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LOCAL LINEARIZATION METHODS FOR THE NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS: AN OVERVIEW

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Abstract

Local Linearization (LL) methods conform a class of one-step explicit integrators for ODEs derived from the following primary and common strategy: the vector field of the differential equation is locally (piecewise) approximated through a first-order Taylor expansion at each time step, thus obtaining successive linear equations that are explicitly integrated. Hereafter, the LL approach may include some additional strategies to improve that basic affine approximation. Theoretical and practical results have shown that the LL integrators have a number of convenient properties. These include arbitrary order of convergence, A-stability, linearization preserving, regularity under quite general conditions, preservation of the dynamics of the exact solution around hyperbolic equilibrium points and periodic orbits, integration of stiff and high-dimensional equations, low computational cost, and others. In this paper, a review of the LL methods and their properties is presented.

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1 Introduction

A number of existing numerical integrators for ordinary differential equations (ODEs), which are usually referred to as exponential methods, have in common the explicit use of exponentials to obtain an approximate solution. Some examples are the methods known as exponential fitting [51, 13, 67, 16, 35], exponential integrating factor [50], exponential integrators [31, 32], exponential time differencing [19, 49], truncated Magnus expansion [39, 6], truncated Fer expansion [68] (also called exponential of iterated commutators in [37]), quadrature schemes based on versions of the variation of constants formula (e.g., [55, 40, 36, 57, 26]), exponential Runge-Kutta [33, 34], local linearization method (see, e.g., [58, 2, 64, 25, 59, 44, 45]) and the high order local linearization methods [21, 22]. The development of exponential methods has been greatly stimulated by their capability of preserving a number of geometric and dynamical features of the underlying systems at the expense of notably less computational effort than implicit integrators and bigger step sizes than conventional explicit integrators. Furthermore, several algorithmic advances have contributed to make them more feasible even for large stiff systems of differential equations, highly oscillatory problems and ODEs whose Jacobian has large imaginary eigenvalues. A number of efficient and stable procedures are now available for computing matrix exponential, e.g. through the Schur decomposition, stable Padé approximations with the scaling and squaring method, Krylov subspace methods and Lie-group based algorithms (see, e.g., [31, 32, 27, 63, 24, 17, 28]). Convenient formulas for the evaluation of some integrals that involve matrix exponential have also been obtained [66, 12].

In particular, the so-called Local Linearization (LL) method yields a one-step exponential integrator from the following strategy: the vector field of the differential equation is locally (piecewise) approximated through a first-order Taylor expansion at each time step, thus obtaining successive linear equations that are explicitly integrated. This approach has also appeared in the literature under other names, such as matricial exponentially fitted method [14], exponential Euler method [7, 52], piece-wise linearized method [59] and exponentially fitted Euler method [32]. An essential and distinctive aspect of the LL method is the local character of the affine approximation of the vector field at each time step, which makes a major difference with the exponential methods proposed in [50, 55, 40, 61, 36, 26] based on global linear approximations. In that way, the LL method attenuates the lack of accuracy of these methods for integrating highly nonlinear ODEs.

Theoretical and practical results have shown that the LL integrator has a number of convenient dynamic properties. These include A-stability, absence of spurious equilibrium points under quite general conditions, and preservation of the dynamics of the exact solution around hyperbolic equilibrium points and periodic orbits [44]. The LL method also allows the integration of stiff equations in a satisfactory way with low computational cost (comparable to conventional explicit schemes). Another appealing feature of the LL approach is its flexibility to be extended to more general kinds of equations, e.g., delay differential equations [47], random differential equations [11]

and stochastic differential equations (e.g., [56, 48, 10, 60] and references therein).

However, a major limitation of the Local Linear approximation resulting from the LL method is its low order of convergence; namely, order two [59, 44]. To overcome this, two classes of higher order local linearization methods were developed in [21] and [22]. These are based on adding a correction term to the Local Linear approximation, which is computed through a truncated Taylor expansion or by solving an auxiliary ODE by means of standard explicit integrators. The first class is called Local Linearization - Taylor (LLT) method, while the second one is called Local Linearization - Runge-Kutta (LLRK) method when the Runge-Kutta method is used to compute the mentioned auxiliary ODE.

Similar to the methods in [19, 55, 40, 26, 33, 34], LLT method yields A-stable integrators that are derived by inserting a polynomial approximation into the remainder term of the variation of constants formula. Likewise some other integrators based on versions of this formula (e.g., [40, 36]) and classical multiderivative integrators, they require the knowledge of higher order derivatives of the exact solution. On this basis the said polynomial is optimally provided by a truncated Taylor expansion but at the expense of computing higher derivatives. For this there are known recursive algorithms (see, e.g., [9, 29, 18]), and the use of symbolic computing packages may be helpful. The practical scope of the LLT method focuses on systems of equations for which such a computation is feasible with affordable effort.

In comparison with related approaches, the LLT method has a number of distinctive features: i) the linear term of the LLT integrators is locally determined at each time step (contrary to the global decomposition into linear and nonlinear parts involved in exponential time differencing [19] and exponential Runge-Kutta methods [33, 34]); ii) the said approximating polynomial is obtained through a truncated Taylor expansion and not by means of multistep interpolation or multistage algorithms as in [19, 55, 40, 26, 33, 34]; iii) as a consequence, LLT discretization reduces to the standard LL discretization when the degree of such a polynomial is zero; iv) some simplifications in computing this polynomial arise from the fact that its first two coefficients are null; v) LLT integrators are one-step methods, thus avoiding the inconvenience of determining starting values (in contrast with the multistep integrators in [19, 55, 40]); vi) it is non-iterative (unlike the method introduced in [26]); vii) it does not require the previous computation of a first approximation by some other A-stable method (unlike the approach in [36]); viii) it retains the above mentioned dynamical properties of the LL method; and ix) remarkably, all the numerical work required for computing the integrals of exponential functions involved in the LLT integrators is reduced to evaluate just one matrix exponential of dimension only slightly greater than the dimension differential equation.

Alternatively, LLRK integrators are obtained by splitting, at each time step, the solution of the underlying ODE in two parts: the solution $\mathbf{v}$ of a linear ODE plus the solution $\mathbf{u}$ of an auxiliary ODE. The first one is solved by a LL scheme in such a way that A-stability is ensured, while the second one is integrated by a high order explicit Runge-Kutta (RK) scheme.

Likewise Implicit-Explicit Runge-Kutta (IMEX RK) and conventional splitting methods (see e.g. [53], [1]), the splitting involved in the LLRK approximation is based on the representation of the underlying vector field as the addition of linear and nonlinear components. However, there are notable differences among these methods: i) Typically, in splitting and IMEX methods the vector field decomposition is global instead of local, and it is not based on a first-order Taylor expansion. ii) In contrast with IMEX and LLRK approaches, splitting methods construct an approximate solution by composition of the flows corresponding to the component vector fields. iii) IMEX RK methods are partitioned (more specifically, additive) Runge-Kutta methods that compute a solution $\mathbf{y} = \mathbf{v} + \mathbf{u}$ by solving certain ODE for $(\mathbf{v}, \mathbf{u})$, setting different RK coefficients for each block. LLRK methods also solve a partitioned system for $(\mathbf{v}, \mathbf{u})$, but a different one. In this case, one of the blocks is linear and uncoupled, and it is discretized by the LL method. After inserting the (continuous time) LL approximation into the second block, this is treated as a non-autonomous ODE, for which any extant RK discretization can be used. On the other hand, it is worth noting that the LLRK method can also be thought of a flexible approach to construct new L-stable explicit schemes based on standard explicit RK integrators. In comparison with the well-known Rosenbrock [8, 62] and Exponential Integrators [31, 32], the L-stability of the LLRK schemes is achieved in a different way. Basically, Rosenbrock and Exponential integrators are obtained by inserting a stabilization factor $(1/(1-z)$ or $(e^z - 1)/z$, respectively) into the explicit RK formulas, whose coefficients must then be determined to fulfil both L-stability and order conditions. In contrast, L-stability of an LLRK scheme results from the fact that the component $\mathbf{v}$ associated with the linear part of the vector field is computed through an L-stable LL scheme. Another major difference is that the RK coefficients involved in the LLRK method are not constrained by any stability condition and they may satisfy the usual order conditions for RK schemes. Thus, the coefficients in the LLRK method may be just those of any standard explicit RK scheme. This makes the LLRK approach greatly flexible and allows for simple numerical implementations on the basis of available subroutines for LL and RK methods. With respect to the LLT method, the LLRK method archives all the nice convergence, stability and dynamical properties of it, but with lower computational cost and without the use of high order derivatives of the vector field of the ODEs.

In this paper, a review of the LL methods and their properties is presented. The paper is organized as follows. In sections 2 and 3, the formulations of the LL, LLT and LLRK methods are presented. Sections 4, 5 and 6 deal with the convergence, linear stability and dynamic properties of the LL, LLT and LLRK discretizations. Section 7 focuses on the numerical implementation of these discretizations, that is, on the so-called Local Linearization schemes. Furthermore, unlike the majority of previous papers on exponential integrators, the theoretical study of previous sections is extended to the numerical schemes that implement the LL methods in practice. Finally, a brief comment on the performance of the Local Linearization schemes in simulations is presented in the last section.

2 Local Linear approximation

Let $\mathcal{D} \subset \mathbb{R}^d$ be an open set. Consider the d -dimensional differential equation

$$\begin{aligned} \frac{d\mathbf{x}(t)}{dt} &= \mathbf{f}(t, \mathbf{x}(t)), \quad t \in [t_0, T] && (1) \\ \mathbf{x}(t_0) &= \mathbf{x}_0, && (2) \end{aligned}$$

where $\mathbf{x}_0 \in \mathcal{D}$ is a given initial point, and $\mathbf{f} : [t_0, T] \times \mathcal{D} \longrightarrow \mathbb{R}^d$ is a differentiable function. Lipschitz and smoothness conditions on the function $\mathbf{f}$ are assumed in order to ensure a unique solution of this equation in $\mathcal{D}$.

Let $(t)_h = \{t_n : n = 0, 1, \cdots, N\}$ be a time discretization with maximum step-size h defined as a sequence of times that satisfy the conditions

$$t_0 < t_1 < \cdots < t_N = T,$$

and

$$\sup_n(h_n) \leq h < 1, \tag{3}$$

where $h_n = t_{n+1} - t_n$ for $n = 0, ..., N-1$. Further, let

$$n_t = \max\{n = 0, 1, \cdots, N : t_n \leq t \text{ and } t_n \in (t)_h\}$$

for all $t \in [t_0, T]$.

