Karlsruhe Institute of Technology

Wave phenomena
analysis and numerics

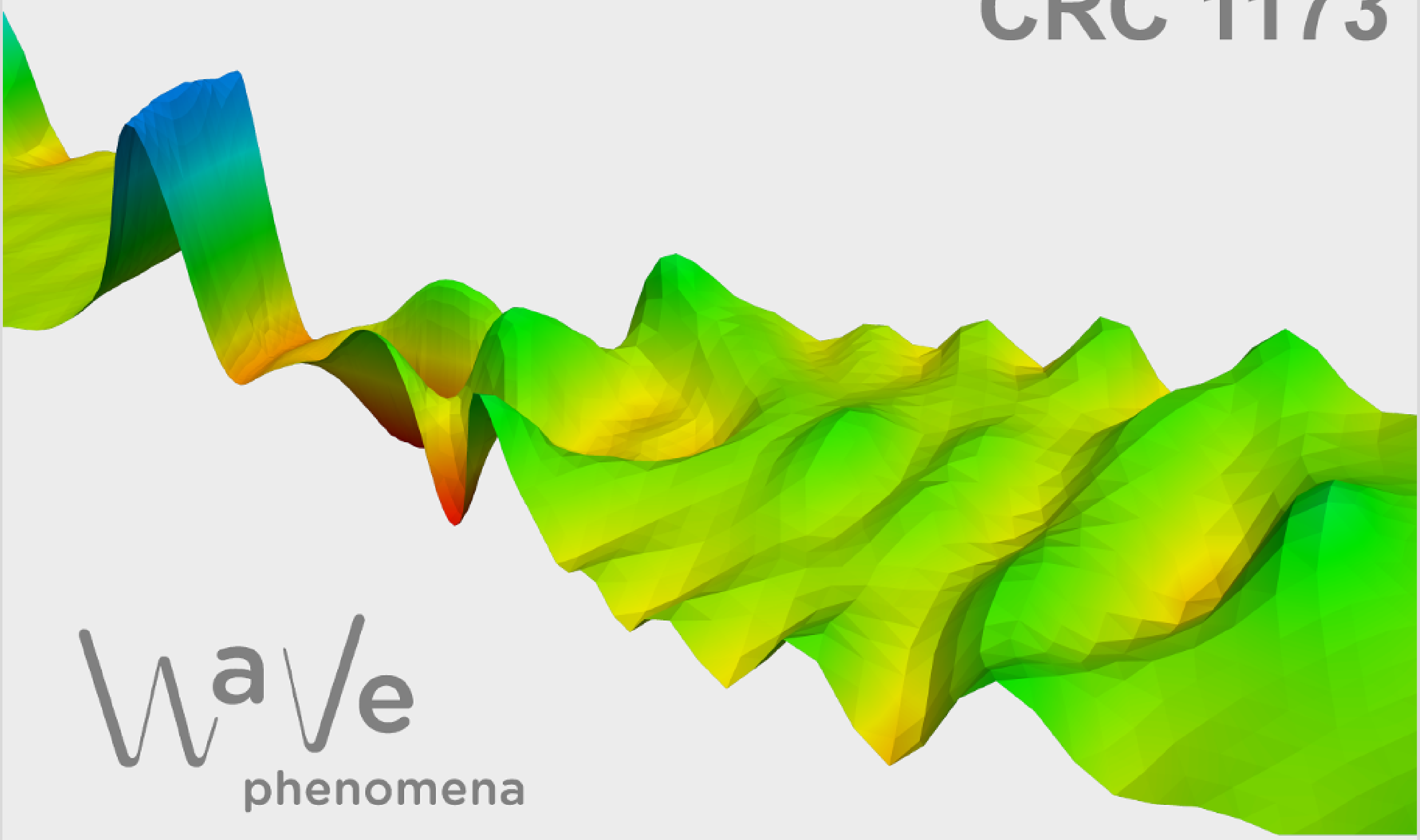
Dynamical low-rank integrators for second-order matrix differential equations

Marlis Hochbruck, Markus Neher, Stefan Schrammer

CRC Preprint 2022/12, February 2022

KARLSRUHE INSTITUTE OF TECHNOLOGY

CRC 1173



Wave phenomena

Participating universities

Funded by

ISSN 2365-662X

Dynamical low-rank integrators for second-order matrix differential equations

Marlis Hochbruck · **Markus Neher** ·
Stefan Schrammer

Received: date / Accepted: date

Abstract In this paper, we construct and analyze a new dynamical low-rank integrator for second-order matrix differential equations. The method is based on a combination of the projector-splitting integrator introduced in [11] and a Strang splitting. We also present a variant of the new integrator which is tailored to stiff second-order problems.

Keywords dynamical low-rank approximation, matrix differential equations

Mathematics Subject Classification (2010) 65L04, 65L05, 65L70

1 Introduction

Dynamical low-rank integrators [9] have been introduced for the approximation of large, time-dependent matrices which are solutions to first-order matrix differential equations that can be well approximated by low-rank matrices. Typically, such matrix differential equations stem from spatially discretized PDEs. The idea is to project the right-hand side of the problem onto the tangent space of the manifold of matrices with small, fixed rank. It was shown in [9], that this ansatz yields differential equations for the factors of a low-rank decomposition resembling a singular value decomposition. Compared to the approximation of the full matrix solution, working only with the factors of the low-rank decomposition significantly reduces the computational costs and the required storage. Unfortunately, the integrator of [9] suffers from ill-conditioning in the presence of small singular values, a situation which is called over-approximation, i.e., the rank chosen within the method exceeds the rank of the actual solution. A projector-splitting integrator which is robust in the case of over-approximation was introduced in [11]. It is based on a clever Lie-Trotter splitting of the projected right-hand side, which allows one to solve the subproblems exactly.

Marlis Hochbruck · Markus Neher · Stefan Schrammer
Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, Germany,
E-mail: marlis.hochbruck@kit.edu, markus.neher@kit.edu, stefan.schrammer@kit.edu

A variant of this approach was recently presented in [2]. This new unconventional integrator is especially suited for strongly dissipative problems.

Both the projector-splitting integrator and the unconventional integrator have been applied to a variety of first-order matrix differential equations, e.g., for Schrödinger equations in [2], for the Vlasov–Poison equation in [3], for Vlasov–Maxwell equations in [4], and for Burgers' equation with uncertainty in [10]. However, to the best of our knowledge, for second-order matrix differential equations of the form

$$A''(t) = F\big(A(t)\big), \quad A(t) \in \mathbb{C}^{m\times n}, \qquad A(0) = A_0, \quad A'(0) = B_0, \tag{1}$$

with large m,n, such integrators have not been considered so far. The obvious technique of reformulating (1) into a first-order system and applying the projector-splitting integrator [11] for first-order matrix differential equations behaved poorly in our numerical experiments. The reason might be that the inherent structure of the second-order problem is ignored by this procedure, causing the approximation quality to deteriorate. Therefore, we propose to combine the projector-splitting integrator with a Strang splitting and call this new scheme ST-LO method (Strang splitting combined with the method by Lubich and Oseledets). It yields a robust and reliable dynamical low-rank integrator for second-order equations of type (1), provided that the exact solution $A(t)$ and its derivative $A'(t)$ can be well approximated by matrices of low rank. In the special situation that the exact flows used within the Strang splitting preserve the low rank of the previous approximation, our integrator reduces to the leapfrog scheme if the rank chosen in the method is sufficiently large. We also develop a variant of the scheme which is tailored to stiff semilinear second-order equations. For this, we combine our newly developed scheme with the ideas in [12], where a dynamical low-rank integrator for stiff first-order equations was based on the projector-splitting integrator.

