

What ODE-Approximation Schemes of Time-Delay Systems Reveal about Lyapunov-Krasovskii Functionals

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Abstract—The article proposes an approach to complete-type and related Lyapunov-Krasovskii functionals that neither requires knowledge of the delay-Lyapunov matrix function nor does it involve linear matrix inequalities. The approach is based on ordinary differential equations (ODEs) that approximate the time-delay system. The ODEs are derived via spectral methods, e.g., the Chebyshev collocation method (also called pseudospectral discretization) or the Legendre tau method. A core insight is that the Lyapunov-Krasovskii theorem resembles a theorem for Lyapunov-Rumyantsev partial stability in ODEs. For the linear approximating ODE, only a Lyapunov equation has to be solved to obtain a partial Lyapunov function. The latter approximates the Lyapunov-Krasovskii functional. Results are validated by applying Clenshaw-Curtis and Gauss quadrature to a semi-analytical result of the functional, yielding a comparable finite-dimensional approximation. In particular, the article provides a formula for a tight quadratic lower bound, which is important in applications. Examples confirm that this new bound is significantly less conservative than known results.

Index Terms—delay systems, Lyapunov-Krasovskii functional, operator-valued Lyapunov equation, spectral methods, pseudospectral discretization, Gauss quadrature

I. INTRODUCTION

Whenever a control law $u = \gamma(x)$ is constructed for a system $\dot{x} = f(x, u)$, the closed loop description $\dot{x}(t) = f(x(t), \gamma(x(t)))$ hinges on the availability of the instantaneous $x(t)$. In practice, however, measurements, network communication, computation times, or the actuator response cause a delay. The resulting $\dot{x}(t) = f(x(t), \gamma(x(t-h)))$, with a time delay $h > 0$, is a retarded functional differential equation (RFDE) and can no longer be tackled by the well-known stability theory of finite-dimensional ordinary differential equations (ODEs). What changes?

A. Motivation: Delay-free versus Time-Delay System

For delay-free nonlinear time-invariant ODEs we could consider the linearization about the equilibrium (provided it is

hyperbolic and the right-hand side is differentiable) and simply conclude exponential stability from the eigenvalues of A in the resulting $\dot{x} = Ax$, $A \in \mathbb{R}^{n \times n}$. We might be interested in the domain of attraction of the equilibrium. To this end, we could calculate a quadratic Lyapunov function $V(x) = x^\top Px$ for the linearized system by prescribing a desired Lyapunov function derivative $D_{(\dot{x}=Ax)}^+ V(x) = -x^\top Qx$. Solving the associated Lyapunov equation $PA + A^\top P = -Q$ for the matrix P with a standard algorithm is accomplished in one line of Matlab code. The obtained Lyapunov function also gives a negative Lyapunov function derivative in the nonlinear system – at least in a certain domain around the equilibrium [1]. Let this domain be estimated by a norm ball with radius $r > 0$. Then the probably most basic estimation of the domain of attraction, cf. [1, Sec. 8.2], is provided by the set of points $x \in \mathbb{R}^n$ such that $V(x) < k_1 r^2$, where k_1 is the coefficient of the positive-definiteness bound $k_1 \|x\|_2^2 \leq V(x)$. Thus, having a non-conservative result for k_1 is important. It is simply the minimum eigenvalue of P that provides the largest possible coefficient k_1 .

In time-delay systems, analogous steps become more elaborate. Given a nonlinear system, the principle of linearized stability still holds [2], and we are led to the linear RFDE

$$\dot{x}(t) = A_0 x(t) + A_1 x(t-h), \quad (1)$$

$A_0, A_1 \in \mathbb{R}^{n \times n}$, with a discrete delay $h > 0$. The characteristic equation has, generically, an infinite number of roots. Still, to determine stability for a given delay h , we can resort to numerical eigenvalue calculations [3]–[7] or we use other characteristic-equation-based criteria that can prove stability for all delays or all delays smaller than a first critical one [8], [9]. The initial state x_0 is in fact an initial function, the domain of attraction is a set of initial functions, the state x_t at time $t \geq 0$ represents the solution segment on the past delay interval $[t-h, t]$, and instead of a Lyapunov function, a Lyapunov-Krasovskii (LK) functional $V(x_t)$ is required. Analogously to the delay-free case discussed above, we can explicitly prescribe the desired LK functional derivative and determine the corresponding LK functional. The LK functional derivative along trajectories of (1) is commonly [10] set as

$$D_{(1)}^+ V(x_t) = -x^\top(t) Q_0 x(t) - x^\top(t-h) Q_1 x(t-h) - \int_{-h}^0 x^\top(t+\theta) Q_2 x(t+\theta) d\theta, \quad (2)$$

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with freely chosen $Q_0, Q_1 \succ 0_{n \times n}$, $Q_2 \succeq 0_{n \times n}$. This derivative is accomplished by so-called complete-type (if $Q_{0,1,2} \succ 0_{n \times n}$) or related LK functionals [11], [10, Thm. 2.11]. Their determination is far more elaborate than the simple Lyapunov equation for ODEs: the known formula for the solution of (2)

$$\begin{aligned} V(x_t) = & x^\top(t) \Psi(0; \tilde{Q}) x(t) + 2 \int_{-h}^0 x^\top(t) \Psi(-h - \eta; \tilde{Q}) A_1 x(t + \eta) d\eta \\ & + \int_{-h}^0 \int_{-h}^0 x^\top(t + \xi) A_1^\top \Psi(\xi - \eta; \tilde{Q}) A_1 x(t + \eta) d\eta d\xi \\ & + \int_{-h}^0 x^\top(t + \eta) [Q_1 + (h + \eta) Q_2] x(t + \eta) d\eta \end{aligned} \quad (3)$$

requires the so-called delay Lyapunov matrix function¹ $\Psi(\cdot; \tilde{Q}): [-h, h] \rightarrow \mathbb{R}^{n \times n}$ associated with $\tilde{Q} = Q_0 + Q_1 + hQ_2$. This matrix-valued function Ψ is defined via a matrix-valued time-delayed boundary-value problem [10, Def. 2.5] that first has to be solved semi-analytically or numerically. The lower bound of interest on $V(x_t)$, e.g., needed in an estimation of the domain of attraction [12, Thm. 1], is described by

$$k_1 \|x(t)\|^2 \leq V(x_t). \quad (4)$$

In contrast to the ODE case, where the minimum eigenvalue of P gives the best possible coefficient k_1 , nothing is reported about the conservativity of known formulae [10], [12] for (4).

B. Objectives and Related Results

In light of the previous section, we intend to benefit from the enormous simplification that comes along with the treatment of ODEs in contrast to RFDEs. To this end, we use schemes of ODEs that approximate the RFDE. Based on these, the paper aims to provide a new numerical approach to complete-type or related LK functionals which only requires to solve (a sequence of) Lyapunov equations. Moreover, a main objective is to get an improved coefficient k_1 in (4). Additionally, we hope to make the Lyapunov-Krasovskii theory more transparent, by interpreting the results in terms of Lyapunov-Rumyantsev partial stability of the approximating ODE.

Numerical approaches to complete-type and related LK functionals are a recent field of research. However, existing results either rely on the knowledge of the delay Lyapunov matrix function¹ Ψ , [13]–[20], or they aim to determine Ψ , [21]–[24]. In contrast, the procedure in the present paper directly leads to an approximation of the overall LK functional (3). Our main focus is not to provide a stability criterion, but, as outlined in Section I-A, we are interested in the functional itself and, in particular, in its lower bound (4).

We are going to use so-called *discretization of the infinitesimal generator* approaches, which are well-established for numerical eigenvalue calculations [3]. These approaches provide an ODE approximation of the RFDE. To analyze that ODE is also the core idea, e.g., in [25]–[27]. The involved ODE can be obtained by various methods. We resort exemplarily to the Chebyshev collocation method, also known as pseudospectral discretization [28], and to the Legendre tau method [29].

¹ $\Psi(s; \tilde{Q})$ is commonly denoted by $U(s)$ in the literature

Even in the context of more general LK functionals, a discretization of the RFDE in whatever form seems to be rarely considered in the literature. An early existence proof for quadratic LK functionals [30], as well as a recent approach to so-called safety functionals [31], also employ discretizations. These, however, do not lead to ODEs, but to difference equations (so-called *discretization of the solution operator* approaches [32]). Moreover, in [33], a discretization occurs in a proof of a linear-matrix-inequality stability criterion.

The core of the approach in the present paper is a Lyapunov equation from the ODE system matrix. The system matrices from both used discretization schemes are already known to give applicable Lyapunov, or, more generally, Riccati equation solutions. Concerning Chebyshev collocation, the resulting system matrix has successfully been employed for Lyapunov equations in the context of H_2 -norm computations [22], [34], [35], where the delay Lyapunov matrix $\Psi(0; \tilde{Q})$ at $s = 0$ is of interest. Further calculations are mentioned in [22] to obtain, at least under the assumption of an exponentially stable RFDE equilibrium, the matrix-valued function Ψ for the LK functional formula (3). The Lyapunov equation is a common element with the present paper, but only a submatrix of the Lyapunov equation solution is used in [22, Prop. 2.1], the product with a matrix exponential is required for any value of s in $\Psi(s; \tilde{Q})$, and the integral expressions in (3) still would have to be evaluated to obtain a LK functional value. Concerning Legendre tau, the system matrix (respectively a similar matrix) has already successfully been used for algebraic Riccati equations in the context of optimal control [36].

Structure. The paper is organized as follows. Sec. II describes the numerical approach, and Sec. III gives the formula for the quadratic lower bound, which is applied to an example in Sec. IV. In Sec. V, we interpret the approach in terms of partial stability of the approximating ODE. Finally, Sec. VI addresses convergence, before Sec. VII concludes the paper.

Notation. The space of continuous \mathbb{R}^n -valued functions on the interval $[a, b]$ is denoted by $C([a, b], \mathbb{R}^n)$, in short C , and square integrable functions by $L_2([a, b], \mathbb{R}^n)$ or L_2 . We write $(w_k)_{k \in \mathcal{I}}$ for a vector with entries w_k , e.g., $(w_k)_{k \in \{0, \dots, N\}} = [w_0, \dots, w_N]^\top$, or $(w_k)_k$ if the index set is clear from the context. Similar holds for matrices. The set of eigenvalues of $A \in \mathbb{R}^{n \times n}$ is $\sigma(A)$, and A is said to be Hurwitz if all eigenvalues have negative real parts. Moreover, $Q \succ 0_{n \times n}$ ($Q \succeq 0_{n \times n}$) denotes positive (semi)definiteness of $Q \in \mathbb{R}^{n \times n}$, implicitly requiring that $Q = Q^\top$. The zero vector in \mathbb{R}^n is 0_n , the vector-valued zero function on $[a, b]$ is $0_{n[a, b]}$, the $m \times n$ zero matrix $0_{m \times n}$, and the identity matrix in $\mathbb{R}^{n \times n}$ is I_n . Given $x \in \mathbb{R}^n$, we write $\|x\|_2$ for the Euclidean norm, whereas $\|x\|$ can be any arbitrary norm in \mathbb{R}^n . The Kronecker product of two matrices A and B is $A \otimes B$, and A^- denotes a generalized inverse. To emphasize the structure of a block matrix, e.g., $A = [A_1 \ A_2]$, with differently sized submatrices, $A_1 \in \mathbb{R}^{n \times nN}$, $A_2 \in \mathbb{R}^{n \times n}$, we write $A = [\text{---} A_1 \text{---} \ A_2]$. We use $\stackrel{!}{=}$ to mark a requirement, and $\stackrel{(\dots)}{=}$ if the relation is explained by (\dots) . The set of class-K functions is defined by $\mathcal{K} = \{\kappa \in C([0, \infty), \mathbb{R}_{\geq 0}) : \kappa(0) = 0, \text{ strictly increasing}\}$. For the formal definition of $D_{(\text{eq})}^+ V$, see, e.g., [37, Sec. 5.2].

II. THE NUMERICAL APPROACH

A. ODE-Approximation Schemes of RFDEs

Given a continuous initial function $x_0 \in C([-h, 0], \mathbb{R}^n)$, the state $x_t \in C([-h, 0], \mathbb{R}^n)$ of the RFDE at time $t \geq 0$ is defined by $x_t(\theta) = x(t + \theta)$, $\theta \in [-h, 0]$. Thus, it represents the solution segment on $[t - h, t]$, cf. Fig. 1a/1b. An ODE approximation has to address a finite-dimensional state vector instead. In the simplest case, this state vector $y(t)$ at time t approximates the values of the segment x_t in $N + 1$ ordered points $\tilde{\theta}_0 = -h, \dots, \tilde{\theta}_N = 0$,

$$\begin{bmatrix} x(t-h) \\ x(t+\tilde{\theta}_1) \\ \vdots \\ x(t+\tilde{\theta}_{N-1}) \\ x(t) \end{bmatrix} = \begin{bmatrix} x_t(-h) \\ x_t(\tilde{\theta}_1) \\ \vdots \\ x_t(\tilde{\theta}_{N-1}) \\ x_t(0) \end{bmatrix} \approx \underbrace{\begin{bmatrix} y^0(t) \\ y^1(t) \\ \vdots \\ y^{N-1}(t) \\ y^N(t) \end{bmatrix}}_{y(t) \in \mathbb{R}^{n(N+1)}} =: \begin{bmatrix} z^0(t) \\ z^1(t) \\ \vdots \\ z^{N-1}(t) \\ \hat{x}(t) \end{bmatrix}. \quad (5)$$

Henceforth, upper indices $k \in \{0, \dots, N\}$ address vector-valued components $y^k(t) \in \mathbb{R}^n$. Whenever the special interest in y^N shall be emphasized, we use the indicated decomposition $y = [z^\top, \hat{x}^\top]^\top$. For $\tilde{\theta}_k$ in (5), a non-equidistant grid

$$\tilde{\theta}_k = \frac{h}{2}(\tilde{\vartheta}_k - 1), \quad \text{with } \tilde{\vartheta}_k = -\cos\left(\frac{k}{N}\pi\right), \quad (6)$$

$k \in \{0, \dots, N\}$, built from shifting and scaling classical Chebyshev nodes² $\tilde{\vartheta}_k \in [-1, 1]$ to $\tilde{\theta}_k \in [-h, 0]$, has proven to be advantageous [38]. The latter is also at the core of the open-source Matlab toolbox Chebfun by Trefethen and co-workers [39], from which we can benefit in the implementations.

It remains to find the ODE

$$\dot{y}(t) = A_y y(t), \quad (7)$$

$A_y \in \mathbb{R}^{n(N+1) \times n(N+1)}$, that describes the dynamics of y . To this end, we use exemplarily the Chebyshev collocation method and the Legendre tau method combined with a change of basis. The resulting system matrices A_y are given by (63) and (68) in the appendix. Fig. 1c shows how a solution of (7) looks like, provided the initial condition $y(0)$, given by the blue points, is a discretization of the initial function $x_0 \in C([-h, 0], \mathbb{R}^n)$, cf. (12) with $\phi = x_0$.