Suppose that, for all $t_n \in (t)_h$, $\mathbf{y}_n \in \mathcal{D}$ is a point close to $\mathbf{x}(t_n)$. Consider the first order Taylor expansion of the function $\mathbf{f}$ around the point $(t_n, \mathbf{y}_n)$

$$\mathbf{f}(s, \mathbf{u}) \approx \mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)(\mathbf{u} - \mathbf{y}_n) + \mathbf{f}_t(t_n, \mathbf{y}_n)(s - t_n)$$

for $s \in \mathbb{R}$ and $\mathbf{u} \in \mathcal{D}$, where $\mathbf{f}_{\mathbf{x}}$ and $\mathbf{f}_t$ denote the partial derivatives of $\mathbf{f}$ with respect to the variables $\mathbf{x}$ and t, respectively. Adopting this linear approximation for $\mathbf{f}$ at each time t_n, the solution of (1)-(2) can be locally approximated on each interval $[t_n, t_{n+1})$ by the solution of the linear ODE

$$\begin{aligned} \frac{d\mathbf{y}(t)}{dt} &= \mathbf{A}_n\mathbf{y}(t) + \mathbf{a}_n(t), \quad t \in [t_n, t_{n+1}) && (4) \\ \mathbf{y}(t_n) &= \mathbf{y}_n\ , && (5) \end{aligned}$$

where $\mathbf{A}_n = \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)$ is a constant matrix and $\mathbf{a}_n(t) = \mathbf{f}_t(t_n, \mathbf{y}_n)(t - t_n) + \mathbf{f}(t_n, \mathbf{y}_n) - \mathbf{A}_n\mathbf{y}_n$ is a linear vector function of t. According to the variation of the constants formula, such a solution is given by

$$\mathbf{y}(t) = e^{\mathbf{A}_n(t-t_n)}(\mathbf{y}_n + \int_0^{t-t_n} e^{-\mathbf{A}_n u}\mathbf{a}_n(t_n + u)\, du). \tag{6}$$

Furthermore, by using the identity

$$\int_0^{\Delta} e^{-\mathbf{A}_n u} du\ \mathbf{A}_n = -(e^{-\mathbf{A}_n\Delta} - \mathbf{I}), \qquad \Delta \geq 0 \tag{7}$$

and simple rules from the integral calculus, the expression (6) can be rewritten as

$$\mathbf{y}(t) = \mathbf{y}_n + \phi(t_n, \mathbf{y}_n; t - t_n), \tag{8}$$

where

$$\begin{aligned} \phi(t_n, \mathbf{y}_n; t - t_n) &= \int_0^{t-t_n} e^{\mathbf{A}_n(t-t_n-u)}(\mathbf{A}_n\mathbf{y}_s + \mathbf{a}_n\,(t_n + u))\,du \\ &= \int_0^{t-t_n} e^{\mathbf{f}_{\mathbf{x}}(t_n,\mathbf{y}_n)(t-t_n-u)}(\mathbf{f}\,(t_n, \mathbf{y}_n) + \mathbf{f}_t\,(t_n, \mathbf{y}_n)\,u)du. \end{aligned} \tag{9}$$

In this way, by setting $\mathbf{y}_0 = \mathbf{x}(t_0)$ and iteratively evaluating the expression (8) at t_{n+1} (for $n = 0, 1..., N-1$), a sequence of points $\mathbf{y}_{n+1}$ can be obtained as an approximation to the solution $\mathbf{x}$ of (1)-(2) at each point $t_{n+1} \in (t)_h$. This is formalized in the following definition.

Definition 1 *For a given time discretization $(t)_h$, the Local Linear discretization of the ODE (1)-(2) at each point $t_{n+1} \in (t)_h$ is defined by the recursive expression*

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \phi(t_n, \mathbf{y}_n; h_n), \tag{10}$$

starting with $\mathbf{y}_0 = \mathbf{x}_0$.

Moreover, an approximation for $\mathbf{x}$ in the whole interval $[t_0, T]$ is stated in the next definition.

Definition 2 *For a given time discretization $(t)_h$, the Local Linear approximation of the solution of (1)-(2) is defined by the function*

$$\mathbf{y}\,(t) = \mathbf{y}_{n_t} + \phi(t_{n_t}, \mathbf{y}_{n_t}; t - t_{n_t}) \tag{11}$$

for all $t \in [t_0, T]$, where $\mathbf{y}_{n_t}$ is the Local Linear discretization (10) at n_t.

It is clear that the Local Linear approximation is a continuous function that coincides with the Local Linear discretization at each point of the time discretization $(t)_h$.

In next sections a number of properties of the Local Linear approximation will be demonstrated. This includes a convergence rate of order 2, A-stability, correct reproduction of phase portraits near hyperbolic equilibrium points and cycles of the underlying differential equations, and others. Furthermore, a variety of numerical implementations of the Local Linear discretization, called Local Linearization schemes, will be presented as well. It will be shown that these numerical schemes essentially differ with respect to the algorithm used to compute the recursion (10), and so, in the dynamical properties that they inherit from the Local Linear discretization.

3 High Order Local Linear approximations

In this section a modification of the LL method is introduced in order to improve its order of convergence while retaining desirable stability and dynamical properties. For this purpose, observe that the solution of the local linear ODE (4)-(5) is an approximation to the solution of the local nonlinear ODE

$$\begin{aligned} \frac{d\mathbf{z}(t)}{dt} &= \mathbf{f}(t, \mathbf{z}(t)), \quad t \in [t_n, t_{n+1}) \\ \mathbf{z}(t_n) &= \mathbf{y}_n \ , \end{aligned}$$

which can be rewritten as

$$\begin{aligned} \frac{d\mathbf{z}(t)}{dt} &= \mathbf{A}_n \mathbf{z}(t) + \mathbf{a}_n(t) + \mathbf{g}(t_n, \mathbf{y}_n; t, \mathbf{z}(t)), \quad t \in [t_n, t_{n+1}) \\ \mathbf{z}(t_n) &= \mathbf{y}_n, \end{aligned}$$

where $\mathbf{g}(t_n, \mathbf{y}_n; t, \mathbf{z}(t)) = \mathbf{f}(t, \mathbf{z}(t)) - \mathbf{A}_n \mathbf{z}(t) - \mathbf{a}_n(t)$, and $\mathbf{A}_n$, $\mathbf{a}_n(t)$ are defined as in the previous section. From the variation of constants formula the solution $\mathbf{z}$ of this equation can be written as

$$\mathbf{z}(t) = \mathbf{l}(t; t_n, \mathbf{y}_n) + \mathbf{r}(t; t_n, \mathbf{y}_n),$$

where

$$\mathbf{l}(t; t_n, \mathbf{y}_n) = \mathbf{y}_n + \phi(t_n, \mathbf{y}_n; t - t_n) \tag{12}$$

is the solution of the linear equation (4)-(5) and

$$\mathbf{r}(t; t_n, \mathbf{y}_n) = \int_0^{t-t_n} e^{\mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)(t - t_n - u)} \mathbf{g}(t_n, \mathbf{y}_n; t_n + u, \mathbf{z}(t_n + u))\, du \tag{13}$$

is the remainder term of the Local Linear approximation (12) to $\mathbf{z}$. Consequently, if $\mathbf{e}_r$ is an approximation to $\mathbf{r}$ of order $r > 2$, then $\mathbf{y}(t) = \mathbf{l}(t; t_n, \mathbf{y}_n) + \mathbf{e}_r(t; t_n, \mathbf{y}_n)$ should provide a better estimate to $\mathbf{z}(t)$ than the Local Linear approximation $\mathbf{y}(t) = \mathbf{l}(t; t_n, \mathbf{y}_n)$ for all $t \in [t_n, t_{n+1})$. This motivates the definition of the following High Order Local Linear (HOLL) discretization.

Definition 3 *For a given time discretization $(t)_h$, the order γ Local Linear discretization of the ODE (1)-(2) is defined by the recursive expression*

$$\mathbf{y}_{n+1} = \mathbf{l}(t_n + h_n; t_n, \mathbf{y}_n) + \mathbf{e}_r(t_n + h_n; t_n, \mathbf{y}_n), \tag{14}$$

starting with $\mathbf{y}_0 = \mathbf{x}_0$, where $\mathbf{e}_r$ is an approximation to the remainder term (13) such that $\|\mathbf{x}(t_n) - \mathbf{y}_n\| = O(h^\gamma)$ for all $t_n \in (t)$, with $\gamma > 2$.

By analogy with definitions 1 and 2 in previous section, it follows

Definition 4 *For a given time discretization $(t)_h$, the order γ Local Linear approximation of the solution of (1)-(2) is defined by the function*

$$\mathbf{y}(t) = \mathbf{l}(t; t_{n_t}, \mathbf{y}_{n_t}) + \mathbf{e}_r(t; t_{n_t}, \mathbf{y}_{n_t})$$

for all $t \in [t_0, T]$, where $\mathbf{y}_{n_t}$ is the order γ Local Linear discretization (14) at n_t. Here, $\mathbf{e}_r$ is assumed to provide an approximation to the remainder term (13) such that $\sup_{t\in[t_0,T]} \|\mathbf{x}(t) - \mathbf{y}(t)\| = O(h^\gamma)$.

For expediency, in what follows, the Local Linear discretization (10) (and consequently the Local Linear approximation (11)) will be named also as order 2 Local Linear discretization (approximation, respectively).

In the next subsections two classes of HOLL approximations are presented. In these classes the remainder term $\mathbf{r}$ is approximated through a truncated Taylor expansion or by a standard explicit integrator that solves an auxiliary ODE. The first class is called Local Linearization - Taylor (LLT) method, while the second one is called Local Linearization - Runge-Kutta (LLRK) method when the Runge-Kutta method is used to compute the mentioned auxiliary ODE.

