \tag{C.1}$$

  where $\mathbf{1} = [1] \in \mathbb{R}^s$.
- Order two:

$$\mathbf{b}^{\mathsf{T}}\mathbf{c} = \frac{1}{2}. \tag{C.2}$$

- Order three:

$$\mathbf{b}^{\mathsf{T}}\mathbf{A}\mathbf{c} = \frac{1}{6}. \tag{C.3}$$

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