B. An Approximation Scheme for the LK Functional

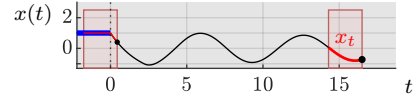
We are going to set up a Lyapunov function $V_y: \mathbb{R}^{n(N+1)} \rightarrow \mathbb{R}$ for the approximating ODE (7) (in fact, a partial Lyapunov function, see Sec. V). To this end, we make the quadratic ansatz

$$V_y(y) = y^\top P_y y, \quad (8)$$

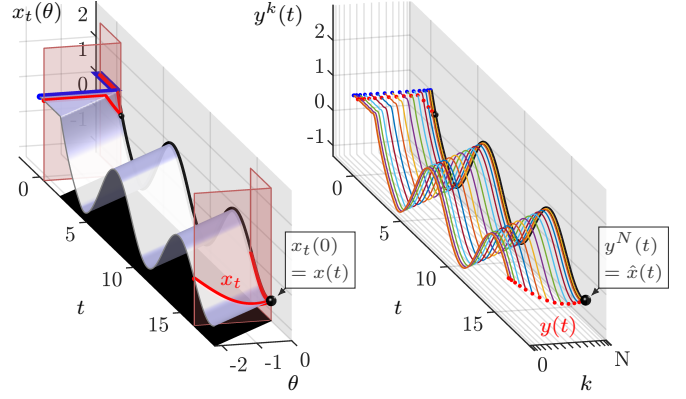
with $P_y = P_y^\top \in \mathbb{R}^{n(N+1) \times n(N+1)}$ to be determined. The derivative of V_y along solutions shall be $-y^\top Q_y y$ with a prescribed symmetric matrix Q_y

$$D_{(7)}^+ V_y(y) = y^\top (P_y A_y + A_y^\top P_y) y \stackrel{!}{=} -y^\top Q_y y, \quad (9)$$

²also called Gauss-Lobatto Chebyshev nodes (cf. Table II) or Chebyshev points of the second kind (despite of referring to extrema of the 'Chebyshev polynomials of the first kind') or endpoints-and-extrema Chebyshev nodes.



(a) RFDE solution, state x_t as solution segment



(b) evolution of the RFDE state x_t (c) components $y^k(t)$ of the ODE solution ($N = 16$, A_y from (63))

Fig. 1: Solution of $\dot{x}(t) = -0.5x(t) - x(t-2.2)$ for the initial function $x_0(\theta) \equiv 1$.

$\forall y \in \mathbb{R}^{n(N+1)}$. Thus, the unknown matrix P_y is obtained by solving the Lyapunov equation

$$P_y A_y + A_y^\top P_y = -Q_y. \quad (10)$$

See Appendix A.3.a for a description in Legendre coordinates (indicated by a subscript ζ at the matrices). We construct the right-hand side of (9) according to a discretization of the right-hand side of (2) with freely chosen matrices $Q_0, Q_1 \succ 0_{n \times n}$, $Q_2 \succeq 0_{n \times n}$. Hence, a straightforward choice of Q_y in (10) becomes visible from

$$\begin{aligned} D_{(7)}^+ V_y(y) &\stackrel{!}{=} -(y^N)^\top Q_0 y^N - (y^0)^\top Q_1 y^0 - \sum_{k=0}^N (y^k)^\top Q_2 y^k w_k \\ &= -y^\top \left(\begin{bmatrix} Q_1 & & & \\ & 0_{n \times n} & & \\ & & \ddots & \\ & & & 0_{n \times n} \\ & & & & Q_0 \end{bmatrix} + \begin{bmatrix} w_0 Q_2 & & & \\ & w_1 Q_2 & & \\ & & \ddots & \\ & & & & w_N Q_2 \end{bmatrix} \right) y \\ &=: -y^\top Q_y y, \end{aligned} \quad (11)$$

where $w_k \in \mathbb{R}$ are integration weights, see Appendix B. Sec. VI-B will present discretization-scheme-dependent modifications of Q_y that aim at improved convergence properties.

Altogether, we solve a discretization of the original problem (2), and thus $V_y(y)$ in (8) is intended to be an approximation of the LK functional $V(\phi)$. Convergence aspects will be addressed in Sec. VI. Hence, given a prescribed argument $\phi \in C([-h, 0], \mathbb{R}^n)$, which might be $\phi = x_t$ for some $t \geq 0$, or, without loss of generality, $\phi = x_0$ at $t = 0$, we can obtain a numerical approximation for the evaluation $V(\phi)$. To this end, the argument y in $V_y(y)$ must be chosen correspondingly. Such a discretization y of ϕ can be obtained by evaluating the

vector-valued function ϕ at the gridpoints (6) and stacking these $(N + 1)$ vectors in

$$y = \begin{bmatrix} | \\ z \\ | \\ \hat{x} \end{bmatrix} = \begin{bmatrix} \phi(-h) \\ \phi(\tilde{\theta}_1) \\ \vdots \\ \phi(\tilde{\theta}_{N-1}) \\ \phi(0) \end{bmatrix}. \quad (12)$$

Strictly speaking, (12) is the interpolatory discretization presupposed in the Chebyshev collocation method. If ϕ is a polynomial of order N or less, (12) also agrees with the coordinate transform (67) of the discretization in the Legendre tau method (73), but otherwise the latter might give a slightly deviating vector y (pointwise evaluations of the approximating polynomial).

To sum up, we only have to solve the Lyapunov equation (10), to obtain the approximation $V(\phi) \approx V_y(y)$.

C. Existence, Uniqueness, and Non-Negativity

Note that Q_y in (11) is a positive semidefinite, but not necessarily positive definite matrix. Let us revisit some properties of the Lyapunov equation (10) in this rather uncommon semidefinite case, without further assumptions on the involved matrices. See [40, p. 284], and [41, Thm. 1] for Lemma 2.1c.

Lemma 2.1: Consider $PA + A^\top P = -Q$, $A, Q \in \mathbb{R}^{\nu \times \nu}$.

- (a) If $\sigma(A) \cap (-\sigma(A)) = \emptyset$, then a unique solution P exists.
- (b) If $Q = Q^\top$ and P is a solution, then P^\top is also a solution. If, additionally, (a) holds, then $P = P^\top$.
- (c) If $Q \succeq 0_{\nu \times \nu}$, $P = P^\top$, and $i_0(A) = 0$, then $i_+(P) \leq i_-(A)$ and $i_-(P) \leq i_+(A)$, where $i_{-,0,+}$ are the numbers of eigenvalues with negative, zero, and positive real parts. \blacktriangleleft

Remark 2.1: Existence of the LK functional V in (2) is analogously ensured by the time-delay counterpart of Lemma 2.1a, the so-called Lyapunov condition [10, Def. 2.6]. \blacktriangleleft

Proposition 2.1: Let $Q_y \succeq 0_{n(N+1) \times n(N+1)}$ be given. If A_y is Hurwitz, then there exists a unique solution P_y in (10). Moreover, $P_y = P_y^\top$ is positive semidefinite. \blacktriangleleft

Proof: Lemma 2.1a with $\sigma(A) \subset \mathbb{C}^-$, Lemma 2.1b, and Lemma 2.1c with $i_0(A) = i_+(A) = 0$. \blacksquare

Consequently, if the zero equilibrium of the ODE approximation (7) is asymptotically stable, and $D_{(7)}^+ V_y(y)$ is chosen according to (11) and thus nonpositive, then existence, uniqueness, and nonnegativity of $V_y(y)$ in Sec. II-B are ensured.

D. Structure of the Result

To get an impression of how the Lyapunov equation solution P_y looks like, we consider an example with $n = 1$. As will be demonstrated, only little implementation effort is required.

Example 2.1: Let $\dot{x}(t) = -0.5x(t) - x(t-2.2)$ and $Q_0 = Q_1 = 1$, $Q_2 = 0$ in (11). We get the solution P_y of (10) via³
 $Q = \text{blkdiag}(Q_1, \text{zeros}(n*(N-1)), Q_0)$; $P = \text{lyap}(A', Q)$; in Matlab, provided A_y is assigned to A (see Rem. 1.1 or Rem. 1.3 in the appendix). The structure of P_y for $N = 40$ is depicted in Fig. 2. It stems from the Legendre tau method,

³If $Q_2 \neq 0_{n \times n}$ and $A_y = A_y^L$, then $\text{Tcy}' * Q_2 * \text{Tcy}$ from (37) is added to Q , with $Q_2 = \text{kron}(\text{delay} * \text{diag}([1./ (2*(0:(N-1)+1), 1)], Q_2)$.

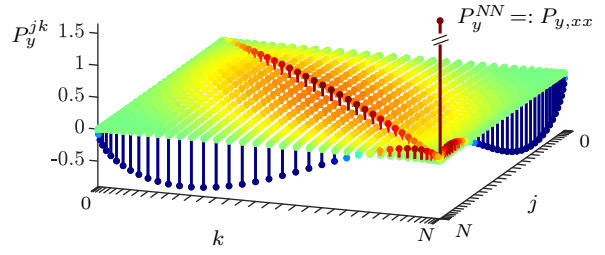


Fig. 2: Entries of the matrix P_y in Example 2.1 ($N = 40$).

i.e., $A_y = A_y^L$ from (68) is used in the Lyapunov equation (or, equivalently, $A_\zeta = A_\zeta^L$ from (66) in the Lyapunov equation from Appendix A.3.a). However, Chebyshev collocation with $A_y = A_y^C$ from (63) gives almost the same picture of P_y . \blacktriangleleft

In Fig. 2, the combs on the last column, the last row, and the diagonal as well as the striking right lower element of the matrix P_y are also existent with a refined grid. Thus, $V_y(y) = y^\top P_y y = \sum_{j=0}^N \sum_{k=0}^N (y^j)^\top P_y^{jk} y^k$ is not the discretized version of a Lebesgue integral $\int_{-h}^0 \int_{-h}^0 \phi^\top(\xi) P(\xi, \theta) \phi(\theta) d\theta d\xi$. Instead, the combs suggest that

$$\begin{aligned} V_y(y) &= y^\top P_y y = \begin{bmatrix} | \\ z \\ | \\ \hat{x} \end{bmatrix}^\top \begin{bmatrix} P_{y,zz} & P_{y,zz}^\top \\ -P_{y,xz} & P_{y,xx} \end{bmatrix} \begin{bmatrix} | \\ z \\ | \\ \hat{x} \end{bmatrix} \quad (13) \\ &= \hat{x}^\top P_{y,xx} \hat{x} + 2 \sum_{k=0}^{N-1} \hat{x}^\top P_{y,xz}^k z^k + \sum_{j=0}^{N-1} \sum_{\substack{k=0 \\ k \neq j}}^{N-1} (z^j)^\top P_{y,zz}^{jk} z^k \\ &\quad + \sum_{k=0}^{N-1} (z^k)^\top P_{y,zz}^{kk} z^k \quad (14) \end{aligned}$$

describes, through the (discrete \leftrightarrow continuous) correspondences indicated by (12) and by k vs. θ in Fig. 1

$$\begin{aligned} z^k &= \phi(\tilde{\theta}_k), \quad k \in \{0, \dots, N-1\} &\leftrightarrow \phi(\theta), \quad \theta \in [-h, 0), \\ z^j &= \phi(\tilde{\theta}_j), \quad j \in \{0, \dots, N-1\} &\leftrightarrow \phi(\xi), \quad \xi \in [-h, 0), \\ \hat{x} &= \phi(0) &\leftrightarrow \phi(0), \end{aligned}$$

the discrete version of some

$$\begin{aligned} V(\phi) &= \phi^\top(0) P_{xx} \phi(0) + 2 \int_{-h}^0 \phi^\top(0) P_{xz}(\theta) \phi(\theta) d\theta \\ &\quad + \int_{-h}^0 \int_{-h}^0 \phi^\top(\xi) P_{zz}(\xi, \theta) \phi(\theta) d\theta d\xi \\ &\quad + \int_{-h}^0 \phi^\top(\theta) P_{zz, \text{diag}}(\theta) \phi(\theta) d\theta. \quad (15a) \end{aligned}$$

Note that the latter exactly reflects the known structure of complete-type and related LK functionals given in (3).

E. Validation via Numerical Integration

To be more precise, the structure of complete-type and related LK functionals is the one in (15a), and the kernel functions can be identified in (3) as

$$\begin{aligned} P_{zz}(\xi, \theta) &= A_1^\top \Psi(\xi - \theta; \tilde{Q}) A_1, \quad P_{xz}(\theta) = \Psi(-h - \theta; \tilde{Q}) A_1, \\ P_{zz, \text{diag}}(\theta) &= Q_1 + (h + \theta) Q_2, \quad P_{xx} = \Psi(0; \tilde{Q}). \quad (15b) \end{aligned}$$

For the sake of validation, we also go the other way around and discretize the known formula of $V(\phi)$ by interpolatory quadrature rules (cf. Table II). That is, replacing the integrals in (15a) by weighted sums from evaluations at the grid points. In Appendix B, we write the result as a quadratic form

$$V(\phi) \approx y^\top P_y^{\text{quad}} y \quad (16)$$

like (13). Taking for Ψ in (15b) the semi-analytical solution approach from [23], the picture of the resulting P_y^{quad} for Example 2.1 is indeed hardly distinguishable from Fig. 2. See Sec. IV for further numerical comparisons.

Remark 2.2: Both the ODE-based approach from Sec. II-B and the numerical-integration-based approach from Sec. II-E provide an approximation $V_y(y) = y^\top P_y y$. The former seeks for an approximative solution of the defining equation (2). In contrast, the latter already starts with the exact knowledge of the LK functional (3), presupposing knowledge of Ψ , and only has to describe a discretization thereof. In so far, the numerical-integration-based approach is related to discretizations of the known $V(\phi)$ already proposed in the literature – be it based on piecewise cubic polynomials that approximate ϕ [16], [17] or, recently, on a Legendre series truncation of ϕ [19] (also used in [42], [43]), or a certain fundamental-matrix-dependent discontinuous approximation of ϕ [13], [14], [20]. With the exception of the latter approach (which addresses zero Q_0 and Q_2), integral terms with Ψ must still be evaluated. To our best knowledge, applying interpolatory quadrature rules (cf. Table II) to (15) has not yet been considered. ◀

III. THE QUADRATIC LOWER BOUND

As a result of the preceding section, we have an approximation of the LK functional. However, in applications, we also need the quadratic lower bound (4). If $Q_0, Q_1 \succ 0_{n \times n}, Q_2 \succeq 0_{n \times n}$, existence of a non-zero⁴ coefficient $k_1 > 0$ is proven in [10, Lem. 2.10], given the RFDE equilibrium is exponentially⁵ stable. In a discrete version for the approximation V_y , the bound (4) becomes $\forall y = [z^\top, \hat{x}^\top]^\top, z \in \mathbb{R}^{nN}, \hat{x} \in \mathbb{R}^n$:

$$k_1 \|\hat{x}\|_2^2 \leq V_y(y). \quad (17)$$

Since solely $\hat{x} = y^N$ is considered, (17) does not refer to the common $\lambda_{\min}(P_y) \|y\|_2^2 \leq V_y(y)$ mentioned in the introduction. Why this discrete version of (4) still also makes sense in a Lyapunov analysis of the approximating ODE, will be explained in Sec. V.

The main contribution of the present section, Lemma 3.1, immediately leads to the searched bound (17) in Thm. 3.1. For the sake of readability, we consider a general positive semidefinite matrix P with a left upper submatrix Z , instead of P_y and $P_{y,zz}$ introduced in (13). The lemma is based on the generalized Schur complement (19), cf. [44], where Z^- is a generalized matrix inverse of Z , e.g., the Moore-Penrose inverse. If Z is nonsingular, then $Z^- = Z^{-1}$.

⁴In contrast to quadratic forms from finite-dimensional matrices, in infinite dimensions coercivity of the associated bilinear form (existence of a quadratic lower bound) is a stronger concept than positive definiteness (positivity for any nonzero element). The same holds for the partial concepts. Consequently, despite of V_y being partially positive definite w.r.t. \hat{x} (Def. 5.3), the largest possible coefficient in (17) as $N \rightarrow \infty$ could become $k_1 \rightarrow 0$, cf. Rem. 4.2.