3.1 Local Linear - Taylor approximations

Suppose that $\mathbf{f}$ is r-times continuous differentiable on $[t_0, T] \times \mathcal{D}$, and let $r > 2$. Then the function $\mathbf{g}(t_n, \mathbf{y}_n; \cdot)$ in (13) can be approximated by its order $r-1$ Taylor expansion around $t = t_n$. That is

$$\mathbf{g}(t_n, \mathbf{y}_n; t, \mathbf{z}(t)) \approx \sum_{j=0}^{r-1} \mathbf{c}_j(t_n, \mathbf{y}_n) \frac{(t-t_n)^j}{j!}, \tag{15}$$

where the coefficient

$$\mathbf{c}_j(t_n, \mathbf{y}_n) = \begin{cases} \frac{d^j}{dt^j}\mathbf{f}(t_n, \mathbf{y}_n) - \frac{\partial}{\partial \mathbf{x}}\mathbf{f}(t_n, \mathbf{y}_n)\frac{d^{j-1}}{dt^{j-1}}\mathbf{f}(t_n, \mathbf{y}_n) & \text{for } j \geq 2 \\ 0 & \text{for } j = 0, 1 \end{cases}$$

is the j-th derivative of $\mathbf{g}(t_n, \mathbf{y}_n; \cdot)$ with respect to t evaluated at $(t_n, \mathbf{z}(t_n))$. Substituting the right-hand term of (15) in (13) the approximation

$$\mathbf{e}_r(t; t_n, \mathbf{y}_n) = \int_0^{t-t_n} e^{\mathbf{f}_\mathbf{x}(t_n, \mathbf{y}_n)(t-t_n-u)} \sum_{j=0}^{r-1} \mathbf{c}_j(t_n, \mathbf{y}_n) \frac{u^j}{j!} du \tag{16}$$

to $\mathbf{r}$ is obtained. Then, from (14), it follows that

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \phi_r(t_n, \mathbf{y}_n, h_n), \tag{17}$$

where

$$\phi_r(\tau, \xi; \delta) = \int_0^\delta e^{(\delta-s)\mathbf{f}_\mathbf{x}(\tau,\xi)} \left(\mathbf{f}(\tau, \xi) + \mathbf{f}_t(\tau, \xi) u + \sum_{j=2}^{r-1} \mathbf{c}_j(\tau, \xi) \frac{u^j}{j!} \right) du.$$

This recursion, starting with $\mathbf{y}_0 = \mathbf{x}_0$, is called the Local Linear - Taylor discretization of (1)-(2). More precisely:

Definition 5 *An order γ Local Linear - Taylor (LLT) discretization is an order γ Local Linear discretization of the form (14), where expression (16) defines the approximation to the remainder term (13).*

Notice that the LLT discretization (17) reduces to the Local Linear discretization (10) for $r = 2$.

Definition 6 *An order γ Local Linear - Taylor (LLT) approximation is an order γ Local Linear approximation of the form*

$$\mathbf{y}(t) = \mathbf{y}_{n_t} + \phi_r(t_{n_t}, \mathbf{y}_{n_t}; t - t_{n_t}) \tag{18}$$

for all $t \in [t_0, T]$, where the function ϕ_r is defined as in (17).

In the following sections it will be demonstrated that the LLT approximations can reach a higher order of convergence than the LL approximation without losing the stability and dynamical properties of that approximation. However, this is achieved at the expense of computing higher order derivatives of the vector field of the equation, which could be highly demanding for a number of ODEs.

3.2 Local Linear - Runge-Kutta approximations

In this subsection an alternative approach for constructing higher order LL integrators is introduced. This is also based on the addition of a correction term to the Local Linear discretization, but now this is determined by the numerical solution of an auxiliary ODE.

Specifically, by taking derivatives with respect to t in (13), it is obtained that $\mathbf{r}(t; t_n, \mathbf{y}_n)$ satisfies the differential equation

$$\frac{d\mathbf{u}(t)}{dt} = \mathbf{q}(t_n, \mathbf{y}_n; t, \mathbf{u}(t)), \quad t \in [t_n, t_{n+1}], \tag{19}$$

$$\mathbf{u}(t_n) = \mathbf{0}, \tag{20}$$

with vector field

$$\mathbf{q}(t_n, \mathbf{y}_n; s, \xi) = \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)\xi + \mathbf{g}\left(t_n, \mathbf{y}_n; s, \mathbf{y}_n + \phi\left(t_n, \mathbf{y}_n; s - t_n\right) + \xi\right),$$

which can be written as

$$\mathbf{q}(t_n, \mathbf{y}_n; s, \xi) = \mathbf{f}(s, \mathbf{y}_n + \phi\left(t_n, \mathbf{y}_n; s - t_n\right) + \xi) - \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)\phi\left(t_n, \mathbf{y}_n; s - t_n\right) - \mathbf{f}_t\left(t_n, \mathbf{y}_n\right)(s - t_n) - \mathbf{f}\left(t_n, \mathbf{y}_n\right),$$

where ϕ is the vector function (9) that defines the Local Linear discretization (10). Thus, an approximation $\mathbf{e}_r$ to $\mathbf{r}$ can be obtained by solving the above ODE (19)-(20) through any conventional numerical integrator. Namely, if $\mathbf{u}_{n+1} = \mathbf{u}_n + \mathbf{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{u}_n; h_n)$ is some one-step numerical integrator for this equation, then $\mathbf{e}_r(t_n + h_n; t_n, \mathbf{y}_n) = \mathbf{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{0}; h_n)$.

In particular, we will focus on the approximation $\mathbf{e}_r$ obtained by means of an explicit RK scheme of order r. Specifically, let us consider an s-stage explicit RK scheme with coefficients

$\mathbf{c} = [c_i]$, $\mathbf{A} = [a_{ij}]$, $\mathbf{b} = [b_j]$ applied to the equation (19)-(20), i.e., the approximation defined by the map

$$\rho\left(t_n, \mathbf{y}_n; t - t_n\right) = (t - t_n) \sum_{j=1}^{s} b_j \mathbf{k}_j, \qquad t \in [t_n, t_{n+1}), \tag{21}$$

where

$$\mathbf{k}_i = \mathbf{q}(t_n, \mathbf{y}_n;\ t_n + c_i\,(t - t_n)\,,\ (t - t_n) \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j).$$

Then, from (14), it follows that

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \phi_r(t_n, \mathbf{y}_n, h_n), \tag{22}$$

where

$$\phi_r(t_n, \mathbf{y}_n, h_n) = \phi\left(t_n, \mathbf{y}_n; h_n\right) + h_n \sum_{j=1}^{s} b_j \mathbf{k}_j.$$

This recursion, starting with $\mathbf{y}_0 = \mathbf{x}_0$, is known as the *Local Linear - Runge-Kutta* discretization of (1)-(2). More precisely:

Definition 7 *An order γ Local Linear - Runge-Kutta (LLRK) discretization is an order γ Local Linear discretization of the form (14), where expression (21) defines the approximation to the remainder term (13).*

Consequently, the corresponding continuous time approximation is defined as follows.

Definition 8 *An order γ Local Linear - Runge-Kutta (LLRK) approximation is an order γ Local Linear approximation of the form*

$$\mathbf{y}\left(t\right) = \mathbf{y}_{n_t} + \phi_r\left(t_{n_t}, \mathbf{y}_{n_t}; t - t_{n_t}\right) \tag{23}$$

for all $t \in [t_0, T]$, where the function ϕ_r is defined as in (22).

In the sections bellow, it will be demonstrated that, like the LLT approximations, the LLRK approximations can reach a higher order of convergence than that the LL approximation without losing the stability and dynamical properties of that approximation. However, this is achieved without computing higher order derivatives of the vector field of the underlying equation, which has a clear advantage over the LLT approximations. Furthermore, a number of general hints for the efficient implementation of the LLRK discretizations will be discussed, some of which will be applied to derive particular LLRK schemes in an illustrative way.

4 Convergence analysis

In this section, the convergence of the Local Linear approximations is studied. For this purpose, let us rewrite the Local Linear discretizations with the Henrici's notation

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_n \varphi_r(t_n, \mathbf{y}_n; h_n), \tag{24}$$

where

$$\varphi_r(t_n, \mathbf{y}_n; h_n) = \frac{1}{h_n}\phi_r\left(t_n, \mathbf{y}_n; h_n\right)$$

is the so-called *increment function,* and the function ϕ_r is defined as in (17) for the LL and LLT discretizations or as in (22) for the LLRK discretizations. Thus, the Local Linear approximations can be rewritten as

$$\mathbf{y}\left(t\right) = \mathbf{y}_{n_t} + \left(t - t_{n_t}\right)\ \varphi_r\left(t_{n_t}, \mathbf{y}_{n_t}; t - t_{n_t}\right)$$

for all $t \in [t_0, T]$.

In what follows, conditions for the uniform convergence of the different kinds of Local Linear approximations will be presented. This includes the conventional results on both the local truncation errors

$$L_{n+1} = \|\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - h_n\varphi_\gamma(t_n, \mathbf{x}(t_n); h_n)\|$$

and the global errors

$$E_{n_T} = \left\|\mathbf{x}(T) - \mathbf{y}_{n_T}\right\|,$$

where $\mathbf{x}$ denotes the solution of the ODE to be integrated on $[t_0, T]$.

4.1 LL approximation

The next theorem states conditions for the uniform convergence of the Local Linear approximation.

Theorem 9 *Let $\mathbf{x}(\cdot; \mathbf{x}_0)$ be the solution of the ODE (1)-(2). Suppose that the vector field $\mathbf{f} \in \mathcal{C}([t_0, T]\times\mathcal{D}, \mathbb{R}^d)$ is a twice differentiable function with bounded second partial derivatives. Further, suppose that $\mathbf{f}(t, \cdot)$ and its first partial derivatives are Lipschitz functions on $\mathcal{D}$ with Lipschitz constants independent of t. Then, for all $t_n \in (t)_h$ and h small enough, there exist positive constants $C_1(\mathbf{x}_0)$ and $C_2(\mathbf{x}_0)$ such that*

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - \phi(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h_n)\| \leq C_1(\mathbf{x}_0)h_n^3$$

and

$$\sup_{t\in[t_0,T]} \|\mathbf{x}(t; \mathbf{x}_0) - \mathbf{y}\left(t\right)\| \leq C_2(\mathbf{x}_0)\ h^2 \tag{25}$$

hold for the Local Linear approximation (11).

Proof. As in [43] ■

The theorem above states the local truncation error of the Local Linear discretization under the same weak assumptions of the existence and uniqueness theorem for ODEs plus some additional differentiability conditions. In practice, the continuity of functions is easier to verify than Lipschitz condition. In this case, Theorem 10 for the local truncation error of the LLT discretization is applicable with $\gamma = 2$ to the Local Linear discretization. Additionally, uniform

convergence of the Local Linear approximations can be obtained under a number of other assumptions on the vector field $\mathbf{f}$. In that respect, see [47], [11] and [42] for the case where DDEs, RDEs and SDEs reduce to ODEs.