For the projector-splitting integrator, a detailed error analysis was provided in [8]. It relies on an exactness property of the integrator, namely that it provides the exact solution if this solution preserves the (low) rank of the initial value for all times and the exact initial value is used to start the integrator. Unfortunately, this is no longer true for the ST-LO scheme because of the Strang splitting. Nevertheless, we will provide error bounds under similar assumptions as in [8].

The paper is organized as follows: In Section 2, we briefly recall the projector-splitting integrator introduced in [11] by Lubich and Oseledets. The construction of the ST-LO scheme is presented in Section 3 and its error analysis in Section 4. A modification of the ST-LO scheme which also works for stiff second-order problems is developed in Section 5.

Throughout this paper, m,n, and r are natural numbers, where w.l.o.g. $m \geq n \gg r$. If $n > m$, we consider the equivalent differential equation for the transpose. By $\mathscr{M}_r$ we denote the manifold of complex $m \times n$ matrices with rank r,

$$\mathscr{M}_r = \{\widehat{Y} \in \mathbb{C}^{m\times n} \mid \operatorname{rank}(\widehat{Y}) = r\}.$$

The Stiefel manifold of $m \times r$ unitary matrices is denoted by

$$\mathscr{V}_{m,r} = \{U \in \mathbb{C}^{m\times r} \mid U^H U = I_r\},$$

where I_r is the identity matrix of dimension r and U^H is the conjugate transpose of U.

The singular value decomposition of a matrix $Y \in \mathbb{C}^{m\times n}$ is given by

$$Y = U\Sigma V^H, \quad U \in \mathscr{V}_{m,m}, \quad V \in \mathscr{V}_{n,n}, \quad \Sigma = \operatorname{diag}(\sigma_1,\dots,\sigma_n) \in \mathbb{C}^{m\times n},$$

where $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$ are its singular values. It is well known that for $r < n$, the rank-r best-approximation to Y w.r.t. the Frobenius norm $\|\cdot\|$ is given by

$$\widehat{Y} = U\widetilde{\Sigma}V^H = \widehat{U}\widehat{\Sigma}\widehat{V}^H,$$

where $\widetilde{\Sigma} = \operatorname{diag}(\sigma_1,\dots,\sigma_r,0,\dots,0)$ and

$$\widehat{U} = U[I_r\ 0] \in \mathscr{V}_{m,r}, \qquad \widehat{V} = V[I_r\ 0] \in \mathscr{V}_{n,r}, \qquad \widehat{\Sigma} = \operatorname{diag}(\sigma_1,\dots,\sigma_r).$$

For a given step size τ we use the notation $t_k = k\tau$ for any k with $2k \in \mathbb{N}_0$.

2 The projector-splitting integrator

In this section, we briefly review dynamical low-rank approximations as introduced in [9, 11]. We start with the following problem: Given some time-dependent matrix $A(t)$, find a low-rank approximation $\widehat{A}(t) \in \mathscr{M}_r$ such that

$$\widehat{A}(t) \approx A(t) \qquad \text{for all} \quad t \in [0,T].$$

In [9], this is done by imposing that $\widehat{A}'(t)$, which is contained in the tangent space $\mathscr{T}_{\widehat{A}(t)}\mathscr{M}_r$ to $\mathscr{M}_r$ at $\widehat{A}(t)$, satisfies

$$\|\widehat{A}'(t) - A'(t)\| = \min! \tag{2}$$

For an initial value $\widehat{A}(0) = \widehat{A}_0 \in \mathscr{M}_r$, condition (2) is equivalent to a Galerkin condition. In fact, then $\widehat{A}$ solves the evolution equation

$$\widehat{A}'(t) = P\big(\widehat{A}(t)\big)A'(t), \qquad \widehat{A}(0) = \widehat{A}_0 \in \mathscr{M}_r, \tag{3}$$

where $P\big(\widehat{A}(t)\big)$ denotes the orthogonal projection onto the tangent space $\mathscr{T}_{\widehat{A}(t)}\mathscr{M}_r$. A natural choice for the initial value $\widehat{A}_0$ of (3) is the rank-r best approximation to $A(0)$.

For all $\widehat{A} \in \mathscr{M}_r$ there is a non-unique low-rank factorization

$$\widehat{A} = \widehat{U}\widehat{S}\widehat{V}^H, \qquad \widehat{U} \in \mathscr{V}_{m,r}, \quad \widehat{V} \in \mathscr{V}_{n,r}, \quad \widehat{S} \in \mathbb{C}^{r\times r} \text{ invertible}, \tag{4}$$

which allows us to write the orthogonal projector $P(\widehat{A})$ onto $\mathscr{T}_{\widehat{A}(t)}\mathscr{M}_r$ as

$$P(\widehat{A})Z = Z\widehat{V}\widehat{V}^H - \widehat{U}\widehat{U}^H Z\widehat{V}\widehat{V}^H + \widehat{U}\widehat{U}^H Z, \tag{5}$$

cf., [9, Lemma 4.1]. The dynamical low-rank integrator constructed in [11] is based on a Lie-Trotter splitting, applied to the differential equation (3) with $P(\widehat{A})$ given in

(5). Given a step size $\tau > 0$, the first integration step consists of solving the three subproblems

$$
\begin{aligned}
Y_\alpha' &= A'\widehat{V}_\alpha\widehat{V}_\alpha^H, & Y_\alpha(0) &= \widehat{A}_0, && \text{(6a)}\\
Y_\beta' &= -\widehat{U}_\beta\widehat{U}_\beta^H A'\widehat{V}_\beta\widehat{V}_\beta^H, & Y_\beta(0) &= Y_\alpha(\tau), && \text{(6b)}\\
Y_\gamma' &= \widehat{U}_\gamma\widehat{U}_\gamma^H A', & Y_\gamma(0) &= Y_\beta(\tau). && \text{(6c)}
\end{aligned}
$$

As shown in [11, Lemma 3.1], all subproblems (6) can be solved exactly on $\mathscr{M}_r$ when the additional conditions

$$\widehat{V}_\alpha'(t) = 0, \qquad \widehat{U}_\beta'(t) = 0,\ \widehat{V}_\beta'(t) = 0, \qquad \widehat{U}_\gamma'(t) = 0,$$

are imposed. Then, the solutions

$$Y_\eta(t) = \widehat{U}_\eta(t)\widehat{S}_\eta(t)\widehat{V}_\eta(t)^H, \qquad \eta \in \{\alpha,\beta,\gamma\},$$

can be written in terms of the increment $\Delta A = A(\tau) - A(0)$,

$$
\begin{aligned}
\widehat{U}_\alpha(t)\widehat{S}_\alpha(t) &= \widehat{U}_\alpha(0)\widehat{S}_\alpha(0) + \Delta A\widehat{V}_\alpha(0), & \widehat{V}_\alpha(t) &= \widehat{V}_\alpha(0),\\
\widehat{S}_\beta(t) &= \widehat{S}_\beta(0) - \widehat{U}_\beta(0)^H\Delta A\widehat{V}_\beta(0), & \widehat{U}_\beta(t) &= \widehat{U}_\beta(0), \quad \widehat{V}_\beta(t) = \widehat{V}_\beta(0),\\
\widehat{V}_\gamma(t)\widehat{S}_\gamma(t)^H &= \widehat{V}_\gamma(0)\widehat{S}_\gamma(0)^H + \Delta A^H\widehat{U}_\gamma(0), & \widehat{U}_\gamma(t) &= \widehat{U}_\gamma(0).
\end{aligned}
$$

The integration process is continued with initial value $Y_\gamma(\tau) \approx \widehat{A}(\tau)$ in the next time step. A single time step of the resultant *projector-splitting integrator* is presented in Algorithm 1, version (α).