Lemma 3.1: Let $P = \begin{bmatrix} Z & B \\ B^\top & X \end{bmatrix}$ with $Z = Z^\top \in \mathbb{R}^{p \times p}, B \in \mathbb{R}^{p \times n}, X = X^\top \in \mathbb{R}^{n \times n}$. If P is positive semidefinite, then

$$\min_{\substack{z \in \mathbb{R}^p \\ x \in \mathbb{R}^n \setminus \{0_n\}}} \frac{1}{\|x\|_2^2} \begin{bmatrix} z \\ x \end{bmatrix}^\top \begin{bmatrix} Z & B \\ B^\top & X \end{bmatrix} \begin{bmatrix} z \\ x \end{bmatrix} = \lambda_{\min}(P/Z), \quad (18)$$

$$\text{where } P/Z = X - B^\top Z^- B. \quad (19)$$

The minimum is attained by $\begin{bmatrix} z \\ x \end{bmatrix} = \begin{bmatrix} -Z^- B v \\ v \end{bmatrix}$, with v being an eigenvector in $(P/Z) v = v \lambda_{\min}(P/Z)$. ◀

Proof: Let us replace z by $w := z + Z^- B x$, which amounts to the coordinate transformation

$$\begin{bmatrix} z \\ x \end{bmatrix} = \begin{bmatrix} I_p & -Z^- B \\ 0_{n \times p} & I_n \end{bmatrix} \begin{bmatrix} w \\ x \end{bmatrix} =: T_{yq} \begin{bmatrix} w \\ x \end{bmatrix}. \quad (20)$$

We arrive at the so-called generalized Aitken block-diagonalization of P in

$$\begin{aligned} \begin{bmatrix} z \\ x \end{bmatrix}^\top \begin{bmatrix} Z & B \\ B^\top & X \end{bmatrix} \begin{bmatrix} z \\ x \end{bmatrix} &= \begin{bmatrix} w \\ x \end{bmatrix}^\top T_{yq}^\top \begin{bmatrix} Z & B \\ B^\top & X \end{bmatrix} T_{yq} \begin{bmatrix} w \\ x \end{bmatrix} \\ &= \begin{bmatrix} w \\ x \end{bmatrix}^\top \begin{bmatrix} Z & -Z Z^- B + B \\ -B^\top Z^- Z + B^\top & X - B^\top Z^- B \end{bmatrix} \begin{bmatrix} w \\ x \end{bmatrix} \\ &= w^\top Z w + x^\top (P/Z) x, \end{aligned} \quad (21)$$

with the last step being based on $-Z Z^- B + B = 0_{p \times n}$, which holds if P is positive semidefinite [44, Thm. 1.19]. The submatrix Z of P is also positive semidefinite due to Cauchy's Interlacing Theorem, and thus (21) is lower bounded by

$$w^\top Z w + x^\top (P/Z) x \geq x^\top (P/Z) x \geq \lambda_{\min}(P/Z) \|x\|_2^2.$$

The bound is attained for $w = 0_p$ and $x = v$. ■

The following theorem is not only useful for the ODE-based approach from Sec. II-B. It is as well applicable to the numerical-integration-based results from Sec. II-E.

Theorem 3.1: If P_y in $V_y(y) = y^\top P_y y$ is positive semidefinite, then the largest possible coefficient in (17) is

$$k_1 = \lambda_{\min}(P_y/P_{y,zz}), \quad (22)$$

where $P_{y,zz}$ denotes the left upper $nN \times nN$ submatrix of P_y and (\cdot/\cdot) is the generalized Schur complement (19). ◀

Proof: Lemma 3.1 applied to $P = P_y$ with $Z = P_{y,zz}$ as in (13). ■

Testing whether P_y is positive semidefinite is not even required if V_y originates from the ODE-based approach in Sec. II-B. If A_y is Hurwitz, the only thing to do is to evaluate (22).

Corollary 3.1: Let $V_y(y) = y^\top P_y y$, where P_y is a solution of (10) for a given positive semidefinite matrix Q_y . If A_y is Hurwitz, then (17) holds with k_1 from (22). ◀

Proof: By Prop. 2.1, P_y is positive semidefinite. Consequently, Thm. 3.1 applies. ■

See Appendix A.3.d for an evaluation in other coordinates.

IV. EXAMPLE AND COMPARISON

We compare the thus obtained bound with known quadratic lower bounds (4) on the LK functional (15). These known formulae for the coefficient in $k_1 \|x(t)\|_2^2 \leq V(x_t)$ are

$$k_1 = \max \alpha \quad [10, \text{Lem. 2.10}]$$

$$\text{s.t. } \begin{bmatrix} Q_0 & 0_{n \times n} \\ 0_{n \times n} & Q_1 \end{bmatrix} + \alpha \begin{bmatrix} A_0^\top + A_0 & A_1 \\ A_1^\top & 0_{n \times n} \end{bmatrix} \succeq 0_{2n \times 2n},$$

$$k_1 = \min \left\{ \frac{\lambda_{\min}(Q_0)}{2\|A_0\|_2 + \|A_1\|_2}, \frac{\lambda_{\min}(Q_1)}{\|A_1\|_2} \right\}, \quad [12, \text{Prop. 1}]$$

provided the equilibrium is exponentially⁵ stable and $Q_0, Q_1 \succ 0_{n \times n}, Q_2 \succeq 0_{n \times n}$. Two issues should be noted.

Firstly, since the LK functional satisfies by construction the monotonicity condition of the common LK theorem, cf. (29), the existence of a quadratic lower bound with $k_1 > 0$ (or actually even $k_1 \geq 0$, cf. Thm. 5.4) is also the crucial missing step that proves asymptotic stability via the LK functional. However, the above formulae are only valid if exponential (equivalently, asymptotic) stability has been proven beforehand. Hence, the stability analysis must already be done by other means in a separate step. For instance, this can be achieved via frequency-domain based methods, e.g., via the eigenvalues of A_y . Having thus A_y already at hand, the approach in the present paper becomes even more convenient.

Remark 4.1: As a consequence of the above issue, how at all to conclude stability from the LK functional (15) or the involved delay Lyapunov matrix function Ψ has long been an open question. It has only recently been resolved by Egorov et al. [14] and Gomez et al. [13]. The criterion is equivalent to requiring that, for some $\tilde{Q} \succ 0_{n \times n}$,

$$\tilde{P}_{zz}(\xi, \eta) := \Psi(\xi - \eta; \tilde{Q}) \quad (23)$$

is a positive definite kernel, in the sense that the block matrix $(\tilde{P}_{zz}(\theta_j, \theta_k))_{jk}$ must be positive semidefinite, with an a priori bound on the discretization resolution of the grid $(\xi, \eta) \in \{\theta_j, \theta_k\}_{jk} \subset [-h, 0] \times [-h, 0]$. Despite of a completely different framework, the result can be brought in relation to Sec. II-E by rewriting the matrix in (16) as

$$P_y^{\text{quad}} = S^\top (\tilde{P}_{zz}(\tilde{\theta}_j, \tilde{\theta}_k))_{jk} S + D, \quad (24)$$

with $S = \text{diag}((w_k)_k) \otimes A_1 + \begin{bmatrix} 0_{n \times nN} & I_n \\ 0_{nN \times nN} & 0_{nN \times n} \end{bmatrix}$ and $D = \text{blkdiag}((w_k(Q_1 + (h + \tilde{\theta}_k)Q_2))_k)$, cf. (79) with (15b). The first term in (24) clearly preserves the positive semidefiniteness of $(\tilde{P}_{zz}(\tilde{\theta}_j, \tilde{\theta}_k))_{jk}$, and D is only an added block diagonal matrix that inherits positive semidefiniteness from Q_1, Q_2 . ◀

Secondly, of course the LK functional changes as the delay changes. Note that, however, the above stated formulae for k_1 do not depend on the value of the delay.

Example 4.1: For all delay values h that are smaller than $h_c := \arccos(-0.9)/\sqrt{1 - 0.9^2} \approx 6.17$, the equilibrium of

$$\dot{x}(t) = \begin{bmatrix} -2 & 0 \\ 0 & -0.9 \end{bmatrix} x(t) + \begin{bmatrix} -1 & 0 \\ -1 & -1 \end{bmatrix} x(t-h) \quad (25)$$

is asymptotically stable [9, Example 3.2]. Let $Q_0 = Q_1 = I_2, Q_2 = 0_{2 \times 2}$. For any given $h > 0$ (affecting A_y), the Lyapunov equation solution P_y can be computed as in Example 2.1. We get k_1 in (22) via the additional lines

```
p=mat2cell(P, n*[N, 1], n*[N, 1]);
k1=min(eig(p{2,2}-p{2,1}*p{1,1}\p{1,2})))
```

in Matlab (as $P_{y,zz}$ is nonsingular). We also consider the numerical-integration-based P_y^{quad} from (79) and (80). Fig. 3a shows the convergence of k_1 for all approaches. ◀

⁵ equivalently, asymptotically since (1) is a linear autonomous RFDE. In linear RFDEs with bounded delays, uniform asymptotic stability and uniform exponential stability are equivalent [37, Thm. 5.3 in Ch. 6]. Moreover, in autonomous or periodic RFDEs (in contrast to neutral FDEs), asymptotic stability is always uniform [37, Lemma 1.1 in Ch. 5].

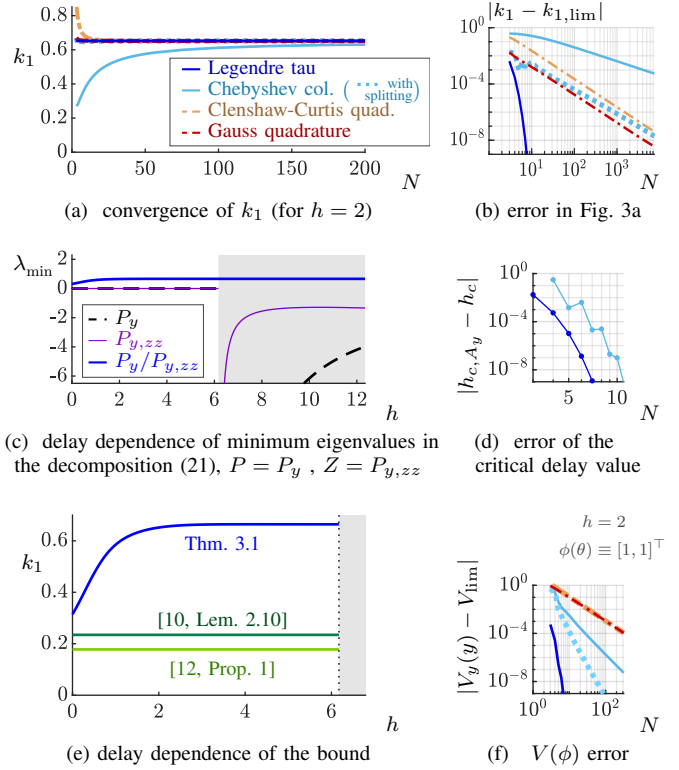


Fig. 3: Example 4.1. In particular, Fig. 3e shows the improved quadratic lower bound. (Figures a,b,d,f share the same legend).

Fig. 3 also gives some further insights. Fig. 3b certifies a surprisingly fast convergence for the Legendre tau method. This is also confirmed by other examples (if $Q_2 \neq 0_{n \times n}$, the Lyapunov equation right-hand side from Sec. VI-B below should be used). For the Chebyshev collocation method, we are going to introduce a splitting approach in Sec. VI-B, which gives an improved rate of convergence, cf. Fig. 3b.

Fig. 3c (Legendre tau, $N = 1000$) shows the interplay of the matrices in (21), once the asymptotic stability is lost for delays larger than $h \approx 6.17$. We are going to prove in Thm. 5.4 that positive semidefiniteness of P_y is indeed necessary and sufficient for A_y being Hurwitz.

Let us consider the boundary $h_{c,Ay}$ between the white and gray delay region in Fig. 3c. It marks the smallest delay at which the matrix A_y is no longer Hurwitz (equivalently, where no longer a positive semidefinite solution P_y exists), which can, e.g., be fine estimated by a bisection method. Already with a rough discretization resolution N , this boundary reflects the analytically known critical delay h_c of (25) quite precisely, and its rapid convergence is shown in Fig. 3d for both the Legendre tau and the Chebyshev collocation method.

Most importantly, Fig. 3e reveals that the largest possible quadratic lower bound depends on the value of the delay. Thm. 3.1 clearly gives a less conservative value of k_1 than the known formulae (green lines). For non-small delays, the bound is even improved by a multiple.

Fig. 3f shows the rapid convergence of the numerical result for $V(\phi)$ with an exemplary argument ϕ .

A remark on non-complete functionals is in order.

| | k_1 | [12, Prop. 1] | [10, Lem. 2.10] | Thm. 3.1 |
|-------------------|--------|---------------|-----------------|----------|
| [12], Example 5.1 | 0.7500 | | 0.8229 | 1.4596 |
| [12], Example 5.2 | 0.6000 | | 2.3238 | 3.8660 |
| [12], Example 5.4 | 0.1464 | | 0.1978 | 0.5229 |

TABLE I: Improvements of the quadratic lower bound for three physical examples from the literature.

Remark 4.2: If $Q_1 = Q_2 = 0_{n \times n}$, only a local cubic lower bound on V is known to exist, and non-existence⁴ of a positive quadratic one is proven for [10, Example 2.1]. Indeed, for this example, k_1 from (22) converges to zero as N increases. ◀

Finally, the reduced conservativity of k_1 , already indicated by Fig. 3e, is confirmed by other examples in Table I.

V. INTERPRETATION IN TERMS OF PARTIAL STABILITY

Note that V_y obtained in Sec. II-B does not necessarily qualify as a Lyapunov function for the ODE (7) since, if $Q_2 = 0_{n \times n}$, the matrix Q_y in the Lyapunov function derivative (11) is not positive definite. Even if $Q_2 \succ 0_{n \times n}$, the involved Q_y is theoretically positive definite for any finite N , but the smallest eigenvalue of Q_y converges to zero as N increases (the denser the grid, the smaller the integration weights w_k). Moreover, the lower bound (17) on V_y does not fit with the classical Lyapunov theory. The present section explains why V_y is still meaningful for a stability analysis of the approximating ODE. Within the presented approach, the lower bound (17) is exactly what is required. First, we clarify what we are actually looking for when we target stability in a RFDE.

A. Stability in RFDEs

Having in mind the classical Lyapunov theorem for ODEs, one might wonder why the lower bound in (4) relies on $\|x(t)\|$ and not on the norm of the RFDE state x_t . The latter addresses the norm in $C([-h, 0], \mathbb{R}^n)$ defined by

$$\|x_t\|_C = \max_{\theta \in [-h, 0]} \|x_t(\theta)\|. \quad (26)$$

For Lyapunov functions in ODEs, both the positive-definiteness bound ($\kappa_1(\|x\|) \leq V(x)$, $\kappa_1 \in \mathcal{K}$) and the monotonicity requirement ($D_f^+ V(x) \leq -\kappa_3(\|x\|)$, $\kappa_3 \in \mathcal{K}$) refer to the norm of the ODE state. Thus, one would expect (26) at these places when transferring Lyapunov's results from $x(t) \in \mathbb{R}^n$ to $x_t = \phi \in C([-h, 0], \mathbb{R}^n)$. However, this is not the case in the following common LK theorem – neither in the left inequality of (28) nor in (29). Instead of $\|\phi\|_C = \|x_t\|_C$, only $\|\phi(0)\| = \|x_t(0)\| = \|x(t)\|$ occurs. As usual, the theorem refers to general autonomous RFDEs

$$\dot{x}(t) = f(x_t), \quad (27)$$

with $f(0_{n_{[-h, 0]}}) = 0_n$ and f locally Lipschitz.