4.2 LLT approximations

The next theorem states conditions for the uniform convergence of the Local Linear - Taylor approximations.

Theorem 10 *Suppose that the vector field* $\mathbf{f}$ *of the ODE (1)-(2) satisfies the condition*

$$(\mathbf{f} \circ \mathbf{x}(\cdot, \mathbf{x}_0)) \in \mathcal{C}^{\gamma}([t_0, T], \mathbb{R}^d). \tag{26}$$

Then, for all $t_n \in (t)_h$ *and* h *small enough, there exist positive constants* $C_1(\mathbf{x}_0)$ *and* $C_2(\mathbf{x}_0)$ *such that*

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - \phi_{\gamma}(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h_n)\| \leq C_1(\mathbf{x}_0) h_n^{\gamma+1}$$

and

$$\sup_{t \in [t_0, T]} \|\mathbf{x}(t; \mathbf{x}_0) - \mathbf{y}(t)\| \leq C_2(\mathbf{x}_0)\ h^{\gamma}$$

hold for the LLT approximation (18).

Proof. As in [44] for $\gamma = 2$, and in [22] for $\gamma \geq 2$. ■

4.3 LLRK approximations

In general, for HOLL approximations derived from the integration of the auxiliary equations (19)-(20) the following result is useful.

Lemma 11 *Let*

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \phi(t_n, \mathbf{y}_n; h_n) + \mathbf{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{0}; h_n), \quad \text{with } \mathbf{y}_0 = \mathbf{x}_0,$$

be a discretization of the ODE (1)-(2), where ϕ *is defined by (9), and* $\mathbf{u}_{n+1} = \mathbf{u}_n + \mathbf{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{u}_n; h_n)$ *is an order* γ *numerical integrator for the auxiliary equations (19)-(20). Then*

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - hF(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h_n)\| \leq C_1(\mathbf{x}_0) h_n^{\gamma+1}$$

for $t_n, t_{n+1} \in (t)_h$, *where*

$$F(t, \xi; h) = \frac{1}{h}\left\{\phi(t, \xi; h) + \mathbf{\Lambda}^{\xi}(t, \mathbf{0}; h)\right\}$$

and $C_1(\mathbf{x}_0)$ *is a positive constant depending only on* $\mathbf{x}_0$. *In addition, if* F *satisfies the local Lipschitz condition for the second argument, then there exist positive constants* δ_0 *and* $C_2(\mathbf{x}_0)$ *such that*

$$\sup_{t \in [t_0, T]} \|\mathbf{x}(t; \mathbf{x}_0) - \mathbf{y}(t)\| \leq C_2(\mathbf{x}_0)\ h^{\gamma},$$

with $h \leq \delta_0$, *where* $\mathbf{y}(t) = \mathbf{y}_{n_t} + (t - t_{n_t}) F(t_{n_t}, \mathbf{y}_{n_t}; t - t_{n_t})$ *is an approximation to* $\mathbf{x}(t; \mathbf{x}_0)$ *for all* $t \in [t_0, T]$.

Proof. As in [23]. ■

In particular, for the Local Linear - Runge-Kutta approximations the next theorem states conditions of uniform convergence.

Theorem 12 *Suppose that the vector field* $\mathbf{f}$ *of the ODE (1)-(2) satisfies the condition*

$$\mathbf{f} \in \mathcal{C}^{\gamma+1}([t_0, T], \mathbb{R}^d). \tag{27}$$

Then, for all $t_n \in (t)_h$ *and* h *small enough, there exist positive constants* $C_1(\mathbf{x}_0)$ *and* $C_2(\mathbf{x}_0)$ *such that*

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - \phi_\gamma(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h_n)\| \leq C_1(\mathbf{x}_0) h_n^{\gamma+1}$$

and

$$\sup_{t \in [t_0, T]} \|\mathbf{x}(t; \mathbf{x}_0) - \mathbf{y}(t)\| \leq C_2(\mathbf{x}_0)\ h^\gamma,$$

hold for the LLRK approximation (23).

Proof. As in [23]. ■

5 A-stability of the Local Linear discretizations

This section deals with the stability of the Local Linear discretizations when integrating linear ODEs.

Consider the scalar test equation

$$dx(t) = \lambda x(t)\, dt, \tag{28}$$

where λ is a complex number with negative real part.

It is trivial that the Local Linear discretization (10) is A-stable, since it provides the exact solution of any linear ODE.

For the Local Linear - Taylor discretization we have the following result.

Theorem 13 *LLT discretizations are A-stable.*

Proof. Note that for the test equation (28) the function ϕ_γ defined in (17) reduces to the function ϕ defined in (10) for $\gamma > 2$. That is, for that equation, the LLT discretizations reduce to the Local Linear discretization, which concludes the proof. ■

Similarly, for the Local Linear - Runge-Kutta discretizations we have the following result.

Theorem 14 *LLRK discretizations are A-stable.*

Proof. As in [23]. ■

6 Steady states of the Local Linear discretizations

It is well known (see, e.g., [15, 65]) that conventional numerical integrators such as Runge-Kutta, Adams-Bashforth, predictor-corrector methods and others produce seriously misleading when integrate dynamical systems. Typical problems are, for instance, the convergence to spurious steady states, changes in the basis of attraction, appearance of spurious bifurcations, etc. The essence of such difficulties is that dynamic of the numerical schemes (seems as discrete dynamical systems) is far richer than that of their continuous counterpart. Contrary to the popular belief, errors of this type may not be solved by reducing the stepsize of the numerical method. Therefore, these aspects should carefully be studied for each numerical integrator.

In this section the relation between the steady states of the autonomous equation

$$\begin{aligned} \frac{d\mathbf{x}(t)}{dt} &= \mathbf{f}(\mathbf{x}(t)), \quad t \in [t_0, T] && (29) \\ \mathbf{x}(t_0) &= \mathbf{x}_0 \in \mathbb{R}^d && (30) \end{aligned}$$

and those of the Local Linear discretizations is considered. For the sake of simplicity, a uniform time partition $(t)_h$ is adopted.

For this purpose, it is convenient to write the order γ Local Linear discretizations with the Henrici's notation

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\varphi_\gamma(\mathbf{y}_n, h), \tag{31}$$

where the incremental function is now rewritten as

$$\varphi_\gamma(\xi,\delta) = \mathbf{\Phi}_\gamma(\xi,\delta)\mathbf{f}(\xi)$$

for the LLT discretizations, or as

$$\varphi_\gamma(\xi,\delta) = \mathbf{\Phi}_2(\xi,\delta)\mathbf{f}(\xi) + \sum_{i=1}^{s} b_i \mathbf{k}_i(\xi,\delta), \tag{32}$$

for the LLRK ones, with $\xi \in \mathbb{R}^d$ and $\delta \geq 0$. In the above expressions

$$\mathbf{\Phi}_\gamma(\xi,\delta) = \frac{1}{\delta}\int_0^\delta e^{(\delta-s)\mathbf{f}_\mathbf{x}(\xi)} \left(\mathbf{I} + \sum_{j=2}^{\gamma-1} \mathbf{M}_j(\xi)\frac{s^j}{j!}\right) ds \tag{33}$$

and

$$\mathbf{k}_i(\xi,\delta) = \mathbf{q}(\xi;\ c_i\delta,\ \delta\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j(\xi,\delta))$$

with

$$\mathbf{q}(\xi;\delta,\mathbf{u}) = \mathbf{f}(\xi + \mathbf{\Phi}_2(\xi,\delta)\mathbf{f}(\xi)\delta + \mathbf{u}) - \mathbf{f}_\mathbf{x}(\xi)\mathbf{\Phi}_2(\xi,\delta)\mathbf{f}(\xi)\delta - \mathbf{f}(\xi).$$

Expression (33) results from a straightforward application of the chain rule of differential calculus, which implies that the coefficients $\mathbf{c}_j(\xi)$ defined in (17) are linear functions of $\mathbf{f}(\xi)$, say $\mathbf{c}_j(\xi) = \mathbf{M}_j(\xi)\mathbf{f}(\xi)$ for some matrices $\mathbf{M}_j(\xi)$ depending of partial derivatives of $\mathbf{f}$ up to order j.

The following two lemmas provide some useful properties of the matrix function $\mathbf{\Phi}_\gamma$.

Lemma 15 *Let $\Omega \subset \mathbb{R}^d$ and $\mathcal{K} \subset \Omega$ be open and compact sets, respectively, and let*

$$\mathbf{\Phi}_2(\xi, \delta) = \frac{1}{\delta} \int_0^{\delta} e^{\mathbf{f}_{\mathbf{x}}(\xi)u} du \tag{34}$$

be the matrix function defined by (33) with $\gamma = 2$. Thus,

i) if $\mathbf{f} \in \mathcal{C}^{k+1}(\Omega, \mathbb{R}^d)$ with $k \in \mathbb{N}$, then $\mathbf{\Phi}_2 \in \mathcal{C}^k(\Omega \times \mathbb{R}_+, \mathbb{R}^{d\times d})$;

ii) if $\mathbf{f} \in \mathcal{C}^2(\Omega, \mathbb{R}^d)$, then $\mathbf{\Phi}_2(\xi, 0) = \mathbf{I}$ and $\partial\mathbf{\Phi}_2(\xi,0)/\partial\xi = \mathbf{0}$ for all $\xi \in \mathcal{K}$;

iii) if $\mathbf{f} \in \mathcal{C}^1(\Omega, \mathbb{R}^d)$, then $\mathbf{\Phi}_2^{-1}(\xi,\delta)$ exists for all $(\xi, \delta) \in K \times R_+$ such that $\lambda_i(\xi)\delta \neq \pm 2\pi n\sqrt{-1}$ for all $i = 1, .., p$ and $n = 1, 2, ...$ Here, $\lambda_1(\xi), .., \lambda_p(\xi)$ denote the p distinct eigenvalues of $f_{\mathbf{x}}(\xi)$, and $p \leq d$.