The above approach is also suitable for the construction of low-rank approximations to the unknown solution $A(t)$ of the first-order differential equation

$$A'(t) = F\big(A(t)\big), \qquad A(0) = A_0 \in \mathbb{C}^{m\times n}, \qquad t \in [0,T]. \tag{7}$$

As explained in [11, Section 3.4], the only change affects the replacement of the increment ΔA in Algorithm 1 in a way resembling the explicit Euler method,

$$\Delta A = \tau F(\widehat{A}_0),$$

see version (β). The global error of this first-order scheme depends on the quality of the approximation of the exact solution $A(t)$ of (7) by a low-rank matrix (for $t \in [0,T]$) and on properties of the right-hand side F, cf. [8].

Remark 1 The computational complexity of Algorithm 1 is dominated by the two products $\Delta A\widehat{V}$ and $\Delta A^H\widehat{U}$ in lines 7 and 11, respectively, the two QR-decompositions of matrices of dimension $m\times r$ and $n\times r$, respectively, and the three matrix-matrix products in lines 8, 10, and 11. For an efficient implementation, it is important to compute the products $\Delta A\widehat{V}$ and $\Delta A^H\widehat{U}$ without computing ΔA explicitly.

Algorithm 1 Projector-splitting integrator for low-rank approximations to (α) given time-dependent matrices $A(t)$ or (β) the solution of (7), single time step

function PRSI($\widehat{U},\widehat{S},\widehat{V},r,\Delta A$)
  {**input:** factors $\widehat{U},\widehat{S},\widehat{V}$ of rank-r approximation $\widehat{A}=\widehat{U}\widehat{S}\widehat{V}^H \approx A(t)$ with $\widehat{U} \in \mathscr{V}_{m,r}$, $\widehat{V} \in \mathscr{V}_{n,r}$,
    $\widehat{S} \in \mathbb{C}^{r\times r}$, functions for matrix-vector multiplication with ΔA and ΔA^H,
      (α) $\Delta A = A(t+\tau)-A(t)$,
      (β) $\Delta A = \tau F(\widehat{A})$ }

  $\widetilde{K} = \Delta A\widehat{V}$
  $K = \widehat{U}\widehat{S}+\widetilde{K}$
  compute QR-decomposition $\widehat{U}\widehat{S} = K$
  $\widehat{S} = \widehat{S} - \widehat{U}^H\widetilde{K}$
  $L = \widehat{V}\widehat{S}^H + \Delta A^H\widehat{U}$
  compute QR-decomposition $\widehat{V}\widehat{S}^H = L$

  return $\widehat{U},\widehat{S},\widehat{V},L$
  {**output:** factors $\widehat{U},\widehat{S},\widehat{V}$ of rank-r approximation $\widehat{A}=\widehat{U}\widehat{S}\widehat{V}^H \approx A(t+\tau)$ and $L=\widehat{V}\widehat{S}^H$ (optional),
    with $\widehat{U} \in \mathscr{V}_{m,r}$, $\widehat{V} \in \mathscr{V}_{n,r}$, $\widehat{S} \in \mathbb{C}^{r\times r}$}
end function

3 Dynamical low-rank approximation of second-order matrix ODEs

Next, we devise a low-rank integrator for second-order matrix differential equations of the form (1). A straightforward practice would be to rewrite (1) as a first-order system

$$\begin{bmatrix} A \\ B \end{bmatrix}' = \begin{bmatrix} B \\ F(A) \end{bmatrix}, \qquad \begin{bmatrix} A(0) \\ B(0) \end{bmatrix} = \begin{bmatrix} A_0 \\ B_0 \end{bmatrix}, \tag{8}$$

and to apply Algorithm 1. However, numerical tests showed that the quality of the numerical solutions deteriorates over time, possibly caused by the neglection of the structure of the the right-hand side of (8).

We thus use a different ansatz and first split (8) into

$$\begin{bmatrix} A \\ B \end{bmatrix}' = \begin{bmatrix} 0 \\ F(A) \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix}, \tag{9}$$

and then apply a standard Strang splitting. Solving the subproblems exactly leads to the well-known leapfrog or Störmer-Verlet scheme,

$$B_{k+\frac{1}{2}} = B_k + \frac{\tau}{2}F(A_k), \tag{10a}$$

$$A_{k+1} = A_k + \tau B_{k+\frac{1}{2}}, \tag{10b}$$

$$B_{k+1} = B_{k+\frac{1}{2}} + \frac{\tau}{2}F(A_{k+1}), \tag{10c}$$

cf. [5, Section 1.5]. If approximations to $A' = B$ are not required at full time steps, then the most economic implementation of the leapfrog scheme is to combine (10a) and (10c) via

$$B_{k+\frac{1}{2}} = B_{k-\frac{1}{2}} + \tau F(A_k), \quad k \geq 1. \tag{10d}$$

For $k=0$, $B_{\frac{1}{2}}$ is computed from (10a).

A low-rank integrator for the second-order equation (1) is now designed by approximating the exact flows of the subproblems in (9) by their respective low-rank flows using the projector-splitting method [11]. First, we determine initial values $\widehat{A}_0$ and $\widehat{B}_0$ as rank-r_A and rank-r_B best-approximations to A_0 and B_0, respectively. After k time steps, the low-rank approximations $\widehat{A}_k \approx A(t_k)$ and $\widehat{B}_{k-\frac{1}{2}} \approx B(t_{k-\frac{1}{2}})$ are represented by (non-unique) decompositions

$$\widehat{A}_k = \widehat{U}_k \widehat{S}_k \widehat{V}_k^H \in \mathscr{M}_{r_A}, \qquad \widehat{B}_{k-\frac{1}{2}} = \widehat{T}_{k-\frac{1}{2}} \widehat{R}_{k-\frac{1}{2}} \widehat{W}_{k-\frac{1}{2}}^H \in \mathscr{M}_{r_B},$$

where

$$\widehat{U}_k \in \mathscr{V}_{m,r_A},\ \widehat{V}_k \in \mathscr{V}_{n,r_A},\ \widehat{S}_k \in \mathbb{C}^{r_A \times r_A}, \qquad \widehat{T}_{k-\frac{1}{2}} \in \mathscr{V}_{m,r_B},\ \widehat{W}_{k-\frac{1}{2}} \in \mathscr{V}_{n,r_B},\ \widehat{R}_{k-\frac{1}{2}} \in \mathbb{C}^{r_B \times r_B}.$$

The low-rank matrices $\widehat{A}_{k+1} \approx A(t_{k+1})$ and $\widehat{B}_{k+\frac{1}{2}} \approx B(t_{k+\frac{1}{2}})$ are obtained by approximating the solutions of (9) by applying Algorithm 1 to

$$\widetilde{B}'_{k-\frac{1}{2}}(\sigma) = F(\widehat{A}_k), \qquad \widetilde{B}_{k-\frac{1}{2}}(0) = \widehat{B}_{k-\frac{1}{2}}, \qquad \sigma \in [0,\tau], \qquad k \geq 1, \tag{11a}$$

$$\widetilde{A}'_k(\sigma) = \widehat{B}_{k+1/2}, \qquad \widetilde{A}_k(0) = \widehat{A}_k, \qquad \sigma \in [0,\tau], \qquad k \geq 0, \tag{11b}$$

where for $k=0$, we have

$$\widetilde{B}'_0(\sigma) = F(\widehat{A}_0), \qquad \widetilde{B}_0(0) = \widehat{B}_0, \qquad \sigma \in [0, \frac{\tau}{2}]. \tag{11c}$$

Since the exact solutions of (11) read

$$\widetilde{B}_{k-\frac{1}{2}}(\tau) = \widehat{B}_{k-\frac{1}{2}} + \tau F(\widehat{A}_k), \tag{12a}$$

$$\widetilde{A}_k(\tau) = \widehat{A}_k + \tau \widehat{B}_{k+\frac{1}{2}}, \tag{12b}$$

$$\widetilde{B}_0(\frac{\tau}{2}) = \widehat{B}_0 + \frac{\tau}{2} F(\widehat{A}_0), \tag{12c}$$

the increments $\Delta B_{k-\frac{1}{2}}$ and ΔA_k are given explicitly as

$$\begin{aligned}
\Delta B_{k-\frac{1}{2}} &= \widetilde{B}_{k-\frac{1}{2}}(\tau) - \widetilde{B}_{k-\frac{1}{2}}(0) = \tau F(\widehat{A}_k), && k \geq 1, \\
\Delta A_k &= \widetilde{A}_k(\tau) - \widetilde{A}_k(0) = \tau \widehat{B}_{k+\frac{1}{2}}, && k \geq 0, \\
\Delta B_0 &= \widetilde{B}_0(\frac{\tau}{2}) - \widetilde{B}_0(0) = \frac{\tau}{2} F(\widehat{A}_0).
\end{aligned}$$

The resulting dynamical low-rank integrator for second-order matrix ODEs will be named ST-LO method, for ***St**rang splitting combined with the **L**ubich-**O**seledets integrator*. It is presented in Algorithm 2.