Theorem 5.1 (LK Theorem [37, Thm. 5-2.1]): If there is a continuous $V: C([-h, 0], \mathbb{R}^n) \rightarrow \mathbb{R}_{\geq 0}$ such that, for all ϕ in a domain $G \subseteq C([-h, 0], \mathbb{R}^n)$, $0_{n_{[-h, 0]}} \in G$, it holds

$$\kappa_1(\|\phi(0)\|) \leq V(\phi) \leq \kappa_2(\|\phi\|_C) \quad (28)$$

$$D_{(27)}^+ V(\phi) \leq -\kappa_3(\|\phi(0)\|), \quad (29)$$

with some class- \mathcal{K} functions $\kappa_{1,2,3} \in \mathcal{K}$, then the zero equilibrium of (27) is asymptotically stable. ◀

The key to the above question is that there are two, obviously equivalent, definitions of asymptotic stability in the RFDE. Starting from the same norm ball for the initial function x_0 , they differ in the condition on the implication side: Either the state x_t with the norm (26) is taken into account (Def. 5.1a), or the pointwise solution $x(t) \in \mathbb{R}^n$ is considered (Def. 5.1b).

Definition 5.1 (Lyapunov stability in RFDEs): The zero equilibrium of (27) is asymptotically stable if

- a) $\forall \varepsilon > 0, \exists \delta > 0 : \|x_0\|_C < \delta \implies \forall t \geq 0 : \|x_t\|_C < \varepsilon$
and $\exists r > 0 : \|x_0\|_C < r \implies \|x_t\|_C \rightarrow 0$ as $t \rightarrow \infty$
or, equivalently,
b) $\forall \varepsilon > 0, \exists \delta > 0 : \|x_0\|_C < \delta \implies \forall t \geq 0 : \|x(t)\| < \varepsilon$
and $\exists r > 0 : \|x_0\|_C < r \implies \|x(t)\| \rightarrow 0$ as $t \rightarrow \infty$. ◀

In terms of the whole state x_t , the pointwise consideration in Def. 5.1b refers only to the boundary value $x(t) = x_t(0)$ in Fig. 1b. The classical LK theorem, Thm. 5.1, addresses Def. 5.1b since, $\forall t \geq 0$,

$$\kappa_1(\|x(t)\|) \stackrel{(28)}{\leq} V(x_t) \stackrel{(29)}{\leq} V(x_0) \stackrel{(28)}{\leq} \kappa_2(\|x_0\|_C) \quad (30)$$

gives a pointwise estimation $\|x(t)\| \leq \kappa_1^{-1}(\kappa_2(\|x_0\|_C))$ to indicate stability. A theorem that addresses Def. 5.1a would instead rely on $\kappa_1(\|\phi\|_C)$ in (28) and $\kappa_3(\|\phi\|_C)$ in (29), as has been expected above. Such a theorem is also valid [45, Thm. 30.1], but these bounds are quite restrictive and not satisfied by common LK functionals.

B. Partial Stability in ODEs

In the approximating ODE, cf. Fig. 1c, the state $y(t) \in \mathbb{R}^{n(N+1)}$ represents the RFDE state $x_t \in C([-h, 0], \mathbb{R}^n)$, and its last vector-valued component $y^N(t) = \hat{x}(t) \in \mathbb{R}^n$ represents the pointwise solution value $x(t) \in \mathbb{R}^n$. While Def. 5.1a translates to the usual⁶ definition of asymptotic stability in the ODE, Def. 5.1b amounts to the concept of partial asymptotic stability with respect to (w.r.t.) \hat{x} . Again, we give the definition for a general class of systems. These are ODEs where $y(t)$ is partitioned into two parts, $z(t) \in \mathbb{R}^p$ and $\hat{x}(t) \in \mathbb{R}^n$, with $\dim(y(t)) = p+n$, and the latter part $\hat{x}(t)$ is of special interest. That is, we consider autonomous ODEs

$$\frac{d}{dt} \begin{bmatrix} z(t) \\ \hat{x}(t) \end{bmatrix} = \begin{bmatrix} f^z(z(t), \hat{x}(t)) \\ f^x(z(t), \hat{x}(t)) \end{bmatrix} \quad (31)$$

with $\begin{bmatrix} f^z(0_p, 0_n) \\ f^x(0_p, 0_n) \end{bmatrix} = 0_{p+n}$ and $f^{z,x}$ locally Lipschitz.

Definition 5.2 (Lyapunov-Rumyantsev partial stability): The zero equilibrium of (31) is partially stable w.r.t. \hat{x} if

$$\forall \varepsilon > 0, \exists \delta > 0 : \left\| \begin{bmatrix} z(0) \\ \hat{x}(0) \end{bmatrix} \right\| < \delta \implies \forall t \geq 0 : \|\hat{x}(t)\| < \varepsilon.$$

It is partially asymptotically stable w.r.t. \hat{x} if, additionally,

$$\exists r > 0 : \left\| \begin{bmatrix} z(0) \\ \hat{x}(0) \end{bmatrix} \right\| < r \implies \|\hat{x}(t)\| \rightarrow 0 \text{ as } t \rightarrow \infty. \quad \blacktriangleleft$$

⁶The choice of the norm $\|y\|_\infty = \max_{k \in \{0, \dots, N\}} \|y^k\|$ is irrelevant due to the equivalence of norms in finite-dimensional spaces.

For an in-depth discussion of this stability concept, see [46]. As in Def. 5.1b for stability in RFDEs, the initial value deviations consider the whole state, but the implications address only the part \hat{x} that is of special interest.

The following partial stability theorem fits well with Thm. 5.1 (note that an upper bound $V_y([\frac{z}{\hat{x}}]) \leq \kappa_2(\|\frac{z}{\hat{x}}\|)$ always exists).

Theorem 5.2 (Peiffer and Rouche 1969 [47, Thm. II]): . If there is a continuous $V_y: \mathbb{R}^{p+n} \rightarrow \mathbb{R}_{\geq 0}$, $V_y(0_{p+n}) = 0$, such that, for all $[\frac{z}{\hat{x}}]$ in a domain $G \subseteq \mathbb{R}^{p+n}$, $0_{p+n} \in G$, it holds

$$\kappa_1(\|\hat{x}\|) \leq V_y([\frac{z}{\hat{x}}]), \quad (32)$$

with $\kappa_1 \in \mathcal{K}$, and $D_{(31)}^+ V_y([\frac{z}{\hat{x}}]) \leq 0$, then the zero equilibrium of (31) is partially stable w.r.t. \hat{x} . If, additionally, $\forall [\frac{z}{\hat{x}}] \in G$:

$$D_{(31)}^+ V_y([\frac{z}{\hat{x}}]) \leq -\kappa_3(\|\hat{x}\|) \quad (33)$$

with $\kappa_3 \in \mathcal{K}$, and there exists $r > 0$ such that $\left\| \begin{bmatrix} z(0) \\ \hat{x}(0) \end{bmatrix} \right\| < r$ implies that $\|f^x(z(t), \hat{x}(t))\|$ is bounded for all $t \geq 0$, then it is partially asymptotically stable w.r.t. \hat{x} . ◀

As in the classical LK theorem for RFDEs (Thm. 5.1), both the (partial) positive-definiteness condition (32) and the monotonicity requirement⁷ (33) consider only the part of special interest $\hat{x}(t) = y^N(t) \approx x(t) = x_t(0)$. We call V in Thm. 5.2 a *partial Lyapunov function*.

To sum up, the discretization of Def. 5.1b for RFDE stability is exactly the definition of Lyapunov-Rumyantsev partial stability w.r.t. \hat{x} (Def. 5.2). Moreover, the Lyapunov-Krasovskii theorem for stability in the RFDE (Thm. 5.1) becomes Peiffer and Rouche's theorem for partial stability (Thm. 5.2).

C. Equivalence of Stability and Partial Stability in the Approximating ODE

In general ODEs, the concept of partial stability is a weaker concept than stability. We can still focus without doubt on partial stability if the equivalence between Def. 5.1a and 5.1b is reflected by the ODE approximation, so that proving partial stability w.r.t. \hat{x} is already sufficient for proving stability.

Condition 5.1: The zero equilibrium of the ODE approximation (7) is (asymptotically) stable if and only if it is partially (asymptotically) stable w.r.t. \hat{x} . ◀

To verify this condition for the discretization schemes at hand, we consider a result from the realm of total stability.

Lemma 5.1: [49, Thm. 3.11.3]. If the zero equilibrium of the auxiliary system

$$\dot{z} = f^z(z, 0_n) \quad (34)$$

is asymptotically stable, then, in (31), partial (asymptotic) stability w.r.t. \hat{x} of the zero equilibrium implies (asymptotic) stability of the zero equilibrium. ◀

Loosely speaking, for reasonable approximations the latter seems to be a matter of course since, if $x(t)$ for $t \geq 0$ could be forced to remain zero, then, for $t \geq h$, the solution segment x_t is zero, which should at least asymptotically be reflected by $z(t) \rightarrow 0_p$ as $t \rightarrow \infty$. In terms of the linear

⁷Criteria that come without the boundedness condition below (33) require a full monotonicity condition $D_{(31)}^+ V_y(y) \leq -\kappa_3(\|y\|)$, $\kappa_3 \in \mathcal{K}$, cf. [48].

ODE (7), Lemma 5.1 only refers to the submatrix $A_{y,zz} := (A_y^{jk})_{j,k \in \{0, \dots, N-1\}}$. For collocation schemes like $A_y = A_y^C$ in Appendix A.1, stability of this submatrix is clearly neither affected by the RFDE coefficient matrices A_0, A_1 (occurrence only in the last block-row), nor the delay h (scalar factor), nor the dimension n (Kronecker product with I_n). For tau methods, an analogous independence can be achieved by first applying a change of basis w.r.t. the z -coordinates. In appropriate coordinates, setting, e.g., $A_0 = A_1 = 0_{n \times n}$ does not alter the submatrix eigenvalues. The next lemma formulates the thus motivated coordinate invariant form of Lemma 5.1 for the linear ODE. Whether it applies is, consequently, no question of A_0, A_1, h , but it is rather a question of the discretization scheme.

Corollary 5.1: Consider the linear ODE (7). If there exists a change of coordinates w.r.t. z , where $[z^\top, \hat{x}^\top]^\top = T[v^\top, \hat{x}^\top]^\top$, such that the left upper $nN \times nN$ submatrix of $T^{-1}A_y T$ is Hurwitz, then Condition 5.1 holds. ◀

Proof: Lemma 5.1 with (31) given by $\frac{d}{dt} [\frac{v}{\hat{x}}] = T^{-1}A_y T [\frac{v}{\hat{x}}]$. ◀

For $A_y = A_y^C$ from the Chebyshev collocation method (A.1), the submatrix $A_{y,zz}$ can indeed proven to be Hurwitz for any discretization resolution N [26, Prop. 2], [50]. Thus, by Corollary 5.1 (with $v = z$), Condition 5.1 holds. For other discretization schemes we refer to [51, Sec. 4.3.2]. For the Legendre tau method, we consider the coordinates described in (76), where $v = [(\zeta^0)^\top, \dots, (\zeta^{N-1})^\top]^\top$ consists of the first N of the $N+1$ Legendre coordinates. Then, Corollary 5.1 (with $T^{-1}A_y T = T_{\chi\zeta} A_\zeta T_{\chi\zeta}^{-1}$ and $T_{\chi\zeta}$ from (76)) can numerically shown to be true for relevant values of N .

Consequently, Condition 5.1 is not only a reasonable assumption for an ODE that approximates an RFDE, but, regarding the discretization of a RFDE, it can even be confirmed as a property of the underlying discretization schemes.

D. Proving Stability in the ODE via $V_y(y)$

The main result of this section, Thm. 5.3, shows that V_y from Sec. II-B indeed always qualifies as a partial Lyapunov function for (7) if the equilibrium is asymptotically stable. As a side effect, Thm. 5.4 gives a necessary and sufficient stability criterion in terms of P_y . We introduce the following wording.

Definition 5.3: Let \hat{x} -pd be the abbreviation for 'partially positive definite w.r.t. the components \hat{x} '. We call

(a) a function $U: \mathbb{R}^{p+n} \rightarrow \mathbb{R}$; $y = [\frac{z}{\hat{x}}] \mapsto U(y)$ \hat{x} -pd on $\Omega \subseteq \mathbb{R}^{p+n}$ if it is positive semidefinite ($\forall y \in \Omega: U(y) \geq 0$, $U(0_{p+n}) = 0$) and $\forall y = [\frac{z}{\hat{x}}] \in \Omega$ with $\|\hat{x}\| \neq 0: U(y) > 0$.

(b) a symmetric matrix $M = M^\top \in \mathbb{R}^{(p+n) \times (p+n)}$ \hat{x} -pd if $U(y) = y^\top M y$ is \hat{x} -pd on \mathbb{R}^{p+n} . ◀

Analogously to local, or in terms of $U(y) = y^\top M y$ even global, positive definiteness, cf. [1, Lemma 4.3], partial positive definiteness can be expressed via a class-K function.

Lemma 5.2: $M = M^\top \in \mathbb{R}^{(p+n) \times (p+n)}$ is \hat{x} -pd if and only if $\exists \kappa \in \mathcal{K}$ such that $\forall [\frac{z}{\hat{x}}] \in \mathbb{R}^{p+n}: \kappa(\|\hat{x}\|) \leq [\frac{z}{\hat{x}}]^\top M [\frac{z}{\hat{x}}]$. ◀

Regarding $y^\top Q_y y = -D_{(31)}^+ V_y(y)$, Lemma 5.2 refers to the class-K function in (33). For Q_y in (11) or (37), we can choose

$$\kappa_3(\|\hat{x}\|_2) := \lambda_{\min}(Q_0) \|\hat{x}\|_2^2 \leq y^\top Q_y y. \quad (35)$$

Rather decisive is whether the Lyapunov equation solution P_y is also \hat{x} -pd, as it is required in (32) with $V_y(y) = y^\top P_y y$.

Lemma 5.3: Let $P_y = P_y^\top$ be a solution of (10) for a \hat{x} -pd Q_y . If P_y is positive semidefinite, then it is even \hat{x} -pd. ◀

Proof: The result is shown by contradiction. Assume there exists a $y_c = \begin{bmatrix} z_c \\ \hat{x}_c \end{bmatrix}$ with $\|\hat{x}_c\| \neq 0$ such that $y_c^\top P_y y_c = 0$. Then $P_y y_c = 0_{n(N+1)}$ (cf. a decomposition $P_y = C^\top C$ in $y_c^\top P_y y_c = \|C y_c\|_2^2 = 0$, $C^\top C y_c = 0_{n(N+1)}$), which leads by (10) to $y_c^\top Q_y y_c = 0$, contradicting that Q_y is \hat{x} -pd. ■

Lemma 5.4: Let $P_y = P_y^\top$ be a solution of (10) for a \hat{x} -pd Q_y . Consider Thm. 5.2 in terms of partial asymptotic stability w.r.t. $y^N = \hat{x}$ for the zero equilibrium in (7). If P_y is positive semidefinite, then, under Cond. 5.1, $V_y(y) = y^\top P_y y$ satisfies the conditions on a partial Lyapunov function in Thm. 5.2. ◀

Proof: In Thm. 5.2, (32) and (33) hold by Lemma 5.3 and 5.2. The boundedness condition on $\|f^x(z(t), \hat{x}(t))\|$ in Thm. 5.2 is also ensured: due to Cond. 5.1, the already provable partial stability implies stability, which is accompanied by compactness of the trajectories, and the image under the continuous mapping f^x remains compact. ■

We are led to the desired interpretation of the function V_y whenever the ODE equilibrium is asymptotically stable.

Theorem 5.3: If A_y is Hurwitz and Cond. 5.1 applies, then V_y from Sec. II-B is a partial Lyapunov function for (7). ◀

Proof: If A_y is Hurwitz, P_y is positive semidefinite by Prop. 2.1. As Q_y in Sec. II-B is \hat{x} -pd, Lemma 5.4 applies. ■

Our focus is not preliminary on a stability criterion in terms of P_y because we can simply compute the eigenvalues of A_y to conclude stability. Nevertheless, the following result might still be of interest since it shows that V_y must only be tested for positive semidefiniteness. Proving existence of κ_1 in (32) is not required due to Lemma 5.3.