Proof. As in [44] ■

Lemma 16 *Let $\Omega \subset \mathbb{R}^d$ and $\mathcal{K} \subset \Omega$ be open and compact sets, respectively, and let $\mathbf{\Phi}_\gamma$ be the matrix function defined in (33). Thus,*

i) if $\mathbf{f} \in \mathcal{C}^{\gamma+k-1}(\Omega, \mathbb{R}^d)$ with $k \in \mathbb{N}$, then $\mathbf{\Phi}_\gamma \in \mathcal{C}^k(\Omega \times \mathbb{R}_+, \mathbb{R}^{d\times d})$;

ii) if $\mathbf{f} \in \mathcal{C}^\gamma(\Omega, \mathbb{R}^d)$, then $\mathbf{\Phi}_\gamma(\xi, 0) = \mathbf{I}$ and $\partial\mathbf{\Phi}_\gamma(\xi,0)/\partial\xi = \mathbf{0}$ for all $\xi \in \mathcal{K}$;

iii) if $\mathbf{f} \in \mathcal{C}^{\gamma-1}(\Omega, \mathbb{R}^d)$, then there exists a positive constant δ_0 such that $\mathbf{\Phi}_\gamma^{-1}(\xi,\delta)$ exists for all $(\xi, \delta) \in \mathcal{K} \times [0, \delta_0]$.

Proof. As in [22] ■

The next lemma states some useful properties of the functions φ_γ on neighborhoods of invariant sets of ODEs.

Lemma 17 *Let $\Sigma \subset \mathbb{R}^d$ be an invariant set for the flow of the equation (29). Let $\mathcal{K}$ and Ω be, respectively, compact and bounded open sets such that $\Sigma \subset \mathcal{K} \subset \Omega$. Suppose that the solution $\mathbf{x}$ of that equation satisfies the condition*

$$\mathbf{x}(t; \mathbf{x}_0) \subset \Omega \text{ for all initial point } \mathbf{x}_0 \in \mathcal{K} \text{ and } t \in [t_0, T]. \tag{35}$$

and the vector field $\mathbf{f}$ fulfils the continuity condition

$$\mathbf{f} \in \mathcal{C}^\gamma(\Omega, \mathbb{R}^d) \text{ or } \mathbf{f} \in \mathcal{C}^{\gamma+1}(\Omega, \mathbb{R}^d). \tag{36}$$

If

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\varphi_\gamma(\mathbf{y}_n, h)$$

represents an order γ LLT or LLRK discretization, then

i) $\varphi_\gamma \to \mathbf{f}$ *and* $\partial\varphi_\gamma/\partial\mathbf{y}_n \to \mathbf{f}_\mathbf{x}$ *as* $h \to 0$ *uniformly in* $\mathcal{K}$,

ii) $\|(\mathbf{x}(t_0+h;\mathbf{x}_0)-\mathbf{x}_0)/h - \varphi_\gamma(\mathbf{x}_0,h)\| = O(h^\gamma)$ *uniformly for* $\mathbf{x}_0 \in \mathcal{K}$.

Proof. As in [44], [22] and [23] for the LL, LLT and LLRK discretizations, respectively. ■

6.1 Fixed points, regularity and linearization preserving

In this subsection, the vector field $\mathbf{f}$ of the autonomous ODE (29) and its derivatives up to order γ are assumed to be defined and bounded for all $\xi \in \mathbb{R}^d$ in such a way that function φ_γ in (31) is well defined.

A numerical integrator is said to be regular if no fixed point (called ghost or spurious fixed point) occurs in the scheme that is not an equilibrium point of the ODE [38].

Theorem 18 *Let* $\lambda_1(\xi),..,\lambda_p(\xi)$ *be the* p *distinct eigenvalues of* $\mathbf{f}_\mathbf{x}(\xi)$, $p \leq d$. *The following assertions hold:*

i) All equilibrium points of an ODE are fixed points of the LL discretization.

ii) If $\mathbf{f} \in \mathcal{C}^1$, *then the LL discretization with step-size* h *is regular if* $\lambda_i(\xi)h \neq \pm 2\pi n\sqrt{-1}$ *for all* $\xi \in \mathbb{R}^d$, $i = 1,..,p$ *and* $n = 1,2,....$

iii) If $\mathbf{f} \in \mathcal{C}^1$, *then for a given step-size* h *the unique possible ghost points of the LL discretization are the points* $\xi \in \mathbb{R}^d$ *such that* $\mathbf{f}(\xi) \neq \mathbf{0}$, $\lambda_i(\xi)h = \pm 2\pi n\sqrt{-1}$ *for some* $1 \leq i \leq p$ *and* $n = 1,2...$, *and* $\mathbf{f}(\xi)$ *is in the null space of the matrix* $\mathbf{\Phi}_2(\xi,h)$.

iv) If $\mathbf{f}$ *is a differentiable Lipschitz function, then the LL discretization is regular for step-size* h *small enough.*

Proof. As in [44]. ■

Theorem 18 implies that, for any h, the Local Linear discretization is regular for one-dimensional ODEs and for any $d-$ dimensional ODE whose vector field $\mathbf{f}$ has symmetric Jacobian matrix $\mathbf{f}_\mathbf{x}$ at every $\xi \in \mathbb{R}^d$. In general, for h small enough, the theorem guarantees regularity for any ODE. This is a remarkable property of the Local Linearization method compared with conventional methods for ODEs.

For the Local Linear - Taylor discretization the next result follows.

Theorem 19 *The following assertions hold:*

i) All equilibrium points of an ODE are fixed points of any LLT discretization.

ii) If $\mathbf{f} \in \mathcal{C}^{\gamma-1}$, *then any LLT discretization is regular for step-size* h *small enough.*

Proof. As in [22]. ■

Analogously, Local Linear - Runge-Kutta discretization satisfies the following.

Theorem 20 *The following assertions hold:*

i) All equilibrium points of an ODE are fixed points of any LLRK discretization.

ii) If $\mathbf{f} \in \mathcal{C}^1$*, then any LLRK discretization is regular for step-size* h *small enough.*

Proof. As in [23]. ■

A numerical integrator $\mathbf{u}_{n+1} = \mathbf{u}_n + \mathbf{\Lambda}(t_n, \mathbf{u}_n; h_n)$ is linearization preserving at an equilibrium point ξ of the ODE (29), if from the Taylor series expansion of $\mathbf{\Lambda}(t_n, \cdot; h_n)$ around ξ it is obtained that

$$\mathbf{u}_{n+1} - \xi = e^{h\mathbf{f}_x(\xi)}(\mathbf{u}_n - \xi) + O(\|\mathbf{u}_n - \xi\|^2).$$

Furthermore, an integrator is said to be linearization preserving if it is linearization preserving at all equilibrium points of the ODE [54].

This last property ensures that the integrator correctly captures all eigenvalues of the linearized system at every fixed point of the ODE, which guarantees the exact preservation (in type and parameters) of a number of local bifurcations of the underlying equation [54]. Certainly, this results in a correct reproduction of the local dynamics before, during and after a bifurcation anywhere in the phase space by the numerical integrator.

Theorem 21 *LL and LLRK discretizations are linearization preserving.*

Proof. As in [54] and [23], for the LL and LLRK discretization, respectively. ■

The next section deals with a more precise analysis of the dynamical behavior of the LL discretizations in the neighborhood of some steady states.

6.2 Phase portrait near equilibrium points

Let $\mathbf{0}$ be a hyperbolic equilibrium point of the equation (29). Let $X_s, X_u \subset \mathbb{R}^d$ be the stable and unstable subspaces of the linear vector field $\mathbf{f}_{\mathbf{x}}(\mathbf{0})$ such that $\mathbb{R}^d = X_s \oplus X_u$, $(\mathbf{x}_s, \mathbf{x}_u) = \mathbf{x} \in \mathbb{R}^d$ and $\|\mathbf{x}\| = \max\{\|\mathbf{x}_s\|, \|\mathbf{x}_u\|\}$. It is well-known that the local stable and unstable manifolds at $\mathbf{0}$ may be represented as $M_s = \{(\mathbf{x}_s, p(\mathbf{x}_s)) : \mathbf{x}_s \in \mathcal{K}_{\varepsilon,s}\}$ and $M_u = \{(q(\mathbf{x}_u), \mathbf{x}_u)) : \mathbf{x}_u \in \mathcal{K}_{\varepsilon,u}\}$, respectively, where the functions $p : \mathcal{K}_{\varepsilon,s} = \mathcal{K}_\varepsilon \cap X_s \to \mathcal{K}_{\varepsilon,u} = \mathcal{K}_\varepsilon \cap X_u$ and $q : \mathcal{K}_{\varepsilon,u} \to \mathcal{K}_{\varepsilon,s}$ are as smooth as $\mathbf{f}$, and $\mathcal{K}_\varepsilon = \{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\| \leq \varepsilon\}$ for $\varepsilon > 0$.

Theorem 22 *Suppose that assumptions (35)-(36) of Lemma 17 hold on a neighborhood* Ω *of* $\mathbf{0}$*. Then, there exist constants* C*,* ε*,* ε_0*,* $h_0 > 0$ *such that the local stable* M_s^h *and unstable* M_u^h *manifolds of the order* γ *Local Linear discretization (31) at* $\mathbf{0}$ *are of the form*

$$M_s^h = \{(\mathbf{x}_s, p^h(\mathbf{x}_s)) : \mathbf{x}_s \in \mathcal{K}_{\varepsilon,s}\} \text{ and } M_u^h = \{(q^h(\mathbf{x}_u), \mathbf{x}_u) : \mathbf{x}_u \in \mathcal{K}_{\varepsilon,u}\},$$

where $p^h = p + O(h^\gamma)$ *uniformly in* $\mathcal{K}_{\varepsilon,s}$ *, and* $q^h = q + O(h^\gamma)$ *uniformly in* $\mathcal{K}_{\varepsilon,u}$*. Moreover, for any* $\mathbf{x}_0 \in \mathcal{K}_\varepsilon$ *and* $h \leq h_0$*, there exists* $\mathbf{z}_0 = \mathbf{z}_0(\mathbf{x}_0, h) \in \mathcal{K}_{\varepsilon_0}$ *satisfying*

$$sup\{\|\mathbf{x}(t_n;\mathbf{x}_0) - \mathbf{y}_n(\mathbf{z}_0)\| : \mathbf{x}(t;\mathbf{x}_0) \in \mathcal{K}_\varepsilon \text{ for } t \in [t_0, t_n]\} \leq Ch^\gamma. \tag{37}$$

Correspondingly, for any $\mathbf{z}_0 \in \mathcal{K}_\varepsilon$ *and* $h \leq h_0$*, there exists* $\mathbf{x}_0 = \mathbf{x}_0(\mathbf{z}_0, h) \in \mathcal{K}_{\varepsilon_0}$ *that fulfils (37), where the sup is taken over all* n *satisfying* $\mathbf{y}_j(\mathbf{z}_0) \in \mathcal{K}_\varepsilon$*,* $j = 0, .., n$*.*

Proof. As in [44], [22] and [23] for the LL, LLT and LLRK discretizations, respectively. ■

Theorem 22 shows that the phase portrait of a continuous dynamical system near a hyperbolic equilibrium point is correctly reproduced by any order γ Local Linear discretization with step-sizes small enough. It states that any trajectory of the dynamical system can be correctly approximated by a trajectory of such discretizations if the discrete initial value is conveniently adjusted. It also affirms that, any trajectory of a Local Linear discretization approximates some trajectory of the continuous system with a suitably selection of the starting point. In both case, these results are valid for sufficiently small step-size and as long as the trajectories stay within some neighborhood of the equilibrium point. Moreover, the theorem states that the local stable and unstable manifolds of a Local Linear discretization at the equilibrium point converge to those of the continuous system as the step-size tends to zero.