There is a close relationship between the ST-LO and the leapfrog schemes:

Theorem 2 *If for all $t \in [0,T]$ the exact solutions $A(t)$ and $B(t)$ of the subproblems* (9) *with* $\operatorname{rank} A_0 = r_A, \operatorname{rank} B_0 = r_B$ *stay of rank r_A and r_B, respectively, then the solutions of the* ST-LO *and leapfrog schemes coincide.*

Proof The ST-LO scheme is derived by exchanging the exact flows of the leapfrog scheme by their corresponding low-rank flows. Since the exact flows preserve the rank by assumption, the application of the exactness property of the projector-splitting integrator [11, Theorem 4.1] yields the desired result. □

Algorithm 2 DLR integrator for second-order ODEs (1), ST-LO scheme, single time step

function ST-LO($\tau, F, \widehat{U}, \widehat{S}, \widehat{V}, \widehat{T}, \widehat{R}, \widehat{W}, r_A, r_B$)
  {**input:** step size τ, right-hand side F,
    factors $\widehat{U}, \widehat{S}, \widehat{V}$ of rank-r_A approximation $\widehat{A} = \widehat{U}\widehat{S}\widehat{V}^H \approx A(t)$ with $\widehat{U} \in \mathscr{V}_{m,r_A}$, $\widehat{V} \in \mathscr{V}_{n,r_A}$,
    $\widehat{S} \in \mathbb{C}^{r_A \times r_A}$,
    factors $\widehat{T}, \widehat{R}, \widehat{W}$ of rank-r_B approximation $\widehat{B} = \widehat{T}\widehat{R}\widehat{W}^H \approx A'(t - \frac{\tau}{2})$ with $\widehat{T} \in \mathscr{V}_{m,r_B}$,
    $\widehat{W} \in \mathscr{V}_{n,r_B}$, $\widehat{R} \in \mathbb{C}^{r_B \times r_B}$}

  $\widehat{B}$-step: $\widehat{T}, \widehat{R}, \widehat{W}, L = \text{PRSI}\big(\widehat{T}, \widehat{R}, \widehat{W}, r_B, \Delta B\big)$ where $\Delta B = \tau F(\widehat{U}\widehat{S}\widehat{V}^H)$

  $\widehat{A}$-step: $\widehat{U}, \widehat{S}, \widehat{V} = \text{PRSI}\big(\widehat{U}, \widehat{S}, \widehat{V}, r_A, \Delta A\big)$ where $\Delta A = \tau \widehat{T} L^H$

  return $\widehat{U}, \widehat{S}, \widehat{V}, \widehat{T}, \widehat{R}, \widehat{W}$
  {**output:** factors $\widehat{U}, \widehat{S}, \widehat{V}$ of rank-r_A approximation $\widehat{A} = \widehat{U}\widehat{S}\widehat{V}^H \approx A(t+\tau)$ with $\widehat{U} \in \mathscr{V}_{m,r_A}$,
    $\widehat{V} \in \mathscr{V}_{n,r_A}$, $\widehat{S} \in \mathbb{C}^{r_A \times r_A}$,
    factors $\widehat{T}, \widehat{R}, \widehat{W}$ of rank-r_B approximation$\widehat{B} = \widehat{T}\widehat{R}\widehat{W}^H \approx A'(t + \frac{\tau}{2})$ with $\widehat{T} \in \mathscr{V}_{m,r_B}$,
    $\widehat{W} \in \mathscr{V}_{n,r_B}$, $\widehat{R} \in \mathbb{C}^{r_B \times r_B}$}
end function

Algorithm 3 DLR integrator for second-order ODEs (1), ST-LO_VAR scheme, single time step

function ST-LO_VAR($\tau, \omega_3^2, F, \widehat{U}, \widehat{S}, \widehat{V}, \widehat{T}, \widehat{R}, \widehat{W}, r_A, r_B$)
  {**input:** step size τ, weight ω_3^2, right-hand side F,
    factors $\widehat{U}, \widehat{S}, \widehat{V}$ of rank-r_A approximation $\widehat{A} = \widehat{U}\widehat{S}\widehat{V}^H \approx A(t)$ with $\widehat{U} \in \mathscr{V}_{m,r_A}$, $\widehat{V} \in \mathscr{V}_{n,r_A}$,
    $\widehat{S} \in \mathbb{C}^{r_A \times r_A}$,
    factors $\widehat{T}, \widehat{R}, \widehat{W}$ of rank-r_B approximation $\widehat{B} = \widehat{T}\widehat{R}\widehat{W}^H \approx A'(t)$ with $\widehat{T} \in \mathscr{V}_{m,r_B}$, $\widehat{W} \in \mathscr{V}_{n,r_B}$,
    $\widehat{R} \in \mathbb{C}^{r_B \times r_B}$}

  $\widehat{B}$-step: $\widehat{T}, \widehat{R}, \widehat{W}, L = \text{PRSI}\big(\widehat{T}, \widehat{R}, \widehat{W}, r_B, \Delta B\big)$ where $\Delta B = \frac{\tau}{2} F(\widehat{U}\widehat{S}\widehat{V}^H)$

  $\widehat{A}$-step: $\widehat{U}, \widehat{S}, \widehat{V} = \text{PRSI}\big(\widehat{U}, \widehat{S}, \widehat{V}, r_A, \Delta A\big)$ where $\Delta A = \omega_3^2 \tau \widehat{T} L^H$

  $\widehat{B}$-step: $\widehat{T}, \widehat{R}, \widehat{W} = \text{PRSI}\big(\widehat{T}, \widehat{R}, \widehat{W}, r_B, \Delta B\big)$ where $\Delta B = \frac{\tau}{2} F(\widehat{U}\widehat{S}\widehat{V}^H)$

  return $\widehat{U}, \widehat{S}, \widehat{V}, \widehat{T}, \widehat{R}, \widehat{W}$
  {**output:** factors $\widehat{U}, \widehat{S}, \widehat{V}$ of rank-r_A approximation to $\widehat{A} = \widehat{U}\widehat{S}\widehat{V}^H \approx A(t+\tau)$ with $\widehat{U} \in \mathscr{V}_{m,r_A}$,
    $\widehat{V} \in \mathscr{V}_{n,r_A}$, $\widehat{S} \in \mathbb{C}^{r_A \times r_A}$,
    factors $\widehat{T}, \widehat{R}, \widehat{W}$ of rank-r_B approximation to $\widehat{B} = \widehat{T}\widehat{R}\widehat{W}^H \approx A'(t+\tau)$ with $\widehat{T} \in \mathscr{V}_{m,r_B}$,
    $\widehat{W} \in \mathscr{V}_{n,r_B}$, $\widehat{R} \in \mathbb{C}^{r_B \times r_B}$}
end function

Clearly, in general the ST-LO scheme does not inherit the exactness property of the projector-splitting integrator, because of the splitting error. A detailed error analysis of the ST-LO scheme will be presented in Section 4.