Theorem 5.4: Assume Cond. 5.1 holds. Let $P_y = P_y^\top$ be a solution of (10) for a \hat{x} -pd matrix Q_y (e.g., (11) or (37)). The zero equilibrium of the approximating ODE (7) is asymptotically stable if and only if P_y is positive semidefinite. ◀

Proof: If $P_y \succeq 0_{n(N+1) \times n(N+1)}$, then Lemma 5.4 applies. Thus, partial asymptotic stability w.r.t. \hat{x} can be proven by Thm. 5.2. The latter implies asymptotic stability by Cond. 5.1. Conversely, if A_y is Hurwitz, then $P_y \succeq 0_{n(N+1) \times n(N+1)}$ because of Prop. 2.1. ■

We conclude Sec. V as follows. The function V_y obtained in Sec. II-B does not necessarily qualify as a classical Lyapunov function. Instead, it is a partial Lyapunov function for a system in which proving partial stability is already sufficient for proving stability.

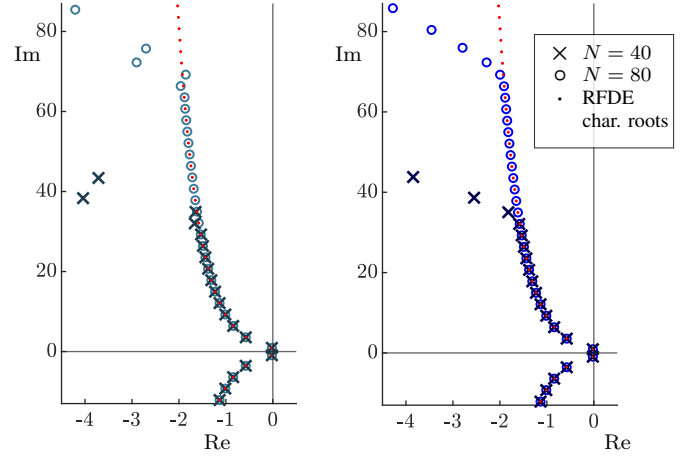
VI. CONVERGENCE

A sequence of refined results with enlarged N s should always be considered. It remains to discuss convergence aspects.

A. Stability Properties of the Approximating ODEs

The discretization scheme used in the proposed ODE-based approach should be stability preserving in the following sense.

Condition 6.1: Provided the discretization resolution N is chosen sufficiently large, the zero equilibrium of the approximating ODE is exponentially stable if and only if the zero equilibrium of the RFDE is exponentially stable. ◀



(a) Chebyshev collocation: eigenvalues of A_y^C in (63)

(b) Legendre tau: eigenvalues of A_y^L in (66) or, equivalently, A_y^L (68)

Fig. 4: Characteristic roots (A_0, A_1, h from Example 2.1).

Chebyshev collocation has successfully been applied in various fields [22], [25], [27], [28], [52] where Cond. 6.1 is also desirable. It is known that eigenvalues of A_y^C converge to the characteristic roots of the RFDE, i.e., to the solutions s of $\det(sI_n - A_0 - e^{-sh}A_1) = 0$, or, equivalently, to the eigenvalues of the infinitesimal generator of the C_0 -semigroup of solution operators, see [28]. The red points in Fig. 4a show typical eigenvalue chains in RFDEs, and the crosses and circles demonstrate how this chain is approached by the eigenvalues of A_y^C . There are also some additional spurious eigenvalues that do not match with RFDE characteristic roots. These, however, are easily identifiable as they do not persist when N changes [28, Prop. 3.7]. See, in Fig. 4a, the crosses ($N = 40$) that do not match with circles ($N = 80$). Moreover, from numerical observations, they are not expected to hamper Cond. 6.1, see also the discussions in [27, p. 361], [22, p. 853]. Thus, despite of not being proven, Cond. 6.1 in practice is a tenable assumption for the Chebyshev Collocation method.

The Legendre tau method is similarly powerful in approximating eigenvalues, see Fig. 4b. Stability preservation of this method (Cond. 6.1) is proven in [7, Thm. 5.3].

As a consequence, the stability-dependent characterization of P_y from Sec. V-D is also meaningful for the RFDE.

Corollary 6.1: Assume the discretization scheme satisfies Cond. 6.1 and 5.1. Provided N is sufficiently large, then P_y from Sec. II-B is positive semidefinite if and only if the zero equilibrium of the RFDE is asymptotically stable. ◀

Proof: Thm. 5.4 combined with Cond. 6.1. ■

B. Scheme-Dependent Improvements

1) *Chebyshev collocation:* Consider the ODE-based approach with the Chebyshev collocation method. To improve the convergence properties (indicated in Fig. 3), we transform the problem of approximating $V(\phi)$ to a problem of approximating a modified $V_0(\phi)$ with Q_1 and Q_2 being zero. To this end, we choose the shift matrices $\tilde{Q}_1 = Q_1$ and $\tilde{Q}_2 = Q_2$ in the following splitting lemma. The idea is closely related to the derivation of complete-type functionals in [10, Thm. 2.11].

Lemma 6.1 (Splitting): For $Q_0, Q_1, Q_2 \in \mathbb{R}^{n \times n}$, let $V(\phi) = V(\phi; Q_0, Q_1, Q_2)$ denote a solution of (2). Then

$$V(\phi; Q_0, Q_1, Q_2) = V_0(\phi) + V_1(\phi) + V_2(\phi) \quad \text{with} \quad (36)$$

$$V_0(\phi) = V(\phi; (Q_0 + \tilde{Q}_1 + h\tilde{Q}_2), (Q_1 - \tilde{Q}_1), (Q_2 - \tilde{Q}_2))$$

$$V_1(\phi) = V(\phi; -\tilde{Q}_1, \tilde{Q}_1, 0_{n \times n}) = \int_{-h}^0 \phi^\top(\eta) \tilde{Q}_1 \phi(\eta) d\eta$$

$$V_2(\phi) = V(\phi; -h\tilde{Q}_2, 0_{n \times n}, \tilde{Q}_2) = \int_{-h}^0 \phi^\top(\eta) (h + \eta) \tilde{Q}_2 \phi(\eta) d\eta$$

for arbitrarily chosen shifts $\tilde{Q}_1, \tilde{Q}_2 \in \mathbb{R}^{n \times n}$. ◀

Proof: For $\phi(\eta) = x_t(\eta) = x(t + \eta)$, the derivatives

$$\frac{d}{dt} \int_{t-h}^t x^\top(\xi) \tilde{Q}_1 x(\xi) d\xi = x^\top(t) \tilde{Q}_1 x(t) - x^\top(t-h) \tilde{Q}_1 x(t-h),$$

$$\begin{aligned} \frac{d}{dt} \int_{t-h}^t x^\top(\xi) [(h + \xi - t) \tilde{Q}_2] x(\xi) d\xi \\ = hx^\top(t) \tilde{Q}_2 x(t) - \int_{t-h}^t x^\top(\xi) \tilde{Q}_2 x(\xi) d\xi \end{aligned}$$

give $D_{(1)}^+ V_1(x_t)$ and $D_{(1)}^+ V_2(x_t)$. They compensate in (36) the difference between $D_{(1)}^+ V_0(x_t)$ and $D_{(1)}^+ V(x_t)$ from (2). ■

The first term $V_0(\phi)$ in (36) can be approximated by $y^\top P_{y,0} y$ from a Lyapunov equation with Q_0 in (11) being replaced by $Q_0 + Q_1 + hQ_2$, and Q_1 and Q_2 being replaced by zero. Since $V_1(\phi)$ and $V_2(\phi)$ in (36) are analytically known, these terms can be treated by a numerical integration. Their contributions are added on the (block-)diagonal of $P_{y,0}$, i.e. $V(\phi) \approx y^\top P_y y$,

$P_y = P_{y,0} + \text{diag}((w_k)_k) \otimes Q_1 + \text{diag}((w_k(h + \tilde{\theta}_k))_k) \otimes Q_2$, where w_k are integration weights, cf. Appendix B.1.

2) *Legendre tau:* A separate numerical treatment of V_1 and V_2 in (36) is not required if the Legendre-tau-based approach is used. However, if Q_2 is nonzero, the following modification of Q_y in (11) should be used in (71) or (10)

$$\begin{aligned} Q_y &= \text{blkdiag}(Q_1, 0_{n(N-1) \times n(N-1)}, Q_0) + T_{\zeta y}^\top Q_{\zeta,2} T_{\zeta y} \\ &\text{with } Q_{\zeta,2} := \text{diag}([\frac{h}{2} \frac{2}{k+1}]_{k \in \{0, \dots, N-1\}}, h) \otimes Q_2 \quad (37) \end{aligned}$$

(the right lower component hQ_2 in $Q_{\zeta,2}$ is motivated by Lemma 1.2 in the appendix). Despite of not being treated separately in the numerical approach, the arising contributions for $V_1(\phi)$ and $V_2(\phi)$ within the approximation of $V(\phi)$ are still of interest for the proofs in the next sections. They can be obtained by solving Lyapunov equations with $Q_{0,1,2}$ being replaced by the matrices behind the semicolon in $V_1(\phi) = V(\phi; \dots)$ and $V_2(\phi) = V(\phi; \dots)$ from Lemma 6.1. Appendix A.3.c shows that the resulting Legendre-tau-based approximations of $V_1(\phi)$ and $V_2(\phi)$ give even the exact value for any ϕ that is a polynomial of order $N - 1$ or less.

C. Convergence Towards the Functional

We are interested in the following convergence statement.

Condition 6.2: For any given $\phi \in C([-h, 0], \mathbb{R}^n)$, the scalar value $V_y(y)$ converges to $V(\phi)$ as N increases. ◀

More formally, we use the notation $y = \pi_y(\phi)$ to emphasize that the discretization $y \in \mathbb{R}^{n(N+1)}$ is uniquely determined from $\phi \in C$ (depending on the discretization scheme). Additionally, to keep track of the discretization resolution N , a

superscript $[N]$ is added, e.g., in $V_y^{[N]}(\cdot) = V_y(\cdot)$ and $\pi_y^{[N]}(\cdot) = \pi_y(\cdot)$. Thus, Cond. 6.2 can be rewritten as

$$\forall \phi \in C : V_y^{[N]}(\pi_y^{[N]}(\phi)) \rightarrow V(\phi), \quad (N \rightarrow \infty). \quad (38)$$

Motivated by the numerical results in Sec. IV, we focus in this section on the Legendre tau method. Moreover, for this discretization scheme, we benefit from existing convergence proofs for the approximation of algebraic Riccati equations from the context of optimal control [7], [36], [53].

1) *Operator-based description:* Henceforth, we use that any argument $\phi \in C$ for $V(\phi)$ gives rise to an element

$$[\phi(0)] \in C \times \mathbb{R}^n \subset L_2 \times \mathbb{R}^n = M_2 \quad (39)$$

in the product space $M_2 = L_2([-h, 0], \mathbb{R}^n) \times \mathbb{R}^n$. Note that $(M_2, \langle \cdot, \cdot \rangle_{M_2})$ is a Hilbert space with the natural inner product

$$\langle [\phi_1], [\phi_2] \rangle_{M_2} = \int_{-h}^0 \phi_1^\top(\theta) \phi_2(\theta) d\theta + r_1^\top r_2, \quad (40)$$

$\phi_{1,2} \in L_2$, $r_{1,2} \in \mathbb{R}^n$. Similarly to the well-known $V_{\mathbb{R}^n}(x) = \langle x, Px \rangle_{\mathbb{R}^n} = x^\top Px$ in the finite-dimensional ODE setting for $x \in \mathbb{R}^n$, a complete-type LK functional can be written as

$$V(\phi) = V_{M_2}([\phi(0)]) = \langle [\phi(0)], \mathcal{P}[\phi(0)] \rangle_{M_2} \quad (41)$$

with a self-adjoint operator $\mathcal{P} : M_2 \rightarrow M_2$. Consider the splitting $V = V_0 + V_{12}$ with $V_{12} = V_1 + V_2$ from Lemma 6.1 ($\tilde{Q}_1 = Q_1, \tilde{Q}_2 = Q_2$). For the first part, which becomes

$$V_0(\phi) = \langle [\phi(0)], \mathcal{P}_0[\phi(0)] \rangle_{M_2}, \quad (42)$$

the self-adjoint operator $\mathcal{P}_0 : M_2 \rightarrow M_2$ is described by suboperators on L_2 and \mathbb{R}^n according to

$$\mathcal{P}_0 \begin{bmatrix} \phi \\ r \end{bmatrix} = \begin{bmatrix} \mathcal{P}_{zz} \phi + \mathcal{P}_{zx} r \\ \mathcal{P}_{xz} \phi + \mathcal{P}_{xx} r \end{bmatrix} = \begin{bmatrix} v \\ w \end{bmatrix}, \quad \text{with} \quad (43)$$

$$\begin{bmatrix} v(\theta) \\ w \end{bmatrix} = \begin{bmatrix} \int_{-h}^0 P_{zz}(\theta, \eta) \phi(\eta) d\eta + P_{zx}(\theta) r \\ \int_{-h}^0 P_{xz}(\eta) \phi(\eta) d\eta + P_{xx} r \end{bmatrix}. \quad (44)$$

Thus, (15a) is regained by (42), using (43) with $r = \phi(0)$,

$$V_0(\phi) \stackrel{(40)}{=} \int_{-h}^0 \phi^\top(\theta) v(\theta) d\theta + \phi^\top(0) w \quad (45)$$

$$\stackrel{(44)}{=} \int_{-h}^0 \phi^\top(\theta) \left(\int_{-h}^0 P_{zz}(\theta, \eta) \phi(\eta) d\eta + P_{zx}(\theta) \phi(0) \right) d\theta \\ + \phi^\top(0) \left(\int_{-h}^0 P_{xz}(\eta) \phi(\eta) d\eta + P_{xx} \phi(0) \right) \quad (46)$$

(to be more precise, (15a) with $P_{zz, \text{diag}}(\theta) \equiv 0_{n \times n}$). The missing part $V_{12} = V_1 + V_2$ in (36) can also be written as

$$V_{12}(\phi) = \int_{-h}^0 \phi^\top(\theta) (Q_1 + (h + \theta)Q_2) \phi(\theta) d\theta \quad (47)$$

$$= \langle [\phi(0)], \mathcal{P}_{12}[\phi(0)] \rangle_{M_2} \quad (48)$$

based on the multiplication operator

$$\mathcal{P}_{12} \begin{bmatrix} \phi \\ r \end{bmatrix} = \begin{bmatrix} \mathcal{P}_{zz, \text{diag}} \phi \\ 0_n \end{bmatrix} = \begin{bmatrix} v \\ 0_n \end{bmatrix}, \quad \text{with} \quad (49)$$

$$v(\theta) = P_{zz, \text{diag}}(\theta) \phi(\theta) = (Q_1 + (h + \theta)Q_2) \phi(\theta).$$

Nevertheless, we are going to treat V_{12} separately⁸.

⁸The term $\phi^\top(-h)Q_1\phi(-h)$ would require an unbounded operator \mathcal{Q} in the Lyapunov equation (51). Moreover, \mathcal{P}_{12} is not compact.