6.3 Phase portraits near periodic orbits

Suppose that the equation (29) has a hyperbolic closed orbit $\Gamma = \{\overline{\mathbf{x}}(t) : t \in [0, T]\}$ of period T in an open bounded set $\Omega \subset \mathbb{R}^d$. Let $\overline{\Omega}$ be the closure of Ω.

Theorem 23 *Let the assumptions (35)-(36) of Lemma 17 hold on a neighborhood of* $\overline{\Omega}$*. Then there exist* $h_0 > 0$ *and an open neighborhood* U *of* Γ *such that the Local Linear discretization (31) with order* $\gamma \geq 3$ *has an invariant closed curve* $\Gamma_h \subset U$ *for all* $h \leq h_0$*. More precisely, there exist* $T-$*periodic functions* $\overline{\mathbf{y}}_h : \mathbb{R} \to U$ *and* $\sigma_h - 1 : \mathbb{R} \to \mathbb{R}$ *for* $h \leq h_0$*, which are uniformly Lipschitz and satisfy*

$$\overline{\mathbf{y}}_h(t) + h\varphi_\gamma(\overline{\mathbf{y}}_h(t), h) = \overline{\mathbf{y}}_h(\sigma_h(t)),\ t \in \mathbb{R},$$

and

$$\sigma_h(t) = t + h + O(h^{\gamma+1}) \text{ uniformly for } t \in \mathbb{R}.$$

Furthermore, the curve $\Gamma_h = \{\overline{\mathbf{y}}_h(t) : t \in [0, T]\}$ *converges to* Γ *in the Lipschitz norm. In particular,*

$$\max_{t\in\mathbb{R}} \|\overline{\mathbf{x}}(t) - \overline{\mathbf{y}}_h(t)\| = O(h^\gamma)$$

and

$$\sup_{t_1\neq t_2} \frac{\|(\overline{\mathbf{x}} - \overline{\mathbf{y}}_h)(t_1) - (\overline{\mathbf{x}} - \overline{\mathbf{y}}_h)(t_2)\|}{|t_1 - t_2|} \to 0 \text{ as } h \to 0.$$

Proof. As in [22] and [23] for the LLT and LLRK discretizations, respectively. ■

Note that the previous theorem does not hold for the order 2 LLT discretization, that is, for the simple Local Linear discretization (10). The reason is that the assumption (36) with $\gamma = 2$ is not enough for Theorem 2.1 in [4]. This yields to the following corollary.

Corollary 24 *By replacing condition (36) with* $\mathbf{f} \in \mathcal{C}^3(\Omega, \mathbb{R}^d)$*, Theorem 23 also holds for the order 2 Local Linear discretization.*

Proof. As in [44]. ■

Theorem 23 and its Corollary affirm that, for h sufficiently small, Local Linear discretizations have a closed invariant curve Γ_h , i.e., $(1 + h\varphi(\cdot; h))(\Gamma_h) = \Gamma_h$, which converges to the periodic orbit Γ of continuous system.

The next theorem deals with the behavior of the discrete trajectories of the order γ Local Linear discretization (31) near the invariant curve Γ_h when the ODE (29) has a stable periodic orbit Γ. For $\mathbf{x}_0$ in a neighborhood of Γ, the notations

$$W_h(\mathbf{x}_0) = \{\mathbf{y}_n(\mathbf{x}_0) : n \geq 0\} \quad \text{and} \quad w(\mathbf{x}_0) = \{\mathbf{x}(t; \mathbf{x}_0) : t \geq 0\}$$

will be used. In addition,

$$d(A, B) = max\{\sup_{\mathbf{z}\in A} \text{dist}(\mathbf{z}, B), \sup_{\mathbf{z}\in B} \text{dist}(\mathbf{z}, A)\}$$

will denote the Hausdorff distance between two sets A and B.

Theorem 25 *Let* Γ *be a stable closed orbit of the equation (29). Then, under assumptions of Theorem 23 or its Corollary, there exist* h_0*,* α*,* β*,* C*,* $\rho > 0$*, such that for* $h \leq h_0$ *and* $dist(\mathbf{x}_0, \Gamma_h) \leq \rho$ *the following hold:*

$$dist(\mathbf{y}_n(\mathbf{x}_0), \Gamma_h) \leq C\ e^{-\alpha t_n}\ dist(\mathbf{x}_0, \Gamma_h),\ n \geq 0$$

and

$$dist(\mathbf{y}_n(\mathbf{x}_0), w(\mathbf{x}_0)) \leq C(h^\gamma + min\{h^\gamma e^{\beta t_n}, e^{-\alpha t_n}\}),\ n \geq 0. \tag{38}$$

Moreover, for any $\delta > 0$ *there exist* $\rho(\delta)$*,* $h(\delta) > 0$ *such that*

$$\sup_{n\geq 0} \{dist(\mathbf{y}_n(\mathbf{x}_0), w(\mathbf{x}_0))\} \leq Ch^{\gamma-\delta}$$

for $h \leq h(\delta)$ *and* $dist(\mathbf{x}_0, \Gamma_h) \leq \rho(\delta)$*. Finally,*

$$d(W_h(\mathbf{x}_0), w(\mathbf{x}_0)) \to 0 \text{ as } h \to 0$$

uniformly for $dist(\mathbf{x}_0, \Gamma) \leq \rho$*.*

Proof. As in [22] and [23] for the LLT and LLRK discretizations, respectively. ■

This theorem states the stability of the invariant curve Γ_h and the convergence of the trajectories of a Local Linear discretization to the continuous trajectories of the underlaying ODE when such discretization starts at a point close to the stable periodic orbit Γ.

7 Local Linearization schemes

This section deals with the practical issues of the LL method, that is, with the so-called Local Linearization schemes for ODEs.

Roughly speaking, every numerical implementation of a Local Linear discretization of any order is generically called Local Linearization scheme. More precisely, this can be defined as follows.

Definition 26 *For an order γ Local Linear discretization $\mathbf{y}_{n+1} = \mathbf{y}_n + \phi_\gamma(t_n, \mathbf{y}_n; h_n)$ of the ODE (1)-(2), all recursion of the form*

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\phi}_\gamma(t_n, \mathbf{y}_n; h_n), \qquad \textit{with } \widetilde{\mathbf{y}}_0 = \mathbf{y}_0,$$

where $\widetilde{\phi}_\gamma$ denotes a numerical algorithm to compute ϕ_γ, is generically called Local Linearization scheme.

Regularly, the numerical implementation of the Local Linear discretization (10) is simply called LL scheme, while the numerical implementation of a HOLL discretization is called HOLL scheme. In particular, the numerical implementation of the HOLL discretizations (17) and (22) are usually called LLTp and LLRK p schemes, respectively, where p denotes the order of convergence of the scheme.

7.1 LL schemes

There is a large variety of LL schemes which differ with respect to the algorithm that is used in the numerical implementation of the Local Linear discretization (10). They are derived from one of the three equivalent expressions of the Local Linear discretization, namely (9), (6) or (4).

For instance, depending on the way of computing the integral (9) in (10), different LL schemes can be obtained.

A first way to do that is by means of quadrature formulas (see for instance [36] and [49]). However, this approach requires the construction of a very thin partition of the interval $[0, h]$ and a large number of evaluations of the exponential matrices for an accurate computation of (9). Therefore, quadrature formulas are not recommend from a computational point of view.

In the case that $\mathbf{f}_\mathbf{x}(\mathbf{y}_n)$ is a non singular matrix, an elemental LL scheme for autonomous ODEs can be obtained [58, 2, 52, 56]. Integration by parts in (9) yields to

$$\mathbf{y}_{n+1} = \mathbf{y}_n + (\mathbf{f}_\mathbf{x}(\mathbf{y}_n))^{-1} \left(e^{h_n \mathbf{f}_\mathbf{x}(\mathbf{y}_n)} - \mathbf{I}\right) \mathbf{f}(\mathbf{y}_n), \tag{39}$$

which requires an algorithm for the numerical computation of inverse and exponential of matrices. Thus, this simple expression is computationally expensive and not reliable in case of ill conditioned matrices $\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)$.