In the same way, a variant of the ST-LO scheme is based on the non-staggered version of the leapfrog scheme (10), procuring approximations to A' on the same time-grid as approximations to A. Here, the function F has to be evaluated twice in each time step so that the computational effort is larger when compared to the standard ST-LO scheme. In this version we also allow for a rescaled step size in the A-step (10b). As we will see later, this will be an important detail in the construction of dynamical low-rank integrators for stiff second-order matrix differential equations. The resulting method is called the ST-LO_VAR scheme. It is described in Algorithm 3.

4 Error analysis of ST-LO

In the following, we analyze the error of the ST-LO scheme given in Algorithm 2 when applied to (1) with a right-hand side F which is Lipschitz-continuous with a moderate Lipschitz constant L, i.e., F satisfies

$$\|F(Y) - F(\widetilde{Y})\| \leq L\|Y - \widetilde{Y}\| \qquad \text{for all } Y, \widetilde{Y} \in \mathbb{C}^{m\times n}. \tag{13}$$

Our analysis relies on the error analysis in [8] for the projector-splitting integrator.

Recall that the ST-LO scheme is derived from the leapfrog scheme (10), which is stable under the CFL condition, cf. [7],

$$\tau^2 \leq \tau_{\mathrm{CFL}}^2 = \frac{4}{L}. \tag{14}$$

We therefore assume, that the step size τ always satisfies (14).

Assumption 1 *The exact solution $A : [0,T] \to \mathbb{C}^{m\times n}$ of (1) is in $\mathscr{C}^4([0,T])$. Furthermore, there are low-rank approximations $X_A(t) \in \mathscr{M}_{r_A}, X_B(t) \in \mathscr{M}_{r_B}$ such that*

$$A(t) = X_A(t) + R_A(t), \qquad \|R_A(0)\| \leq \rho_A, \quad \|R_A'(t)\| \leq \rho_A', \tag{15a}$$

$$B(t) = A'(t) = X_B(t) + R_B(t), \qquad \|R_B(0)\| \leq \rho_B, \quad \|R_B'(t)\| \leq \rho_B'. \tag{15b}$$

Additionally, there exist sufficiently large constants γ_A and γ_B, such that (15) is also satisfied for all $Y_A(t), Y_B(t) \in \mathbb{C}^{m\times n}$ with

$$\|A(t) - Y_A(t)\| \leq \gamma_A, \qquad \|B(t) - Y_B(t)\| \leq \gamma_B.$$

For the approximations $\widehat{A}_k \approx A(t_k)$ and $\widehat{B}_{k+\frac{1}{2}} \approx B(t_{k+\frac{1}{2}})$ computed with the ST-LO scheme and for $\widetilde{A}_k$ and $\widetilde{B}_{k-\frac{1}{2}}$ given in (12), we define

$$
\begin{aligned}
&E_A^k = \|A(t_k) - \widehat{A}_k\|, && E_B^{k+\frac{1}{2}} = \|B(t_{k+\frac{1}{2}}) - \widehat{B}_{k+\frac{1}{2}}\|, && k \geq 0, && \text{(16a)}\\
&\widetilde{E}_A^0 = 0, && \widetilde{E}_B^{\frac{1}{2}} = \|B(t_{\frac{1}{2}}) - \widetilde{B}_0(t_{\frac{1}{2}})\|, && && \text{(16b)}\\
&\widetilde{E}_A^k = \|A(t_k) - \widetilde{A}_{k-1}(\tau)\|, && \widetilde{E}_B^{k+\frac{1}{2}} = \|B(t_{k+\frac{1}{2}}) - \widetilde{B}_{k-\frac{1}{2}}(\tau)\|, && k \geq 1, && \text{(16c)}\\
&\widehat{E}_A^0 = E_A^0, && \widehat{E}_B^{\frac{1}{2}} = \|\widetilde{B}_0(t_{\frac{1}{2}}) - \widehat{B}_{\frac{1}{2}}\|, && && \text{(16d)}\\
&\widehat{E}_A^k = \|\widetilde{A}_{k-1}(\tau) - \widehat{A}_k\|, && \widehat{E}_B^{k+\frac{1}{2}} = \|\widetilde{B}_{k-\frac{1}{2}}(\tau) - \widehat{B}_{k+\frac{1}{2}}\|, && k \geq 1. && \text{(16e)}
\end{aligned}
$$

By the triangle inequality, we have

$$
E_B^{k+\frac{1}{2}} \leq \widetilde{E}_B^{k+\frac{1}{2}} + \widehat{E}_B^{k+\frac{1}{2}} \qquad \text{and} \qquad E_A^{k+1} \leq \widetilde{E}_A^{k+1} + \widehat{E}_A^{k+1}, \qquad k \geq 0. \tag{17}
$$

The analysis of the ST-LO scheme is organized in two lemmas and a theorem. Our first result are coupled, recursive inequalities for E_A^{k+1} and $E_B^{k+\frac{1}{2}}$.

Lemma 3 *Let $A : [0,T] \to \mathbb{C}^{m\times n}$ with $A \in \mathscr{C}^4([0,T])$ be the exact solution of (1) with initial values $A_0, B_0 \in \mathbb{C}^{m\times n}$ and $B = A'$. Further, denote by $\widehat{B}_{k-\frac{1}{2}}$ and $\widehat{A}_k$ the low-rank approximations obtained by the* ST-LO *scheme after k steps started with initial values $\widehat{A}_0 \in \mathscr{M}_{r_A}, \widehat{B}_0 \in \mathscr{M}_{r_B}$. Then, the errors introduced in (16) satisfy*

$$
E_B^{\frac{1}{2}} \leq E_B^0 + \frac{\tau}{2} L E_A^0 + \widehat{E}_B^{\frac{1}{2}} + C_B^{LF}\tau^2, \tag{18a}
$$

$$
E_A^1 \leq (1 + \frac{\tau^2}{2} L) E_A^0 + \tau E_B^0 + \tau \widehat{E}_B^{\frac{1}{2}} + \widehat{E}_A^1 + (C_A^{LF} + C_B^{LF})\tau^3 \tag{18b}
$$

and for $k \in \mathbb{N}$ we have

$$
E_B^{k+\frac{1}{2}} \leq E_B^{k-\frac{1}{2}} + \tau L E_A^k + \widehat{E}_B^{k+\frac{1}{2}} + C_B^{LF}\tau^3, \tag{19a}
$$

$$
E_A^{k+1} \leq (1+\tau^2 L) E_A^k + \tau E_B^{k-\frac{1}{2}} + \tau \widehat{E}_B^{k+\frac{1}{2}} + \widehat{E}_A^{k+1} + (C_A^{LF} + C_B^{LF}\tau)\tau^3. \tag{19b}
$$

The constants C_A^{LF} and C_B^{LF} are given explicitly as

$$
C_A^{LF} = \max_{t\in[0,T]} \frac{1}{24}\|A'''(t)\|, \qquad C_B^{LF} = \max\Big\{ \max_{t\in[0,\frac{\tau}{2}]} \frac{1}{8}\|A'''(t)\|, \ \max_{t\in[0,T]} \frac{1}{24}\|A^{(4)}(t)\| \Big\}.
$$