2) *Convergence towards V_0* : The operator \mathcal{P}_0 in (42) satisfies a non-operator-valued Lyapunov equation, c.f. [54], [55]. Its right-hand side is based on the right-hand side of (2). Because of the splitting approach, the latter is $D_{(1)}^+ V_0(x_t) = x^\top(t) \tilde{Q} x(t)$ with $\tilde{Q} = Q_0 + Q_1 + hQ_2$, or, for $x_t = \phi$,

$$D_{(1)}^+ V_0(\phi) = -\phi^\top(0) \tilde{Q} \phi(0) = -\langle [\phi(0)], \mathcal{Q}[\phi(0)] \rangle_{M_2}, \quad (50)$$

$\mathcal{Q}[\phi(0)] = \begin{bmatrix} 0_{n_1 \times n_1} \\ \tilde{Q} \phi(0) \end{bmatrix}$. Therefore, the operator-valued Lyapunov equation for the self-adjoint operator $\mathcal{P}_0 = \mathcal{P}_0^*$ reads

$$\underbrace{\langle \psi, \mathcal{P}_0 \mathcal{A} \psi \rangle_{M_2} + \langle \psi, \mathcal{A}^* \mathcal{P}_0 \psi \rangle_{M_2}}_{=2\langle \psi, \mathcal{P}_0 \mathcal{A} \psi \rangle_{M_2}} = -\langle \psi, \mathcal{Q} \psi \rangle_{M_2}, \quad (51)$$

$\forall \psi \in D(\mathcal{A}) \subset M_2$, cf. [54], [55], where \mathcal{A} is the infinitesimal generator of the C_0 -semigroup of solution operators on M_2 (which for linear RFDEs is as well an appropriate state space), and $D(\mathcal{A})$ is its domain. See, e.g., [54] for background on \mathcal{A} .

From the ODE-based approach in Sec. II-B, we obtain an approximation $V_0(\phi) \approx V_{y,0}(y) = y^\top P_{y,0} y$, or, in the notation of (38), $V_{y,0}^{[N]}(\pi_y^{[N]}(\phi))$. Similarly to the exact $V_0(\phi)$ in (42), this approximation can be described via

$$V_{y,0}^{[N]}(\pi_y^{[N]}(\phi)) = \langle [\phi(0)], \mathcal{P}_0^{[N]} [\phi(0)] \rangle_{M_2} \quad (52)$$

with an approximated operator $\mathcal{P}_0^{[N]}$. Moreover, similarly to the exact operator \mathcal{P}_0 from (51), this approximated operator $\mathcal{P}_0^{[N]}$ also satisfies an operator-valued Lyapunov equation,

$$2\langle \psi, \mathcal{P}_0^{[N]} \mathcal{A}^{[N]} \psi \rangle_{M_2} = -\langle \psi, \mathcal{Q} \psi \rangle_{M_2}, \quad (53)$$

which, however, only relies on an approximation $\mathcal{A}^{[N]}$ instead of \mathcal{A} . See [36] for details. The matrices A_ζ or, equivalently, A_y in Sec. II are coordinate representations of that $\mathcal{A}^{[N]}$.

It has to be shown that, $\forall \phi \in C$, the scalar value $V_0(\phi)$ in (42) is indeed the limit of its approximations in (52) as $N \rightarrow \infty$. In terms of the operators, weak⁹ operator convergence $\mathcal{P}_0^{[N]} \xrightarrow{\text{weakly}} \mathcal{P}_0$ suffices for that objective.

Lemma 6.2: Let (52) describe a Legendre-tau-based result for $V_0(\phi)$. Assume $\{\|\mathcal{P}_0^{[N]}\|\}_N$ is bounded¹⁰, and the existence and uniqueness conditions from Lemma 2.1 and Rem. 2.1 hold. Then $\mathcal{P}_0^{[N]}$ converges weakly to \mathcal{P}_0 as $N \rightarrow \infty$. ◀

Proof: See [36, Thm. 5.1 (i)] with zero input operator and the uniqueness conditions from Sec. II-C. ■

In fact, this result is not at all special to the Legendre tau method. An alternative proof from [53, Thm. 6.7] applies to any discretization scheme that satisfies standard conditions proving convergence of numerical solutions for $(x_t, x(t))$ in M_2 . Lemma 6.2 relies on uniform boundedness and existence

⁹ The operator sequence $\{\mathcal{P}^{[N]}\}_N$ converges weakly to \mathcal{P} if $\forall \varphi, \psi \in M_2$: $\lim_{N \rightarrow \infty} \langle \varphi, \mathcal{P}^{[N]} \psi \rangle_{M_2} = \langle \varphi, \mathcal{P} \psi \rangle_{M_2}$ (i.e., $\forall \psi \in M_2$: $\mathcal{P}^{[N]} \psi \xrightarrow{\text{weakly}} \mathcal{P} \psi$). It converges strongly if $\forall \psi \in M_2$: $\lim_{N \rightarrow \infty} \|\mathcal{P}^{[N]} \psi - \mathcal{P} \psi\|_{M_2} = 0$. The implications ‘operator norm conv.’ \Rightarrow ‘strong conv.’ \Rightarrow ‘weak conv.’ hold.

¹⁰ To compute the norm of the self-adjoint operator $\mathcal{P}_0^{[N]}$ via $P_{y,0}$, $P_{\zeta,0}$, or $P_{\chi,0}$, note that $\|\mathcal{P}_0^{[N]}\| = \sup_{\langle \phi, \phi(0) \rangle_{M_2} \leq 1} \langle [\phi(0)], \mathcal{P}_0^{[N]} [\phi(0)] \rangle_{M_2}$. Considering, e.g., Sec. A.3.d, we obtain $\|\mathcal{P}_0^{[N]}\| = \|P_{\tilde{\chi},0}\|_2$ where $P_{\tilde{\chi},0} = T_{\tilde{\chi}\chi}^{-\top} P_{\chi,0} T_{\tilde{\chi}\chi}^{-1}$ and where $T_{\tilde{\chi}\chi}$ is such that $\inf_{\phi} \langle \phi, \phi(0) \rangle_{M_2}^2 = \chi^\top G_{\chi} \chi = \|T_{\tilde{\chi}\chi} \chi\|_2^2$ with the infimum being taken over all $(\phi, \phi(0)) \in M_2$ that have the discretization χ . The latter is attained by (77) with the metric coefficients $G_\chi = \text{diag}(\left(\frac{h}{2} \frac{2}{2k+1}\right)_{k=0 \dots N-1}, 1) \otimes I_n$. Thus, $T_{\tilde{\chi}\chi} = G_\chi^{1/2}$.

assumptions. In the following we show that these can be ignored in the case of an exponentially stable RFDE equilibrium. Nevertheless, while simplifying the considerations, stability of the equilibrium is no necessary condition in the derivations.

Lemma 6.3: If the RFDE equilibrium is exponentially stable, then the assumptions in Lemma 6.2 hold. ◀

Proof: Let $\mathcal{T}(t) : M_2 \rightarrow M_2; \begin{bmatrix} x_0 \\ x_0(0) \end{bmatrix} \mapsto \begin{bmatrix} x_t \\ x(t) \end{bmatrix} = \mathcal{T}(t) \begin{bmatrix} x_0 \\ x_0(0) \end{bmatrix}$ be the solution operator, and $\mathcal{T}^{[N]}(t)$ its approximation (represented by $e^{A_y^{[N]} t}$). Due to the stability preservation property from [7, Thm. 5.3], $\exists M \geq 1, \beta > 0, \bar{N} \in \mathbb{N}$, such that $\forall N \geq \bar{N} : \|\mathcal{T}^{[N]}(t)\| \leq M e^{-\beta t}$. Therefore, the improper integral formula $\mathcal{P}^{[N]} \psi = \int_0^\infty (\mathcal{T}^{[N]})^*(s) \mathcal{Q} \mathcal{T}^{[N]}(s) \psi ds$ is applicable, see, e.g., [53]. Thus, with $\|\mathcal{Q}\| = \|\tilde{Q}\|_2$, the operators $\mathcal{P}^{[N]}$ are uniformly bounded by $\|\mathcal{P}^{[N]}\| \leq \int_0^\infty \|\tilde{Q}\|_2 \|\mathcal{T}^{[N]}(s)\|^2 ds \leq \|\tilde{Q}\|_2 \frac{M^2}{2\beta}$. Moreover, the existence and uniqueness assumptions hold by Prop. 2.1. ■

The convergence towards $V_0(\phi)$ does not require more than the thus established weak convergence $\mathcal{P}_0^{[N]} \xrightarrow{\text{weakly}} \mathcal{P}_0$. However, the following stronger result will become helpful in Sec. VI-D.

Lemma 6.4: Let (52) describe a Legendre-tau-based result for $V_0(\phi)$. If the RFDE equilibrium is exponentially stable, then $\mathcal{P}_0^{[N]}$ converges in operator norm to \mathcal{P}_0 , i.e., it holds $\|\mathcal{P}_0^{[N]} - \mathcal{P}_0\| \rightarrow 0$ as $N \rightarrow \infty$. ◀

Proof: See [53, Thm. 6.9], where even convergence in the trace norm [53, p. 111] is proven. The result requires that not only the approximations of the solution operator $\mathcal{T}(t)$ converge strongly⁹, but also those of its adjoint $\mathcal{T}^*(t)$, which for the Legendre tau method is proven in [7, Thm. 2.2]. ■

3) *Convergence towards V* : To prove Cond. 6.2 on convergence towards $V = V_0 + V_{12}$, it only remains to include V_{12} .

Theorem 6.1: If the RFDE equilibrium is exponentially stable or, more generally, if the assumptions of Lemma 6.2 hold, then Cond. 6.2 applies for the Legendre-tau-based approach (with the Lyapunov equation right-hand side from (37)). ◀

Proof: Since P_y depends linearly on Q_y in the Lyapunov equation (10), the approximation of V is the superposition of the approximations of V_0 and $V_{12} = V_1 + V_2$ from Lemma 6.1. For the first one, the convergence, $\forall \phi \in C$: $V_{y,0}^{[N]}(\pi_y^{[N]}(\phi)) \rightarrow V_0(\phi)$ as $N \rightarrow \infty$, is a consequence of the weak⁹ convergence of $\mathcal{P}_0^{[N]}$ proven in Lemma 6.2. Concerning the second one, the lemmata in Sec. A.3.c show that $V_{12}(\phi)$ is approximated by $V_{y,12}^{[N]}(\pi_y^{[N]}(\phi)) = V_{12}(\tilde{\phi}^{(N-1)})$, where $\tilde{\phi}^{(N-1)}$ is a Legendre series truncation of ϕ . The convergence, $\forall \phi \in C$: $V_{12}(\tilde{\phi}^{(N-1)}) \rightarrow V_{12}(\phi)$ as $N \rightarrow \infty$, follows from the L_2 -convergence of the involved Legendre series truncation, $\|\phi - \tilde{\phi}^{(N-1)}\|_{L_2} \rightarrow 0$ as $N \rightarrow \infty$ [56, Thm. 6.2.3], combined with the continuity¹¹ of V_{12} in L_2 . ■

D. Quadratic Lower Bound on the Functional

We are going to prove that, for $N \rightarrow \infty$, the quadratic lower bound on the approximation gives also a valid quadratic lower bound on the functional. This holds for any discretization scheme satisfying Cond. 6.2. Moreover, for the Legendre

¹¹ A quadratic form $V(x) = \langle x, \mathcal{P} x \rangle_X$, $\mathcal{P} = \mathcal{P}^*$, in a Hilbert space X is continuous if $\exists k > 0 : \langle x, \mathcal{P} x \rangle_X \leq k \|x\|_X^2$, which by $\inf k = \|\mathcal{P}\|$ holds if \mathcal{P} is bounded. Note that $V_{12}(\phi) = \langle \phi, \mathcal{P}_{zz, \text{diag}} \phi \rangle_{L_2} \leq (\|Q_1\|_2 + h \|Q_2\|_2) \|\phi\|_{L_2}^2$. For $V_{M_2}(\psi) = \langle \psi, \mathcal{P} \psi \rangle_{M_2} \leq k \|\psi\|_{M_2}^2$ see [10, p. 65].

tau method, the thus obtained bound will be shown to be tight, meaning that the largest possible coefficient k_1 in (4) is obtained.

For any discretization resolution N , the largest possible coefficient $k_1^{[N]}$ for the bound (17) on the approximation $V_y^{[N]}$ is given by (22). Note that $k_1^{[N]}$ and, similarly, the largest possible coefficient $k_1 = k_1^{\text{opt}}$ for the bound (4) on the functional V are defined by

$$k_1^{[N]} = \min_{\substack{z \in \mathbb{R}^{nN} \\ \hat{x} \in \mathbb{R}^n \setminus \{0_n\}}} \frac{1}{\|\hat{x}\|_2^2} V_y^{[N]} \left(\begin{bmatrix} z \\ \hat{x} \end{bmatrix} \right), \quad k_1^{\text{opt}} = \inf_{\substack{\phi \in C \\ \phi(0) \neq 0_n}} \frac{1}{\|\phi(0)\|_2^2} V(\phi). \quad (54)$$

However, since both the functional and its approximation are quadratic, with $V(c\phi) = c^2 V(\phi)$ for any $c \in \mathbb{R}$ in (15a) and $V_y^{[N]}(cy) = c^2 V_y^{[N]}(y)$ in (8), definition (54) simplifies to

$$k_1^{[N]} = \min_{\substack{z \in \mathbb{R}^{nN} \\ \hat{x} \in \mathbb{R}^n \setminus \{0_n\}}} V_y^{[N]} \left(\frac{1}{\|\hat{x}\|_2} \begin{bmatrix} z \\ \hat{x} \end{bmatrix} \right), \quad k_1^{\text{opt}} = \inf_{\substack{\phi \in C \\ \phi(0) \neq 0_n}} V \left(\frac{1}{\|\phi(0)\|_2} \phi \right). \quad (55)$$

Theorem 6.2: If Cond. 6.2 holds, then $k_1 = \limsup_{N \rightarrow \infty} k_1^{[N]}$ is a valid quadratic lower bound coefficient in (4). ◀

Proof: Let ϕ_δ give a $V(\phi_\delta)$ that is arbitrarily close to the infimum in (55) according to

$$\forall \delta > 0, \exists \phi_\delta \in C, \|\phi_\delta(0)\|_2 = 1 : \quad V(\phi_\delta) < k_1^{\text{opt}} + \delta. \quad (56)$$

The assumed convergence (38), i.e., $\forall \phi \in C, \forall \varepsilon > 0, \exists \bar{N}(\varepsilon, \phi) \in \mathbb{N}, \forall N \geq \bar{N}(\varepsilon, \phi) : |V_y^{[N]}(\pi_y^{[N]}(\phi)) - V(\phi)| < \varepsilon$, shows that

$$\forall N \geq \bar{N}(\frac{\varepsilon}{2}, \phi_\delta) : \quad |V_y^{[N]}(\pi_y^{[N]}(\phi_\delta)) - \underbrace{V(\phi_\delta)}_{< k_1^{\text{opt}} + \delta}| < \frac{\varepsilon}{2}, \quad (57)$$

and thus, $\forall N \geq \bar{N}(\frac{\varepsilon}{2}, \phi_\delta) :$

$$k_1^{[N]} \stackrel{(55)}{=} \min_{\substack{z \in \mathbb{R}^{nN} \\ \hat{x} \in \mathbb{R}^n \setminus \{0_n\}}} V_y^{[N]} \left(\frac{1}{\|\hat{x}\|_2} \begin{bmatrix} z \\ \hat{x} \end{bmatrix} \right) \leq V_y^{[N]}(\pi_y^{[N]}(\phi_\delta)) \stackrel{(57)}{<} V(\phi_\delta) + \frac{\varepsilon}{2} \stackrel{(56)}{<} k_1^{\text{opt}} + \delta + \frac{\varepsilon}{2}. \quad (58)$$

Choosing $\delta = \frac{\varepsilon}{2}$, (58) becomes $k_1^{[N]} < k_1^{\text{opt}} + \varepsilon$. Hence, $\limsup_{N \rightarrow \infty} k_1^{[N]} \leq k_1^{\text{opt}}$. Any $k_1 \leq k_1^{\text{opt}}$ is admissible in (4). ■

For the Legendre tau method, we are going to prove that $k_1^{[N]}$ converges to the largest admissible coefficient k_1^{opt} . The proof involves the following assumption on the arguments of the minimum in (55): For any N , we consider a vector $\begin{bmatrix} z^{[N]} \\ \hat{x}^{[N]} \end{bmatrix}$, with $\|\hat{x}^{[N]}\|_2 = 1$, such that $V_y^{[N]} \left(\begin{bmatrix} z^{[N]} \\ \hat{x}^{[N]} \end{bmatrix} \right) = k_1^{[N]}$. By (77), any $\begin{bmatrix} z^{[N]} \\ \hat{x}^{[N]} \end{bmatrix}$ represents a function $\phi^{[N]}$ (we use (77) since the minimizing argument is not expected to be continuous at $\theta = 0$). The assumption below is that $\phi^{[N]}$ remains uniformly bounded in L_2 , which, however, could numerically¹² be confirmed for all tested examples that give a nonzero k_1 .