An alternative scheme that does not involve the inverse of a matrix can be directly derived by rewriting (9) as

$$\phi\left(t_n, \mathbf{y}_n; h\right) = \int_0^h e^{\mathbf{f}_{\mathbf{x}}(t_n,\mathbf{y}_n)(h-u)}\mathbf{f}\left(t_n, \mathbf{y}_n\right) du + \int_0^h \int_0^u e^{\mathbf{f}_{\mathbf{x}}(t_n,\mathbf{y}_n)(h-u)}\mathbf{f}_t\left(t_n, \mathbf{y}_n\right) dudv,$$

and applying Theorem 1 in [66] for computing the expression above. In this way, the Local Linear discretization can be rewritten as [41]

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{v}(t_n,\mathbf{y}_n; h_n), \tag{40}$$

where the $d-$dimensional vector $\mathbf{v}$ is defined in the block matrix

$$\left[\begin{array}{cc} - & \mathbf{v}(\mathbf{y}_n; h_n) \\ 0 & 1 \end{array}\right] = e^{h_n\mathbf{D}_n} \qquad \text{with } \mathbf{D}_n = \left[\begin{array}{cc} \mathbf{f}_{\mathbf{x}}(\mathbf{y}_n) & \mathbf{f}(\mathbf{y}_n) \\ 0 & 0 \end{array}\right] \in \mathbb{R}^{(d+1)\times(d+1)}$$

for autonomous ODEs, or in the block matrix

$$\left[\begin{array}{ccc} - & - & \mathbf{v}(t_n, \mathbf{y}_n; h_n) \\ 0 & 1 & - \\ 0 & 0 & 1 \end{array}\right] = e^{h_n\mathbf{D}_n} \qquad \text{with } \mathbf{D}_n = \left[\begin{array}{ccc} \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n) & \mathbf{f}_t(t_n, \mathbf{y}_n) & \mathbf{f}(t_n, \mathbf{y}_n) \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{(d+2)\times(d+2)}$$

for non-autonomous ODEs. Thus, the numerical implementation of the expression (40) is reduced to the use of a conventional algorithm to compute the matrix exponential $e^{h_n\mathbf{D}_n}$, e.g., those based on rational Padé approximations, the Schur decomposition or Krylov subspace methods (see [63] for a recent review). The choice of one of them will mainly depend on the size and structure of the matrix $\mathbf{D}_n$. In many cases, it is sufficient to use the algorithms developed in [66, 24] which take advantage of the special structure of the matrix $\mathbf{D}_n$. For large systems of differential equations the Krylov subspace methods are specially recommended. In this case, the Krylov method is applied to the direct computation of the vector $e^{h_n\mathbf{D}_n}\mathbf{r} = \left[\begin{array}{cc} \mathbf{v}^\intercal(t_n,\mathbf{y}_n; h_n) & - \end{array}\right]^\intercal$, where $\mathbf{r}^\intercal = \left[\begin{array}{cc} \mathbf{0}_{1\times d} & 1 \end{array}\right]$ or $\mathbf{r}^\intercal = \left[\begin{array}{cc} \mathbf{0}_{1\times(d+1)} & 1 \end{array}\right]$ depending of the dimension of $\mathbf{D}_n$. Happy Matlab-users!; just call "expm" function or "expv" from the expokit toolbox [63] for simple implementations of (40). Recently, Lie-group based methods for the computation of matrix exponential have also been developed. These methods are useful in case that the conservation of invariants and/or symmetries is essential (see [17], and references therein).

In contrast with the mentioned LL schemes, other ones are based on approximations to $\phi\left(s, \mathbf{y}_s; h\right)$ that do not involve the explicit computation of matrix exponentials. Examples are the approximations based on the Schur decomposition [5], the truncated Taylor expansion [57], the rational Padé approximations [31] and the Krylov subspace methods [31].

To obtain an LL scheme based on the Schur decomposition or on the truncated Taylor expansion, expression (9) is rewritten as

$$\phi\left(t_n, \mathbf{y}_n; h\right) = \mathbf{R}_0(\mathbf{f}_{\mathbf{x}}\left(t_n, \mathbf{y}_n\right), h)\ \left(\mathbf{f}\left(t_n, \mathbf{y}_n\right) + h\mathbf{f}_t\left(t_n, \mathbf{y}_n\right)\right) - \mathbf{R}_1(\mathbf{f}_{\mathbf{x}}\left(t_n, \mathbf{y}_n\right), h)\ \mathbf{f}_t\left(t_n, \mathbf{y}_n\right),$$

where

$$\mathbf{R}_p(\mathbf{M},h)=\int_0^h e^{\mathbf{M}u}u^p du,$$

with $\mathbf{M}\equiv\mathbf{f}_{\mathbf{x}}\left(t_n,\mathbf{y}_n\right)$ and $p\in\mathbb{N}$.

If $\mathbf{M}$ is not singular, it can be shown by induction that

$$\mathbf{R}_p(\mathbf{M},h)=h^{p+1}p!\{(-\mathbf{M}h)^{-p-1}(\mathbf{I}-e^{\mathbf{M}h})-e^{\mathbf{M}h}\sum_{i=0}^{p-1}(-\mathbf{M}h)^{-i-1}/(p-i)!\}.$$

In general, if $\mathbf{M}$ is singular, then $\mathbf{R}_p(\mathbf{M},h)$ can be defined as the limit of $\mathbf{R}_p(\mathbf{M}_k,h)$ as $\mathbf{M}_k$ tends to $\mathbf{M}$ within the class of nonsingular matrices. This limit is then computed through the Schur decomposition $\mathbf{M}=\mathbf{Q}\mathbf{T}\mathbf{Q}^\intercal$. Define $\mathbf{M}_k=\mathbf{Q}\mathbf{T}_k\mathbf{Q}^\intercal$ whit $\mathbf{T}_k=\mathbf{T}+\mathbf{D}_k$, where $\mathbf{D}_k$ is an invertible diagonal matrix such that $\mathbf{D}_k$ tends to the zero matrix as k goes to infinite. Thus, the LL scheme is defined as

$$\mathbf{y}_{n+1}=\mathbf{y}_n+\lim_{k\to\infty}\{\mathbf{Q}\mathbf{R}_0(\mathbf{T}_k,h_n)\mathbf{Q}^\intercal\ (\mathbf{f}(t_n,\mathbf{y}_n)+h_n\mathbf{f}_t(t_n,\mathbf{y}_n))-\mathbf{Q}\mathbf{R}_1(\mathbf{T}_k,h_n)\mathbf{Q}^\intercal\ \mathbf{f}_t(t_n,\mathbf{y}_n)\},\quad(41)$$

where $\lim_{k\to\infty}\mathbf{R}_0(\mathbf{T}_k,h)$ and $\lim_{k\to\infty}\mathbf{R}_1(\mathbf{T}_k,h)$ are computed by means of the recursive Parlett algorithm [27]. In this way, $\mathbf{R}_p(\mathbf{T}_k,h)$ can be expressed in terms of $\mathbf{R}_p([\mathbf{T}_k]^{ii},h)$, where $[\mathbf{T}_k]^{ii}$ are the diagonal entries of $\mathbf{T}_k$. If $[\mathbf{T}]^{ii}\neq 0$ then $\lim_{k\to\infty}\mathbf{R}_p([\mathbf{T}_k]^{ii},h)=\mathbf{R}_p([\mathbf{T}]^{ii},h)$, whereas if $[\mathbf{T}]^{ii}=0$ then $\lim_{k\to\infty}\mathbf{R}_p([\mathbf{T}_k]^{ii},h)=h^{p+1}/(p+1)$.

For autonomous ODE, the LL schemes based on Taylor, Padé or Krylov approximation can be obtained by rewriting (9) as

$$\mathbf{y}_{n+1}=\mathbf{y}_n+h_n\mathbf{\Phi}(h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n))\ \mathbf{f}(\mathbf{y}_n),\quad(42)$$

where $\mathbf{\Phi}(z)\equiv(e^z-1)/z=\sum_{i=0}^{\infty}z^i/(i+1)!$ is equivalent to $\frac{1}{h}\mathbf{R}_0(z,h)$. That is, by directly applying these approximations to either $\mathbf{\Phi}(h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n))$ or $\mathbf{\Phi}(h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n))\ \mathbf{f}(\mathbf{y}_n)$. For non-autonomous ODEs, the procedure above is applied to the extended formally autonomous system obtained by adding the trivial differential equation $dt/dt=1$.

On the other hand, the Padé and Krylov approximations have also been used to compute directly the variation of constants formula (6) for autonomous equations [63]. For that purpose, that formula is rewritten as

$$\mathbf{y}\left(t\right)=e^{h_{n_t}\mathbf{f}_{\mathbf{x}}(\mathbf{y}_{n_t})}\mathbf{y}_{n_t}+h_{n_t}\mathbf{\Phi}(h_{n_t}\mathbf{f}_{\mathbf{x}}(\mathbf{y}_{n_t}))\left(\mathbf{f}(\mathbf{y}_{n_t})-\mathbf{f}_{\mathbf{x}}(\mathbf{y}_{n_t})\mathbf{y}_{n_t}\right),$$

which yields to the recursive integration

$$\mathbf{y}\left(\tau_{k+1}\right)=\mathbf{y}\left(\tau_k+\Delta_k\right)=\mathbf{y}\left(\tau_k\right)+\Delta_k\mathbf{\Phi}(\Delta_k\mathbf{f}_{\mathbf{x}}(\mathbf{y}_{n_t}))\left(\mathbf{f}_{\mathbf{x}}(\mathbf{y}_{n_t})\left(\mathbf{y}\left(\tau_k\right)-\mathbf{y}_{n_t}\right)+\mathbf{f}\left(t_{n_t},\mathbf{y}_{n_t}\right)\right)\quad(43)$$

of equation (4) on $[t_{n_t},t_{n_t+1}]$ for all increasing sequence of time instants $\tau_k\in[t_{n_t},t_{n_t+1}]$. Thus, LL schemes can be obtained by approximating $\mathbf{\Phi}$ as in the previous paragraph. Observe that (43) includes (42) as a particular case.

Alternately, in [49] an algorithm to compute $\mathbf{\Phi}$ based on a contour integral was proposed. Specifically, by taking a contour $\Gamma \subset \mathbb{C}$ that encloses the eigenvalues of $h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)$, the matrix function $\mathbf{\Phi}$ can be expressed as

$$\mathbf{\Phi}(h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)) = \int_{\Gamma} \mathbf{\Phi}(z)\,(z\mathbf{I} - h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n))^{-1}\,dz = \int_{\Gamma} \frac{e^z - 1}{z}\,(z\mathbf{I} - h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n))^{-1}\,dz,$$

which is numerically computed by the trapezoidal rule with equally spaced points. Simulation results have shown that the resulting scheme overcomes the poor accuracy of (39) when the matrix $h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)$ is nearly singular. However, this is achieved at the expense of computing inverses of a large number of matrices $z_j\mathbf{I} - h_n\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)$ corresponding to the quadrature nodes z_j. Further, the contour Γ is generally problem dependent and difficult to determine in advance.

Another way to compute the Local Linear discretization is by means of conventional numerical schemes for the integration of the linear ODE (4). In particular, implicit integrators should be used in order to keep the A-stability of the Local Linear discretization. Since many of these integrators result to be explicit for linear equations, the resulting LL schemes would be A-stable with moderate computational cost. Moreover, in this linear case, the stability function of various implicit Runge-Kutta schemes reduce to stable Padé approximations to matrix exponential (see Tables 3.1 and 3.2 in [30]), which made this approach equivalent to that of scheme (40). From a practical viewpoint, algorithms that compute matrix exponential usually incorporate additional processing routines to improve accuracy and numerical stability, e.g., squaring and scaling, balancing, etc. (see [28] and references therein). Equivalently, some of these additional pre-processing can be done by the mentioned RK as well, e.g., the recursive application of these RK schemes on a convenient partition of the interval $[0, h]$ is equivalent to squaring and scaling procedure.