Proof By Taylor series expansion, we have

$$
\|A(t_{k+1}) - \big(A(t_k) + \tau B(t_{k+\frac{1}{2}})\big)\| \leq C_A^{\mathrm{LF}}\tau^3, \qquad k \geq 0, \tag{20a}
$$

$$
\|B(t_{k+\frac{1}{2}}) - \big(B(t_{k-\frac{1}{2}}) + \tau F(A(t_k))\big)\| \leq C_B^{\mathrm{LF}}\tau^3, \qquad k \geq 1. \tag{20b}
$$

as well as

$$\|B(t_{\frac{1}{2}}) - \big(B_0 + \frac{\tau}{2}F(A_0)\big)\| \le C_B^{\mathrm{LF}}\tau^2. \tag{20c}$$

Hence for $k = 0$, we have

$$\begin{aligned}\widetilde{E}_B^{\frac{1}{2}} &\le \|B_0 + \frac{\tau}{2}F(A_0) - (\widehat{B}_0 + \frac{\tau}{2}F(\widehat{A}_0))\| + C_B^{\mathrm{LF}}\tau^2 \\ &\le E_B^0 + \frac{\tau}{2}LE_A^0 + C_B^{\mathrm{LF}}\tau^2 \end{aligned}\tag{21}$$

by (20c), (12c), and (13). Employing (17) shows (18a). Using (18a) and (20a) yields

$$\begin{aligned}\widetilde{E}_A^1 &\le \|A_0 + \tau B(\frac{\tau}{2}) - (\widehat{A}_0 + \tau\widehat{B}_{\frac{1}{2}})\| + C_A^{\mathrm{LF}}\tau^3 \\ &\le E_A^0 + \tau E_B^{\frac{1}{2}} + C_A^{\mathrm{LF}}\tau^3 \\ &\le \big(1 + \frac{\tau^2}{2}L\big)E_A^0 + \tau E_B^0 + \tau\widehat{E}_B^{\frac{1}{2}} + (C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}})\tau^3. \end{aligned}\tag{22}$$

Together with (17) this proves (18b).

For $k \ge 1$ we follow the same steps. We have by (12), (13), and (20b)

$$\widetilde{E}_B^{k+\frac{1}{2}} \le E_B^{k-\frac{1}{2}} + \tau LE_A^k + C_B^{\mathrm{LF}}\tau^3 \tag{23}$$

and by (17) thus (19a). Lastly, we have by (20a), using again (12), and inserting (19a)

$$\begin{aligned}\widetilde{E}_A^{k+1} &\le E_A^k + \tau E_B^{k+\frac{1}{2}} + C_A^{\mathrm{LF}}\tau^3 \\ &\le E_A^k + \tau\left(E_B^{k-\frac{1}{2}} + \tau LE_A^k + \widehat{E}_B^{k+\frac{1}{2}} + C_B^{\mathrm{LF}}\tau^3\right) + C_A^{\mathrm{LF}}\tau^3 \\ &= (1 + \tau^2 L)E_A^k + \tau E_B^{k-\frac{1}{2}} + \tau\widehat{E}_B^{k+\frac{1}{2}} + (C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}}\tau)\tau^3, \end{aligned}\tag{24}$$

which together with (17) completes the proof. □

In [8, Section 2.6.1] it was shown that the error between a time-dependent matrix $A(t)$ satisfying (15a) and the rank-r_A approximation $Y_1 \approx A(\tau)$ computed by Algorithm 1 started from $X_A(0) \in \mathscr{M}_{r_A}$ is bounded by

$$\|A(\tau) - Y_1\| \le \rho_A + 7\tau\rho_A'. \tag{25}$$

In the next lemma we eliminate $\widehat{E}_B^{k+\frac{1}{2}}$ and $\widehat{E}_A^{k+1}$ from (19) by using (25).

Lemma 4 *Let the assumptions of Lemma 3 be satisfied. Furthermore, assume that*

$$E_A^0 \le \rho_A, \qquad E_B^0 \le \rho_B. \tag{26}$$

If Assumption 1 is fulfilled, then for all k such that $t_{k+4} \leq T$, the errors $E_B^{k+\frac{1}{2}}$ and E_A^{k+1} defined in (16) satisfy

$$E_B^{k+\frac{1}{2}} \leq \rho_B + 7t_{k+1}\rho_B' + \tau L \sum_{j=0}^{k} E_A^j + C_B^{LF}\tau^2(1+t_k), \tag{27a}$$

$$\begin{aligned} E_A^{k+1} \leq \rho_A + t_{k+1}\rho_B + \tau L \sum_{j=0}^{k} t_{k+1-j}E_A^j + 7t_{k+1}\rho_A' + \frac{7}{2}t_{k+1}t_{k+2}\rho_B' \\ + \left((C_A^{LF} + C_B^{LF})t_{k+1} + \frac{1}{2}t_k t_{k+1} C_B^{LF} \right)\tau^2, \end{aligned} \tag{27b}$$

respectively.

Proof The proof is accomplished by induction on k. First, we show that the errors $\widetilde{E}_A^{k+1}$ and $\widetilde{E}_B^{k+\frac{1}{2}}$ are uniformly bounded by suitable constants γ_A and γ_B. Then the auxiliary solutions $\widetilde{A}$ and $\widetilde{B}$ are sufficiently close to the exact solutions A and B, and hence they admit representations like (15) by Assumption 1. Since the approximations $\widehat{A}$ and $\widehat{B}$ are low-rank approximation to $\widetilde{A}$ and $\widetilde{B}$ computed by Algorithm 1 started from initial values of rank r_A and r_B, respectively, the local errors $\widehat{E}_A^{k+1}$ and $\widehat{E}_B^{k+\frac{1}{2}}$ are bounded by

$$\widehat{E}_B^{\frac{1}{2}} \leq \frac{7}{2}\tau\rho_B', \quad \widehat{E}_B^{k+\frac{1}{2}} \leq 7\tau\rho_B', \quad k \geq 1, \qquad \widehat{E}_A^{k+1} \leq 7\tau\rho_A', \quad k \geq 0, \tag{28}$$

cf. (25). The estimate on the global error then follows from (17).

For $k = 0$ we deduce from (21) and (26)

$$\widetilde{E}_B^{\frac{1}{2}} \leq \rho_B + \frac{\tau}{2}L\rho_A + C_B^{\mathrm{LF}}\tau^2.$$

By Assumption 1, for $\gamma_B \geq \rho_B + \frac{\tau}{2}L\rho_A + C_B^{\mathrm{LF}}\tau^2$, it holds by (18a) and (28) that

$$\begin{aligned} E_B^{\frac{1}{2}} &\leq \rho_B + \frac{\tau}{2}LE_A^0 + 7\frac{\tau}{2}\rho_B' + C_B^{\mathrm{LF}}\tau^2 \\ &< \rho_B + \tau LE_A^0 + 7t_1\rho_B' + C_B^{\mathrm{LF}}\tau^2, \end{aligned} \tag{29}$$

which is (27a) for $k = 0$.

Likewise, by (22), (26), and (29) we have

$$\widetilde{E}_A^1 \leq \rho_A + \tau^2 LE_A^0 + \tau\rho_B + 7\tau^2\rho_B' + (C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}})\tau^3. \tag{30}$$

Choosing γ_A as the right-hand side of (30), by Assumption 1 and (28) we deduce

$$E_A^1 \leq \rho_A + \tau^2 LE_A^0 + t_1\rho_B + 7t_1\rho_A' + \frac{7}{2}t_1 t_2\rho_B' + (C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}})t_1\tau^2,$$

which shows (27b) for $k = 0$.