Theorem 6.3: Consider the Legendre tau method with (37). As described above, for $\phi^{[N]}$ being related to $k_1^{[N]}$, assume that $\exists \beta > 0, \forall N : \|\phi^{[N]}\|_{L_2} < \beta$. Then the quadratic lower bound coefficient $k_1^{[N]}$ from Cor. 3.1 converges to the largest possible quadratic lower bound coefficient on the functional in (4). ◀

¹²The L_2 norm of (77) can be computed from $\|\phi^{[N]}\|_{L_2}^2 = \sum_{k=0}^{N-1} \frac{h}{2} \frac{2}{2k+1} \|\zeta^k\|_2^2$ using the first $N-1$ of the N subvectors in ζ . These are either derived via $\zeta = T_{\zeta y} \begin{bmatrix} z \\ \hat{x} \end{bmatrix}$, cf. Rem. 1.3, where $z = -P_{y,zz}^{-1} P_{y,xz}^\top \hat{x}$ and $\hat{x} = v/\|v\|_2$, see Lemma 3.1, or are directly available if Lemma 3.1 is applied to the coordinates from (76).

Proof: We denote by C_d the set of functions $\phi : [-h, 0] \rightarrow \mathbb{R}^n$ that are continuous on $[-h, 0)$ and possibly have a jump discontinuity at the end point $\phi(0^-) \neq \phi(0)$. Note that $\phi^{[N]} \in C_d$. The functional $V : C \rightarrow \mathbb{R}$ can straightforwardly be extended to arguments in C_d since $V(\phi) = V_{M_2}((\phi, \phi(0)))$ holds by (41), which, in fact, is defined for all $(\phi, \phi(0)) \in L_2 \times \mathbb{R}^n$. Also on this extended set of arguments, the value of interest from (55) is still the infimum $k_1^{\text{opt}} = \inf_{\substack{\phi \in C_d \\ \phi(0) \neq 0_n}} V \left(\frac{1}{\|\phi(0)\|_2} \phi \right)$ (even on $L_2 \times \mathbb{R}^n$ it would be since V_{M_2} is continuous¹¹ in $M_2 = L_2 \times \mathbb{R}^n$ and C is dense in L_2). With a slight abuse of notation we do not alter the name V for the extension on C_d . By construction, the discretization $\pi_y^{[N]}(\phi^{[N]}) = \begin{bmatrix} z^{[N]} \\ \hat{x}^{[N]} \end{bmatrix}$ yields an argument of the minimum in (55). First, we have to show that $\forall \varepsilon > 0, \exists \bar{N}_1(\varepsilon) \in \mathbb{N}$, such that

$$\forall N \geq \bar{N}_1(\varepsilon) : \quad \underbrace{|V_y^{[N]}(\pi_y^{[N]}(\phi^{[N]})) - V(\phi^{[N]})|}_{k_1^{[N]}} < \varepsilon. \quad (59)$$

According to the splitting approach (Lemma 6.1 with $\tilde{Q}_1 = Q_1, \tilde{Q}_2 = Q_2$), we decompose V into three parts $V(\phi^{[N]}) = V_0(\phi^{[N]}) + V_1(\phi^{[N]}) + V_2(\phi^{[N]})$ and its approximation correspondingly. The second and third term, $V_1(\phi^{[N]})$ and $V_2(\phi^{[N]})$, do not contribute to the error in (59) since $\phi^{[N]}(\theta)$ is an $(N-1)$ -th order polynomial on $\theta \in [-h, 0)$ for which the approximation is exact, according to the lemmata of Appendix A.3.c. Therefore, it suffices to show uniform convergence on $\cup_N \{\phi^{[N]}\}$ for the approximations of V_0 . Let $\psi^{[N]} = (\phi^{[N]}, \phi^{[N]}(0)) \in M_2$. By assumption, $\|\psi^{[N]}\|_{M_2}^2 = \|\phi^{[N]}\|_{L_2}^2 + \|\phi^{[N]}(0)\|_2^2 \leq \beta^2 + 1$. Thus, using (42) and (52), the error in (59) becomes $|\langle \psi^{[N]}, \mathcal{P}_0^{[N]} \psi^{[N]} \rangle_{M_2} - \langle \psi^{[N]}, \mathcal{P}_0 \psi^{[N]} \rangle_{M_2}| \leq \|\mathcal{P}_0^{[N]} - \mathcal{P}_0\| (\beta^2 + 1)$. By Lemma 6.4, the latter converges to zero, and thus (59) holds. Consequently, $\forall N \geq \bar{N}_1(\varepsilon)$:

$$k_1^{[N]} \stackrel{(59)}{>} V(\phi^{[N]}) - \varepsilon \geq \inf_{\substack{\phi \in C_d \\ \phi(0) \neq 0_n}} V \left(\frac{1}{\|\phi(0)\|_2} \phi \right) - \varepsilon \stackrel{(55)}{=} k_1^{\text{opt}} - \varepsilon. \quad (60)$$

With $\bar{N}_0(\varepsilon) := \bar{N}(\frac{\varepsilon}{2}, \phi_{\delta=\varepsilon/2})$ from Thm. 6.2, we obtain

$$\forall N \geq \max\{\bar{N}_0(\varepsilon), \bar{N}_1(\varepsilon)\} : \quad k_1^{\text{opt}} - \varepsilon \stackrel{(60)}{<} k_1^{[N]} \stackrel{(58)}{<} k_1^{\text{opt}} + \varepsilon,$$

completing the proof of $|k_1^{[N]} - k_1^{\text{opt}}| \rightarrow 0$ ($N \rightarrow \infty$). ■

VII. CONCLUSION

The present paper shows that the counterpart of LK functionals for RFDEs are not classical Lyapunov functions for ODEs, but rather they correspond to partial Lyapunov functions, i.e., Lyapunov functions that prove partial stability. The latter are still simply obtained by solving a Lyapunov equation. Using the system matrix of an approximating ODE, the result gives an approximation of the LK functional $V(\phi)$. Note that Fig. 2 yields the structure of complete-type LK functionals without any prior knowledge. For an appropriate ODE approximation with a sufficiently large discretization resolution N , the involved matrix P_y is positive semidefinite if and only if the RFDE equilibrium is asymptotically stable. A formula for a partial positive-definiteness bound on the functional approximation is derived. When it is applied to the Legendre-tau ODE-based result, a rapid convergence of the

resulting lower bound coefficient is observed as N increases. Its limit is shown to be the best possible quadratic lower bound coefficient k_1 on the LK functional. Examples demonstrate that the latter significantly improves known results. In particular, the obtained k_1 depends on the delay, which is not the case in existing formulae. For the sake of validation, the present paper also proposes a numerical integration of the LK functional formula by Clenshaw-Curtis and Gauss quadrature rules. For these, the lower bound formula is purposeful as well. However, the ODE-based approach is expected to provide approximations of LK functionals even in more general cases where the LK functional is not known analytically.

APPENDIX

Table II classifies the employed polynomial methods. The following appendix also includes some implementation hints.

A. ODEs that Approximate RFDEs

We consider ODE approximations for (1) from two spectral methods: Chebyshev collocation and Legendre tau.

1) *Chebyshev collocation method*: By interpolation, the vector $y(t)$ at time t in (5), cf. Fig. 1, determines an N -th order approximating polynomial for x_t . More specifically,

$$x_t(\theta) \approx \sum_{k=0}^N y^k(t) \ell_k(\vartheta(\theta)), \quad (61)$$

where $\ell_k: [-1, 1] \rightarrow \mathbb{R}$ are interpolating Lagrange basis polynomials w.r.t. the (Gauss-Lobatto) Chebyshev nodes $\{\tilde{\vartheta}_k\}_{k \in \{0, \dots, N\}}$ on $[-1, 1]$, and where

$$\vartheta: [-h, 0] \rightarrow [-1, 1]; \quad \theta \mapsto \vartheta(\theta) := \frac{2}{h}\theta + 1 \quad (62)$$

maps the argument $\theta \in [-h, 0]$ to this interval.

The exact evolution of x_t in Fig. 1b can be described by an abstract ODE in $C([-h, 0], \mathbb{R}^n)$, see [3] for details. This abstract ODE can be discretized via the collocation method. The result describes the dynamics of the unknown coefficients $y^k(t)$ in (61). It is the ODE (7) with $A_y = A_y^C$,

$$A_y^C := \begin{bmatrix} \frac{2}{h} \ell'_0(\tilde{\vartheta}_0) I_n & \cdots & \cdots & \cdots & \frac{2}{h} \ell'_N(\tilde{\vartheta}_0) I_n \\ \vdots & & & & \vdots \\ \frac{2}{h} \ell'_0(\tilde{\vartheta}_{N-1}) I_n & \cdots & \cdots & \cdots & \frac{2}{h} \ell'_N(\tilde{\vartheta}_{N-1}) I_n \\ A_1 & 0_{n \times n} & \cdots & 0_{n \times n} & A_0 \end{bmatrix}, \quad (63)$$

cf. [25]. The upper part of A_y^C that is given by $\frac{2}{h} (\ell'_k(\tilde{\vartheta}_j))_{j \in \{0, \dots, N-1\}, k \in \{0, \dots, N\}} \otimes I_n$ requires the first N rows of the $(N+1) \times (N+1)$ differentiation matrix $(\ell'_k(\tilde{\vartheta}_j))_{j, k \in \{0, \dots, N\}}$. See [38, p. 54] (with $x_k = -\tilde{\vartheta}_k$).

Remark 1.1 (Implementation of A_y^C): A Matlab implementation of the skew-centrosymmetric differentiation matrix is available from `diffmat` in the Chebfun toolbox [39]. Based on the latter, $A_y^C = A$ is obtained from

$$D = \text{diffmat}(N+1, [-\text{delay}, 0]); \quad A = \text{kron}(D, \text{eye}(n)); \\ A(\text{end}-n+1:\text{end}, :) = [A_1, \text{zeros}(n, n*(N-1)), A_0]$$

(if A_0, A_1, h, n, N are assigned to $A_0, A_1, \text{delay}, n, N$). ◀

¹³orthogonal w.r.t. the (weighted) inner product in which the chosen basis polynomials are orthogonal. In (73), the modified ζ^N makes the projection non-orthogonal, unless the discretization is interpreted in terms of (77).

2) *Legendre tau method*: Let $p_k: [-1, 1] \rightarrow \mathbb{R}$ denote the k -th Legendre polynomial. See, e.g., [57] for formulae and plots. Using $\{p_k(\vartheta(\cdot))\}_{k=0}^N$ as basis, an N -th order approximating polynomial for x_t becomes

$$x_t(\theta) \approx \sum_{k=0}^N \zeta^k(t) p_k(\vartheta(\theta)). \quad (64)$$

The evolution of the coefficients $\zeta^k(t) \in \mathbb{R}^n$, stacked as $\zeta := [(\zeta^0)^\top, \dots, (\zeta^N)^\top]^\top$, shall again be described by

$$\dot{\zeta}(t) = A_\zeta \zeta(t). \quad (65)$$

In [29], this is achieved via Lanczos' tau method (considering a Hilbert space setting, cf. Sec. VI-C). A general introduction to the tau method is given in [57]. We only state the result, which is (65) with $A_\zeta = A_\zeta^L$ having the block entries

$$A_\zeta^{L, jk} = \begin{cases} \frac{2}{h}(2j+1)I_n, & \text{if } j \in \{0, \dots, N-1\}, \\ & k > j \text{ and } j+k \text{ odd} \\ A_0 + (-1)^k A_1 - \frac{2}{h} \frac{k(k+1)}{2} I_n, & \text{if } j = N \\ 0_{n \times n}, & \text{else.} \end{cases} \quad (66)$$

Thus, A_ζ^L exhibits the structure (exemplarily for N even)

$$A_\zeta^L = \begin{bmatrix} 0_{n \times n} & 0_{n \times n} & 0_{n \times n} & \cdots & 0_{n \times n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0_{n \times n} & 0_{n \times n} & 0_{n \times n} & \cdots & 0_{n \times n} \\ A_0 + A_1 & A_0 - A_1 & A_0 + A_1 & \cdots & A_0 - A_1 \end{bmatrix} \\ + \frac{2}{h} \begin{bmatrix} 0 & 1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 3 & 0 & \cdots & 3 \\ 0 & 0 & 0 & 5 & \cdots & 0 \\ \vdots & & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & (2N-1) \\ 0 & -1 & -3 & -6 & \cdots & -\frac{N(N+1)}{2} \end{bmatrix} \otimes I_n.$$

Remark 1.2 (Implementation of A_ζ^L): Written in standard Matlab code, we obtain $A_\zeta^L = A_\zeta$ from

$$\text{Dc} = \text{zeros}(N+1, N+1); \text{Dc}(\text{end}, :) = -(0:N) .* (1:N+1)/2; \\ \text{for } j=0:N-1; \text{Dc}(j+1, (j+1)+1:2:\text{end}) = 2*j+1; \text{end} \\ \text{Ac} = 2/\text{delay} * \text{kron}(\text{Dc}, \text{eye}(n)); \\ \text{Ac}(\text{end}-n+1:\text{end}, :) = \text{Ac}(\text{end}-n+1:\text{end}, :) + \dots \\ \text{kron}(\text{ones}(1, N+1), A_0) + \text{kron}((-1).^ (0:N), A_1)$$

(with $A_0, A_1, \text{delay}, n, N$ as above). ◀

Hence, we have the dynamics (65) of the Legendre coordinates $\zeta(t) \in \mathbb{R}^{n(N+1)}$ that, in (64), describe the approximating polynomial for x_t . However, we can equivalently express the polynomial (64) in interpolation coordinates $y(t) \in \mathbb{R}^{n(N+1)}$, referring to the interpolation basis $\{\ell_k(\vartheta(\cdot))\}_{k=0}^N$ of (61). Let $T_{y\zeta}$ denote the transformation matrix of this change of basis

$$y(t) = T_{y\zeta} \zeta(t). \quad (67)$$

The thus computed $y(t)$ obeys the ODE (7) with $A_y = A_y^L$,

$$A_y^L := T_{y\zeta} A_\zeta^L T_{y\zeta}^{-1}. \quad (68)$$

Note that the first and last block row of $T_{y\zeta}$ in (67) are simply

$$\begin{bmatrix} y^0(t) \\ y^N(t) \end{bmatrix} = \begin{bmatrix} I_n & -I_n & \cdots & (-1)^N I_n \\ I_n & I_n & \cdots & I_n \end{bmatrix} \zeta(t) \quad (69)$$

since $p_k(-1) = (-1)^k$, $p_k(1) = 1$ (and $T_{y\zeta}^{jk} = p_k(\vartheta(\tilde{\theta}_j)) I_n$).

Remark 1.3 (Implementation of A_y^L): Efficient conversion algorithms [59] are found in the Chebfun toolbox. Applying

| polynomial approximation (of functions) | | spectral methods (for differential equations) | | numerical integration (for integral expressions) | |
|---|---|---|-----------------------|--|-------------------------|
| (*) JP stands for Chebyshev, Legendre, or other Jacobi polynomials | | JP: Chebyshev Legendre | | JP: Chebyshev Legendre | |
| interpolation / coincidence in the chosen nodes (natural basis: Lagrange polynomials w.r.t. the chosen nodes), equivalently, 'discrete expansion' with the 0-th to N -th JP as basis, related to an approximation of the series truncation below via quadrature | Gauss-Lobatto nodes (extrema of the N -th JP) | collocation / pseudospectral method / method of selected points / at the nodes vanishing residual | <i>Chebyshev col.</i> | interpolatory quadrature / integration of an interpolating polynomial instead of the original function | <i>Cleenshaw-Curtis</i> |
| | Gauss nodes (roots of the $(N+1)$ -th JP) | | – | | <i>Gauss quad.</i> |
| series truncation / orthogonal ¹³ projection to the 0-th to N -th JP / 'continuous expansion' with the 0-th to N -th JP as basis / generalized Fourier truncation / least squares best approximation | | Galerkin-like methods, e.g., Galerkin method or tau method / Lanczos' tau method / Galerkin with boundary bordering | <i>Legendre tau</i> | – (the projection requires itself integral evaluations) | – |

TABLE II: Classification of the used methods ("–" marks synonymous terms). See [57], [38], [51], [56], [58] for details.

these to the identity matrix yields $T_{y\zeta}$ and $T_{\zeta y} := T_{y\zeta}^{-1}$. Thus,

$$A_y^L = A \text{ can be derived by adding the lines}$$

```
Tyc=kron(legcoeffs2chebvals(eye(N+1)),eye(n));
Tcy=kron(chebvals2legcoeffs(eye(N+1)),eye(n));
A=Tyc*Ac*Tcy
```

to the code given in Remark 1.2. ◀

3) Further notes on the Legendre tau method:

a) *Lyapunov equation in Legendre coordinates:* To obtain an approximation of $V(\phi)$ via the Legendre tau approach, we can resort to (10) with $A_y = A_y^L$ from (68). However, from a numerical point of view, it might be preferable to remain in Legendre coordinates ζ and to use $A_\zeta = A_\zeta^L$, (66), in

$$V_\zeta(\zeta) := \zeta^\top P_\zeta \zeta, \quad P_\zeta = P_\zeta^\top \in \mathbb{R}^{n(N+1) \times n(N+1)} \quad (70)$$

$$D_f^+ V_\zeta(\zeta) = \zeta^\top (P_\zeta A_\zeta + A_\zeta^\top P_\zeta) \zeta \stackrel{!}{=} -\zeta^\top (T_{y\zeta}^\top Q_y T_{y\zeta}) \zeta,$$

$\forall \zeta \in \mathbb{R}^{n(N+1)}$ with $T_{y\zeta}$ from (67). That is, we solve

$$P_\zeta A_\zeta + A_\zeta^\top P_\zeta = -T_{y\zeta}^\top Q_y T_{y\zeta} \quad (71)$$

for P_ζ and, if desired, express the result in y coordinates

$$V_y(y) = V_\zeta(\zeta) = V_\zeta(T_{y\zeta}^{-1}y) = y^\top \underbrace{(T_{y\zeta}^{-1})^\top P_\zeta T_{y\zeta}^{-1}}_{=: P_y} y. \quad (72)$$

With Q_y from (37), only the first and last block rows (69) of $T_{y\zeta}$ are required in (71).

b) *Discretization:* The discretization $\zeta = (\zeta^k)_{k \in \{0, \dots, N\}}$ of a given function ϕ , e.g., an initial condition $x_0 = \phi$ or an argument of the functional $V(\phi)$, is chosen as

$$\zeta^k = \tilde{\zeta}^k, \quad \text{if } k < N, \quad \text{and} \quad \zeta^N = \phi(0) - \sum_{k=0}^{N-1} \zeta^k, \quad (73)$$

where $\{\zeta^0, \dots, \zeta^{N-1}\}$ stem from a truncation of the Legendre series representation $\phi(\theta) = \sum_{k=0}^{\infty} \tilde{\zeta}^k p_k(\vartheta(\theta))$, [29]. The last component ζ^N in (73) is such that the N -th order approximating polynomial $\sum_{k=0}^N \zeta^k p_k(\vartheta(\theta)) \approx \phi(\theta)$, at $\theta = 0$, exactly matches $\phi(0)$ (note that $\vartheta(0) = 1$ and $p_k(1) = 1, \forall k$).

c) V_1 and V_2 : For two important cases of the right-hand side $-Q_\zeta = -T_{y\zeta}^\top Q_y T_{y\zeta}$ in (71), we can give the solution P_ζ , respectively the resulting $V_y(y) = V_\zeta(\zeta) \approx V(\phi)$, analytically.

Lemma 1.1: The Legendre-tau-based approximation of $V_1(\phi)$ in Lemma 6.1 becomes $V_1(\tilde{\phi}^{(N-1)})$, where $\tilde{\phi}^{(N-1)}(\theta) = \sum_{k=0}^{N-1} \tilde{\zeta}^k p_k(\vartheta(\theta))$ is the $(N-1)$ -th order Legendre series truncation of $\phi(\theta) = \sum_{k=0}^{\infty} \tilde{\zeta}^k p_k(\vartheta(\theta))$. ◀

Proof: For $Q_y = \text{diag}([1, 0_{1 \times n(N-1)}, -1]) \otimes \tilde{Q}_1$, and, thus, $Q_\zeta^{jk} = (-1 + (-1)^{j+k}) \tilde{Q}_1$, it can be verified that

$$P_\zeta = \text{diag}([\frac{h}{2} \frac{2}{2k+1}]_{k \in \{0, \dots, N-1\}}, 0] \otimes \tilde{Q}_1 \quad (74)$$

is a solution of (71). Hence, $V_\zeta(\zeta) = \zeta^\top P_\zeta \zeta = \sum_{k=0}^{N-1} \frac{h}{2} \frac{2}{2k+1} \zeta_k^\top \tilde{Q}_1 \zeta_k$. Equivalence with $V_1(\tilde{\phi}^{(N+1)}) = \int_{-h}^0 (\sum_{k=0}^{N-1} \tilde{\zeta}^j p_j(\vartheta(\theta)))^\top \tilde{Q}_1 (\sum_{j=0}^{N-1} \tilde{\zeta}^k p_k(\vartheta(\theta))) d\theta$ follows from (73) and $\int_{-1}^1 p_j(\vartheta) p_k(\vartheta) d\vartheta = \frac{2}{2k+1} \delta_{jk}$ [57, B.1]. ■

Lemma 1.2: Provided (37) is used, the Legendre-tau-based approximation of $V_2(\phi)$ in Lemma 6.1 becomes $V_2(\tilde{\phi}^{(N-1)})$ with $\tilde{\phi}^{(N-1)}$ as above (Lemma 1.1). ◀

Proof: Consider $Q_\zeta = Q_{\zeta,0} + Q_{\zeta,2}$ with $Q_{\zeta,0} = T_{y\zeta}^\top (\text{diag}([0_{1 \times nN}, 1]) \otimes Q_0) T_{y\zeta} = 1_{(N+1) \times (N+1)} \otimes Q_0$ and $Q_{\zeta,2} = \text{diag}([\frac{1}{2k+1}]_{k \in \{0, \dots, N-1\}}, 1] \otimes hQ_2$, where $Q_0 = -h\tilde{Q}_2, Q_2 = \tilde{Q}_2$. It can be verified that P_ζ with

$$P_\zeta^{jk} = \begin{cases} (\frac{h}{2})^2 \frac{2}{2j+1} \frac{k}{2k+1} \tilde{Q}_2 & \text{if } j = k - 1 < N - 1 \\ (\frac{h}{2})^2 \frac{2}{2j+1} \tilde{Q}_2 & \text{if } j = k < N \\ (\frac{h}{2})^2 \frac{2}{2j+1} \frac{k+1}{2k+1} \tilde{Q}_2 & \text{if } j = k + 1 < N \\ 0_{n \times n} & \text{else} \end{cases} \quad (75)$$

solves (71). The equality $\zeta^\top P_\zeta \zeta = V_2(\sum_{k=0}^{N-1} \zeta^k p_k(\vartheta(\theta)))$ is shown by using the three-term recurrence relation [57, (4.17)] $\vartheta p_k(\vartheta) = \frac{k}{2k+1} p_{k-1}(\vartheta) + \frac{k+1}{2k+1} p_{k+1}(\vartheta)$ in V_2 . ■

d) *Combined coordinates:* Besides of Legendre coordinates ζ , and interpolation coordinates $y = [\begin{smallmatrix} z \\ \hat{x} \end{smallmatrix}] = T_{y\zeta} \zeta$, the combination of the first $(N-1)$ of the N Legendre coordinates and the boundary value $\hat{x} = \phi(0)$,

$$\chi = \begin{bmatrix} \zeta^0 \\ \vdots \\ \zeta^{N-1} \\ \hat{x} \end{bmatrix} = \underbrace{\begin{bmatrix} I_{nN} & 0_{nN \times n} \\ I_n & \dots & I_n & I_n \end{bmatrix}}_{T_{\chi\zeta}} \zeta, \quad (76)$$

is, in light of (73), as well an appropriate choice of coordinates. In particular, Lemma 3.1 can directly be applied to $P_\chi = T_{\chi\zeta}^\top P_\zeta T_{\chi\zeta}$, with $T_{\chi\zeta} = T_{\chi\zeta}^{-1} = \begin{bmatrix} I_{nN} & 0_{nN \times n} \\ -1_n^\top \otimes I_n & I_n \end{bmatrix}$, thus obtaining the quadratic lower bound as in Cor. 3.1, but without the need of $P_y = T_{\zeta y}^\top P_\zeta T_{\zeta y}$ (which would require $T_{\zeta y}$ from Rem. 1.3).

e) *Discontinuous basis:* The given coordinates ζ , or equivalently $y = T_{y\zeta} \zeta$, or $\chi = T_{\chi\zeta} \zeta$, uniquely represent an N -th order approximating polynomial $\phi(\theta) \approx \sum_{k=0}^N \zeta^k p_k(\vartheta(\theta)) = \sum_{k=0}^N y^k \ell_k(\vartheta(\theta)) = \sum_{k=0}^{N-1} \chi^k (p_k(\vartheta(\theta)) - p_N(\vartheta(\theta))) + \chi^N p_N(\vartheta(\theta))$. However, if a function with a jump discontinuity

at $\theta = 0$ is of interest, it is convenient¹⁴ to consider as approximating function instead the piecewise defined $(N - 1)$ -th order polynomial with a discontinuous end point

$$\phi(\theta) \approx \begin{cases} \sum_{k=0}^{N-1} \zeta^k p_k(\vartheta(\theta)), & \text{if } \theta < 0 \\ \hat{x}, & \text{if } \theta = 0 \end{cases} \quad (77)$$

(which, in (73), has the same discretization).

B. Numerical Integration of LK Functionals

Sec. II-E proposes to apply interpolatory quadrature rules to the LK functional. We consider Clenshaw-Curtis and Gauss quadrature. See, e.g., [58] for convergence statements.

1) *Clenshaw-Curtis quadrature*: A numerical integration of (15a) by an interpolatory quadrature rule replaces integrals by weighted sums from values at certain grid points. If these grid points are the (Gauss-Lobatto) Chebyshev nodes $\{\tilde{\theta}_k\}_{k \in \{0, \dots, N\}}$ introduced in (6), this amounts to a Clenshaw-Curtis quadrature, cf. [56, Sec. 3.7]. The weights¹⁵ w_k are, e.g., available¹⁶ in the Chebfun toolbox [39]. For (15a), we obtain

$$\begin{aligned} V(\phi) &\approx \phi^\top(0) P_{xx} \phi(0) + 2 \sum_{k=0}^N w_k \phi^\top(0) P_{xz}(\tilde{\theta}_k) \phi(\tilde{\theta}_k) \\ &+ \sum_{j=0}^N w_j \sum_{k=0}^N w_k \phi^\top(\tilde{\theta}_j) P_{zz}(\tilde{\theta}_j, \tilde{\theta}_k) \phi(\tilde{\theta}_k) \\ &+ \sum_{k=0}^N w_k \phi^\top(\tilde{\theta}_k) P_{zz, \text{diag}}(\tilde{\theta}_k) \phi(\tilde{\theta}_k). \end{aligned} \quad (78)$$

Let $y^k = \phi(\tilde{\theta}_k)$, $k \in \{0 \dots, N\}$, where $y^N = \phi(\tilde{\theta}_N) = \phi(0)$. As in (13), the result (78) can be written as a quadratic form (with $p = \dim(z) := \dim([y^0, \dots, y^{N-1}]^\top) = nN$)

$$\begin{aligned} V(\phi) &\approx y^\top P_y^{\text{quad}} y = y^\top \left(\begin{array}{cc} 0_{p \times p} & 0_{p \times n} \\ 0_{n \times p} & P_{xx} \end{array} \right) \\ &+ \begin{bmatrix} 0_{p \times (p+n)} \\ - (P_{xz}(\tilde{\theta}_k) w_k)_k \end{bmatrix} + \begin{bmatrix} 0_{(p+n) \times p} & (w_j P_{zz}^\top(\tilde{\theta}_j))_j \\ & \text{blkdiag}((w_k P_{zz, \text{diag}}(\tilde{\theta}_k))_k) \end{bmatrix} \\ &+ \left(w_j P_{zz}(\tilde{\theta}_j, \tilde{\theta}_k) w_k \right)_{jk} \end{aligned} \quad (79)$$

See (24) for a factorization taking (15b) into account. Note that the right lower component of P_y^{quad} approximately becomes P_{xx} since the other contributions are weighted by w_N , which is quite small in the non-equidistant grid.

2) *Gauss quadrature*: As an alternative, we apply (Legendre) Gauss quadrature. Thus, the integral of a function is approximated by weighted sums from the function values at (Gauss) Legendre nodes. Being Gauss nodes, cf. Table II, they do not contain the boundary points of the domain $[-h, 0]$. That is why we take N (Gauss) Legendre nodes¹⁷ $\tilde{\theta}_k$, and add the zero end point with zero weight to get the

¹⁴See, in [36], the projector Q^N versus L^N .

¹⁵The weights $w_k = \frac{h}{2} \int_{-1}^1 \ell_k(\tilde{\vartheta}) d\tilde{\vartheta}$ are integrals of the Lagrange polynomials in $\int_{-h}^0 u(\theta) d\theta \approx \int_{-h}^0 \sum_{k=0}^N u(\tilde{\theta}_k) \ell_k(\theta) d\theta = \sum_{k=0}^N u(\tilde{\theta}_k) w_k$.

¹⁶implemented via `[theta, w]=chebpts(N+1, [-delay, 0])`

¹⁷via `[thetaL, wL]=legpts(N, [-delay, 0])` using the toolbox [39]

$N+1$ nodes $[(\tilde{\theta}^L)^\top, 0]^\top$ and weights $[(w^L)^\top, 0]^\top$. Therefore, contrary to the Gauss-Lobatto-node-based Clenshaw-Curtis quadrature, the contributions in (79) do not overlap, yielding for $y_G = [\phi^\top(\tilde{\theta}_0^L), \dots, \phi^\top(\tilde{\theta}_{N-1}^L), \phi^\top(0)]^\top$

$$\begin{aligned} V(\phi) &\approx y_G^\top \left[\begin{array}{cc} (w_j^L P_{zz}(\tilde{\theta}_j^L, \tilde{\theta}_k^L) w_k^L)_{jk} & (w_j^L P_{xz}^\top(\tilde{\theta}_j^L))_j \\ - (P_{xz}(\tilde{\theta}_k^L) w_k^L)_k & P_{xx} \end{array} \right] y_G \\ &\text{with } D = \text{blkdiag}((w_k^L P_{zz, \text{diag}}(\tilde{\theta}_k^L))_k). \end{aligned} \quad (80)$$

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