Assuming that (27) holds true for some arbitrary, but fixed $k-1 \in \mathbb{N}_0$, we now prove (27). Applying the Gronwall-type Lemma 6 below, we find from (27b) for $j = 1, \dots, k$

$$E_A^j \leq \mathrm{e}^{\sqrt{L} t_k} M_A^j, \tag{31}$$

where

$$M_A^j = \rho_A + t_j \rho_B + 7 t_j \rho_A' + \frac{7}{2} t_j t_{j+1} \rho_B' + \big((C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}}) t_j + \frac{1}{2} t_{j-1} t_j C_B^{\mathrm{LF}} \big) \tau^2. \tag{32}$$

By (26), this bound is also valid for $j = 0$. From (23) and (27a) we obtain

$$\begin{aligned}
\widetilde{E}_B^{k+\frac{1}{2}} &\leq E_B^{k-\frac{1}{2}} + \tau L E_A^k + C_B^{\mathrm{LF}} \tau^3 \\
&\leq \Big(\rho_B + 7 t_k \rho_B' + \tau L \sum_{j=0}^{k-1} E_A^j + C_B^{\mathrm{LF}} \tau^2 (1 + t_{k-1}) \Big) + \tau L E_A^k + C_B^{\mathrm{LF}} \tau^3 \\
&= \rho_B + 7 t_k \rho_B' + \tau L \sum_{j=0}^{k} E_A^j + C_B^{\mathrm{LF}} \tau^2 (1 + t_k).
\end{aligned} \tag{33}$$

Inserting (31) into (33) for $0 \leq t_{k+4} \leq T$ results in constants $C_B(T), \widetilde{C}_B(T)$ depending on L, ρ_B, ρ_B' and C_B^{LF} such that

$$\widetilde{E}_B^{k+\frac{1}{2}} \leq C_B(T) + \tau^2 \widetilde{C}_B(T).$$

By Assumption 1 for $\gamma_B \geq C_B(T) + \tau^2 \widetilde{C}_B(T)$, (28) shows that $\widehat{E}_B^{k+\frac{1}{2}} \leq 7 \tau \rho_B'$. Thus we obtain from (33) and (17)

$$E_B^{k+\frac{1}{2}} \leq \rho_B + 7 t_{k+1} \rho_B' + \tau L \sum_{j=0}^{k} E_A^j + C_B^{\mathrm{LF}} \tau^2 (1 + t_k),$$

which proves (27a) for all $k \in \mathbb{N}_0$.

Similarly, using (24) and the induction hypothesis, we get

$$\begin{aligned}
\widetilde{E}_A^{k+1} \leq \Big(&\rho_A + t_k \rho_B + \tau L \sum_{j=0}^{k-1} t_{k-j} E_A^j + 7 t_k \rho_A' + \frac{7}{2} t_k t_{k+1} \rho_B' \\
&\qquad + \big((C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}}) t_{k+1} + \frac{1}{2} t_k t_{k+1} C_B^{\mathrm{LF}} \big) \tau^2 \Big) + \tau^2 L E_A^k \\
&+ \tau \Big(\rho_B + 7 t_k \rho_B' + \tau L \sum_{j=0}^{k-1} E_A^j + C_B^{\mathrm{LF}} \tau^2 (1 + t_{k-1}) \Big) \\
&+ 7 \tau^2 \rho_B' + (C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}} \tau) \tau^3 \\
= \rho_A &+ t_{k+1} \rho_B + \tau L \sum_{j=0}^{k} t_{k+1-j} E_A^j + 7 t_k \rho_A' + \frac{7}{2} t_{k+1} t_{k+2} \rho_B' \\
&+ \big((C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}}) t_{k+1} + \frac{1}{2} t_k t_{k+1} C_B^{\mathrm{LF}} \big) \tau^2.
\end{aligned} \tag{34}$$

By employing the bound (31) on E_A^j for $0 \le t_{k+4} \le T$ we define constants $C_A(T)$, $C_A(T)$ depending on $L, \rho_A, \rho_B, \rho_A', \rho_B', C_A^{\mathrm{LF}}$ and C_B^{LF} such that

$$\widetilde{E}_A^{k+1} \le C_A(T) + \tau^2 \widetilde{C}_A(T).$$

Now let Assumption 1 be fulfilled for some $\gamma_A \ge C_A(T) + \tau^2 \widetilde{C}_A(T)$. Then we have $\widehat{E}_A^{k+1} \le 7\tau\rho_A'$ by (28). Finally, we conclude from (34) and (17)

$$\begin{aligned} E_A^{k+1} \le \rho_A + t_{k+1}\rho_B + \tau L \sum_{j=0}^{k} t_{k+1-j} E_A^j + 7t_{k+1}\rho_A' + \frac{7}{2} t_{k+1} t_{k+2} \rho_B' \\ + \left((C_A^{\mathrm{LF}} + C_B^{\mathrm{LF}}) t_{k+1} + \frac{1}{2} t_k t_{k+1} C_B^{\mathrm{LF}} \right) \tau^2. \end{aligned}$$

This completes the proof. □

We are now able to prove a global error bound.

Theorem 5 *If the assumptions of Lemma 4 are satisfied, then the global errors E_A^{k+1} and $E_B^{k+\frac{1}{2}}$ are bounded by*

$$E_A^{k+1} \le \mathrm{e}^{\sqrt{L} t_{k+1}} M_A^{k+1},$$

where M_A^{k+1} is given in (32), and

$$E_B^{k+\frac{1}{2}} \le \mathrm{e}^{\sqrt{L} t_k} M_B^{k+\frac{1}{2}},$$

for

$$M_B^{k+\frac{1}{2}} = \rho_B + t_{k+\frac{1}{2}} L \rho_A + 7t_{k+\frac{1}{2}} \rho_B' + \frac{1}{2} t_k t_{k+1} \rho_A' + \big(\frac{1}{2} t_k t_{k+1} C_A^{LF} + (1+t_k) C_B^{LF} \big) \tau^2,$$

respectively, as long as $t_{k+4} \le T$.

Proof The bound for E_A^{k+1} is a direct consequence of (31) with $j = k+1$. The bound for $E_B^{k+\frac{1}{2}}$ is obtained as for E_A^{k+1} in the proof of Lemma 4, but starting from substituting (19b) into (19a). □

The error of the ST-LO scheme is hence a combination of two error contributions: an error caused by the low-rank approximations, and a time discretization error stemming from the leapfrog scheme. If the low-rank errors ρ_A, ρ_B, ρ_A' and ρ_B' are small, i.e., the solutions A, B of (1) are well-approximated by low-rank matrices, the time discretization error dominates.

In the proofs of Lemma 4 and Theorem 5 we used the following Gronwall-type lemma.

Lemma 6 *Let $\tau, L \geq 0$ and $\{M_k\}_{k\geq 0}$ a nonnegative, monotonically increasing sequence. If the nonnegative sequence $\{E_k\}_{k\geq 0}$ satisfies*

$$E_k \leq M_k + L\tau^2 \sum_{j=0}^{k-1} (k-j)E_j,$$

then

$$E_k \leq M_k \, \mathrm{e}^{\tau k \sqrt{L}}.$$

Proof Define $\varepsilon_k := E_k/M_k$ for all $k \geq 0$. The sequence $\{\varepsilon_k\}_{k\geq 0}$ is nonnegative and satisfies

$$\varepsilon_k \leq 1 + \tau^2 L \sum_{j=0}^{k-1} (k-j)\varepsilon_j \tag{35}$$

due to the monotonicity of $\{M_k\}_{k\geq 0}$. The statement then follows from [1, Lemma 3.8]. □

5 Dynamical low-rank integrator for stiff second-order matrix differential equations

We now consider semilinear second-order equations of the form

$$A'' = -\Omega_1^2 A - A\Omega_2^2 + f(A), \quad t \in [0,T], \quad A(0) = A_0, \quad A'(0) = B_0 \tag{36}$$

with given Hermitian, positive semidefinite matrices $\Omega_1 \in \mathbb{C}^{m\times m}$ and $\Omega_2 \in \mathbb{C}^{n\times n}$ of large norm and a Lipschitz continuous function f with moderate Lipschitz constant. It is well known that explicit methods like the leapfrog scheme (10) require step size restrictions to ensure stability. Hence the same is true for the ST-LO algorithm, since it can be viewed as a low-rank counterpart of the leapfrog scheme. Thus we aim at a scheme which is unconditionally stable (i.e. independent of $\|\Omega_{1,2}\|$).

For first-order equations, such an integrator was proposed in [12]. However, the idea in [12] cannot be applied here directly since it relies on the property that the exact solution of a linear first-order equation with initial value in $\mathscr{M}_r$ stays in $\mathscr{M}_r$ for all times. This is in general not true for linear second-order equations, so that additional considerations are required.

We reformulate (36) into an equivalent first-order problem and split the right-hand side into a linear and a nonlinear part by introducing weights $\omega_i \geq 0$, $i = 1,2,3$ with $\omega_1^2 + \omega_2^2 + \omega_3^2 = 1$

$$\begin{bmatrix} A \\ B \end{bmatrix}' = \begin{bmatrix} B \\ -\Omega_1^2 A - A\Omega_2^2 + f\big(A\big) \end{bmatrix} = \begin{bmatrix} \omega_1^2 B \\ -\Omega_1^2 A \end{bmatrix} + \begin{bmatrix} \omega_2^2 B \\ -A\Omega_2^2 \end{bmatrix} + \begin{bmatrix} \omega_3^2 B \\ f(A) \end{bmatrix}. \tag{37}$$

A natural choice would be $\omega_i^2 = 1/3$, $i = 1,2,3$ but a different weighting is also possible. The split equations can be written as

$$\begin{bmatrix} A \\ B \end{bmatrix}' = \begin{bmatrix} \omega_1^2 B \\ -\Omega_1^2 A \end{bmatrix} = \begin{bmatrix} 0 & \omega_1^2 I \\ -\Omega_1^2 & 0 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}, \tag{38a}$$

$$\begin{bmatrix} A & B \end{bmatrix}' = \begin{bmatrix} \omega_2^2 B & -A\Omega_2^2 \end{bmatrix} = \begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} 0 & -\Omega_2^2 \\ \omega_2^2 I & 0 \end{bmatrix}, \tag{38b}$$

$$\begin{bmatrix} A \\ B \end{bmatrix}' = \begin{bmatrix} \omega_3^2 B \\ f(A) \end{bmatrix}. \tag{38c}$$

The solution of the linear problems (38a) and (38b) can be expressed in terms of the matrix exponential

$$\exp\left(t \begin{bmatrix} 0 & \omega_i^2 I \\ -\Omega_j^2 & 0 \end{bmatrix} \right) = \begin{bmatrix} \cos(\omega_i t \Omega_j) & \omega_i^2 t \operatorname{sinc}(\omega_i t \Omega_j) \\ -t\Omega_j^2 \operatorname{sinc}(\omega_i t \Omega_j) & \cos(\omega_i t \Omega_j) \end{bmatrix}, \qquad j = 1,2. \tag{39}$$

The full splitting scheme reads

$$\begin{bmatrix} \widehat{A}_1 \\ \widehat{B}_1 \end{bmatrix} = \left(\phi_{\frac{\tau}{2}}^{\Omega_1} \circ \phi_{\frac{\tau}{2}}^{\Omega_2} \circ \phi_{\tau}^{\mathscr{S}} \circ \phi_{\frac{\tau}{2}}^{\Omega_2} \circ \phi_{\frac{\tau}{2}}^{\Omega_1} \right) \begin{bmatrix} \widehat{A}_0 \\ \widehat{B}_0 \end{bmatrix}, \tag{40}$$

where $\phi_{\frac{\tau}{2}}^{\Omega_1}$ and $\phi_{\frac{\tau}{2}}^{\Omega_2}$ denote the numerical flows given by Algorithm 1 with step size $\frac{\tau}{2}$ to the exact solutions of (38a) and (38b), respectively. $\phi_{\tau}^{\mathscr{S}}$ denotes the numerical flow of the ST-LO_VAR scheme, described in Algorithm 3, with right-hand side f. The overall method (40) is called ST-LOSTIFF.

When approximations at full time steps are dispensable, the last half step $\phi_{\frac{\tau}{2}}^{\Omega_1}$ in (40) can be combined with the first one of the next time step.

6 Conclusion and Outlook

In the present paper, we developed and analyzed dynamical low-rank integrators for second-order matrix differential equations of the forms (1) or (36), proving second order convergence in time under reasonable assumptions.

Numerical experiments are reported in [6], where we also discuss implementation issues. This includes rank-adaptivity, which turns out to be essential for accomplishing the desired accuracy efficiently.

Acknowledgements Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

References

1. Carle, C., Hochbruck, M., Sturm, A.: On leapfrog-Chebyshev schemes. SIAM J. Numer. Anal. **58**(4), 2404–2433 (2020). URL https://doi.org/10.1137/18M1209453

2. Ceruti, G., Lubich, C.: An unconventional robust integrator for dynamical low-rank approximation. CRC 1173 Preprint 2020/41, Karlsruhe Institute of Technology (2020). URL https://www.waves.kit.edu/downloads/CRC1173_Preprint_2020-41.pdf. Accepted by BIT Numerical Mathematics
3. Einkemmer, L., Lubich, C.: A low-rank projector-splitting integrator for the vlasov–poisson equation. SIAM Journal on Scientific Computing **40**(5), B1330–B1360 (2018). URL https://doi.org/10.1137/18M116383X
4. Einkemmer, L., Ostermann, A., Piazzola, C.: A low-rank projector-splitting integrator for the vlasov–maxwell equations with divergence correction. Journal of Computational Physics **403**, 109,063 (2020). URL https://www.sciencedirect.com/science/article/pii/S0021999119307685
5. Hairer, E., Lubich, C., Wanner, G.: Geometric numerical integration illustrated by the Störmer-Verlet method. Acta Numer. **12**, 399–450 (2003). URL https://doi.org/10.1017/S0962492902000144
6. Hochbruck, M., Neher, M., Schrammer, S.: Rank-adaptive dynamical low-rank integrators for first-order and second-order matrix differential equations. CRC 1173 Preprint 2022/13, Karlsruhe Institute of Technology (2022). DOI 10.5445/IR/1000143198. URL https://www.waves.kit.edu/downloads/CRC1173_Preprint_2022-13.pdf
7. Joly, P., Rodríguez, J.: Optimized higher order time discretization of second order hyperbolic problems: construction and numerical study. J. Comput. Appl. Math. **234**(6), 1953–1961 (2010). URL https://doi.org/10.1016/j.cam.2009.08.046
8. Kieri, E., Lubich, C., Walach, H.: Discretized dynamical low-rank approximation in the presence of small singular values. SIAM J. Numer. Anal. **54**(2), 1020–1038 (2016). URL https://doi.org/10.1137/15M1026791
9. Koch, O., Lubich, C.: Dynamical low-rank approximation. SIAM J. Matrix Anal. Appl. **29**(2), 434–454 (2007). URL https://doi.org/10.1137/050639703
10. Kusch, J., Ceruti, G., Einkemmer, L., Frank, M.: Dynamical low-rank approximation for Burgers' equation with uncertainty. CRC 1173 Preprint 2021/20, Karlsruhe Institute of Technology (2021). URL https://www.waves.kit.edu/downloads/CRC1173_Preprint_2021-20.pdf
11. Lubich, C., Oseledets, I.V.: A projector-splitting integrator for dynamical low-rank approximation. BIT **54**(1), 171–188 (2014). URL https://doi.org/10.1007/s10543-013-0454-0
12. Ostermann, A., Piazzola, C., Walach, H.: Convergence of a low-rank Lie-Trotter splitting for stiff matrix differential equations. SIAM J. Numer. Anal. **57**(4), 1947–1966 (2019). URL https://doi.org/10.1137/18M1177901