Clearly, the error of an LL scheme depends on both the discretization error (25) and the error derived from the numerical implementation of the LL discretization. This is stated in the following theorem.

Theorem 27 *Let* $\mathbf{x}$ *be the solution of the ODE (1)-(2). For a time discretization* $(t)_h$*, let* $\widetilde{\mathbf{y}}$ *be a numerical solution of the piecewise linear ODE*

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{B}_{n_t}\mathbf{z}(t) + \mathbf{b}_{n_t}(t), \tag{44}$$

$$\mathbf{z}(t_{n_t}) = \widetilde{\mathbf{y}}_{n_t}, \tag{45}$$

defined for all $t \in [t_0, T]$*, where* $\mathbf{B}_{n_t} = \mathbf{f}_{\mathbf{x}}(t_{n_t}, \widetilde{\mathbf{y}}_{n_t})$ *is a* $d \times d$ *constant matrix and* $\mathbf{b}_{n_t}(t) = \mathbf{f}_t(t_{n_t}, \widetilde{\mathbf{y}}_{n_t})(t - t_{n_t}) + \mathbf{f}(t_{n_t}, \widetilde{\mathbf{y}}_{n_t}) - \mathbf{B}_{n_t}\widetilde{\mathbf{y}}_{n_t}$ *is a* d*-dimensional constant vector. Suppose that*

$$\sup_{t_n \le t \le t_{n+1}} \|\mathbf{z}(t) - \widetilde{\mathbf{y}}(t)\| \le L h_n^{r+1}$$

for some constants $L > 0$ *and* $r \in \mathbb{N}$*. Then there exists a constant* $M > 0$ *such that*

$$\sup_{t_0 \le t \le T} \|\mathbf{x}(t) - \widetilde{\mathbf{y}}(t)\| \le M h^{\min\{2,r\}} \tag{46}$$

for h small enough.

Proof. As in [45]. ■

Evidently, this theorem can be directly applied to the LL schemes based on conventional numerical methods for the integration of the linear ODE (4)-(5).

Corollary 28 *Let $\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \Lambda\left(t_n, \widetilde{\mathbf{y}}_n; t_{n+1} - t_n\right)$ be an order r conventional numerical integrator for the linear equation (44)-(45). Then, the corresponding Local Linear approximation $\widetilde{\mathbf{y}}$ holds that*

$$\sup_{t_0 \leq t \leq T} \|\mathbf{x}(t) - \widetilde{\mathbf{y}}(t)\| \leq M h^{\min\{2,r\}},$$

where M is a positive constant.

Proof. As in [45]. ■

However, Theorem 27 cannot be straightforwardly applied to the LL schemes derived from some expressions for the exact solution of linear equation (4), e.g., to those based on some numerical implementations of expressions (39)-(43). For these types of schemes we have the following useful result.

Theorem 29 *Denote by $\widetilde{\phi}$ a numerical implementation of ϕ, and by*

$$\widetilde{\mathbf{y}}(t) = \widetilde{\mathbf{y}}_{n_t} + \widetilde{\phi}\left(t_{n_t}, \widetilde{\mathbf{y}}_{n_t}; t - t_{n_t}\right) \tag{47}$$

the numerical implementation of the Local Linear approximation (11) for all $t \in [t_0, T]$. If

$$\left\| \phi\left(t_{n_t}, \widetilde{\mathbf{y}}_{n_t}; t - t_{n_t}\right) - \widetilde{\phi}\left(t_{n_t}, \widetilde{\mathbf{y}}_{n_t}; t - t_{n_t}\right) \right\| \leq C h^{r+1} \tag{48}$$

then,

$$\sup_{t_0 \leq t \leq T} \|\mathbf{x}(t) - \widetilde{\mathbf{y}}(t)\| \leq M h^{\min\{2,r\}},$$

where C and M are positive constants.

Proof. As in [45]. ■

Let us see, for instance, an illustrative example in which the Padé approximation is combined with the "scaling and squaring" strategy to compute the exponential matrix in expression (40) for the Local Linear discretization. To do so note that, according to that expression, the function ϕ can be written as

$$\phi\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) = \mathbf{L} e^{\widetilde{\mathbf{D}}_n h_n} \mathbf{r}, \tag{49}$$

where

$$\widetilde{\mathbf{D}}_n = \begin{bmatrix} \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n) & \mathbf{f}_t(t_n, \widetilde{\mathbf{y}}_n) & \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n) \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{(d+2)\times(d+2)},$$

$\mathbf{L} = \left[\begin{array}{cc} \mathbf{I}_d & \mathbf{0}_{d\times 2} \end{array} \right]$ and $\mathbf{r}^\intercal = \left[\begin{array}{cc} \mathbf{0}_{1\times(d+1)} & 1 \end{array} \right]$ for non-autonomous ODEs; and

$$\widetilde{\mathbf{D}}_n = \left[\begin{array}{cc} \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n) & \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n) \\ 0 & 0 \end{array} \right] \in \mathbb{R}^{(d+1)\times(d+1)},$$

$\mathbf{L} = \left[\begin{array}{cc} \mathbf{I}_d & \mathbf{0}_{d\times 1} \end{array} \right]$ and $\mathbf{r}^\intercal = \left[\begin{array}{cc} \mathbf{0}_{1\times d} & 1 \end{array} \right]$ for an autonomous one.

Theorem 30 *Let* $\widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) = \mathbf{L}\left(\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{D}}_n h_n)\right)^{2^{k_n}} \mathbf{r}$ *, where* $\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{D}}_n h_n)$ *is the* (p,q)*-Padé approximation of* $e^{2^{-k_n}\widetilde{\mathbf{D}}_n h_n}$*,* k_n *is the smallest integer number such that* $\left\|2^{-k_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$*, and matrices* $\widetilde{\mathbf{D}}_n$*,* $\mathbf{L}$*,* $\mathbf{r}$ *are defined as above. Then, under assumptions of Theorem 9, there exist positive constants* C *and* M *such that*

$$\left\|\phi\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) - \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right)\right\| \leq C h^{p+q+1},$$

and the global error of the LL scheme

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) \tag{50}$$

is given by

$$\|\mathbf{x}(t_n) - \widetilde{\mathbf{y}}_n\| \leq M h^{\min\{2, p+q\}}$$

for all $t_n \in (t)_h$ *.*

Proof. As in [45]. ■

Otherwise, when the Krylov method [31] is used, the function ϕ can be approximated by

$$\widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; h_n) = \mathbf{L}\ \mathbf{k}^{p,q}_{m_n,k_n}(h_n, \widetilde{\mathbf{D}}_n, \mathbf{r}),$$

where $\mathbf{k}^{p,q}_{m_n,k_n}(h_n, \widetilde{\mathbf{D}}_n, \mathbf{r})$ denotes the Krylov-Padé approximation of $e^{h_n\widetilde{\mathbf{D}}_n}\mathbf{r}$. More precisely,

$$\mathbf{k}^{p,q}_{m,k}(\delta, \mathbf{A}, \mathbf{v}) = \beta \mathbf{V}_m \mathbf{F}^k_{p,q}(\delta \mathbf{H}_m)\mathbf{e}_1,$$

where $\beta = \|\mathbf{v}\|$, $\mathbf{e}_1$ is the $m-$dimensional unitary vector, and the matrices $\mathbf{V}_m = [\mathbf{v}_1, .., \mathbf{v}_m]$ and $\mathbf{H}_m$ are the orthonormal basis of the Krylov space $\mathcal{K}_m = span(\mathbf{v}, \mathbf{A}\mathbf{v}, ..., \mathbf{A}^{m-1}\mathbf{v})$ and the upper Hessenberg matrix, respectively, resulting both from the well-known Arnoldi algorithm (see for instance [27]). In addition, $\mathbf{F}^k_{p,q}(\delta\mathbf{H}_m) = (\mathbf{P}_{p,q}(2^{-k}\delta\mathbf{H}_m))^{2^k}$ denotes the (p,q)-Padé approximation with "scaling and squaring" procedure for the computation of $e^{\delta\mathbf{H}_m}$, and k is the smallest integer number such that $\left\|2^{-k}\delta\mathbf{H}_m\right\| \leq \frac{1}{2}$.

The next theorem states the convergence rate of the LL scheme resulting from expression (40) and the Krylov-Padé approximation for the exponential matrix.

Theorem 31 *Let* $\widetilde{\phi} = \mathbf{L}\ \mathbf{k}^{p,q}_{m_n,k_n}(h_n, \widetilde{\mathbf{D}}_n, \mathbf{r})$*, where* $\mathbf{k}^{p,q}_{m_n,k_n}(h_n, \widetilde{\mathbf{D}}_n, \mathbf{r})$ *denotes the* $(m_n, p, q)-$*Krylov-Padé approximation of* $e^{h_n\widetilde{\mathbf{D}}_n}\mathbf{r}$*,* k_n *is the smallest integer number such that* $\left\|2^{-k_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$*,*

and $\widetilde{\mathbf{D}}_n$, $\mathbf{L}$, $\mathbf{r}$ *are matrices defined as in (49). Suppose that assumptions of Theorem 9 hold. If* $m_n \geq 2h_n \left\|\widetilde{\mathbf{D}}_n\right\|_2$ *for all* n, *then there exist positive constants* C *and* M *such that*

$$\left\|\phi\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) - \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right)\right\|_2 \leq C h^{\min\{m, p+q+1\}},$$

and the global error of the LL scheme

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right)$$

is given by

$$\|\mathbf{x}(t_n) - \widetilde{\mathbf{y}}_n\|_2 \leq M h^{\min\{2, m-1, p+q\}}$$

for all $t_n \in (t)_h$, *where* $m = \min\{m_n\}$.

Proof. Similar to that given in [46] for LL schemes for random differential equations. ■

In the above theorem the restriction to the norm $\|\cdot\|_2$ results from the condition $m_n \geq 2h_n \left\|\widetilde{\mathbf{D}}_n\right\|_2$, which is required to establish the convergence of the Krylov approximation to the exponential matrices. Nevertheless, depending on the class of the matrix $\widetilde{\mathbf{D}}_n$ and/or the location and shape of its spectrum (see for instance [31] and references in [63]), that condition can be replaced by others, so the mentioned restriction to the norm can be removed.

According to the theorems of this section, a numerical implementation of ϕ with error $O(h^3)$ is sufficient to keep the order of convergence of the Local Linear discretization. However, the high performance of the current computers has allowed professional mathematical softwares (i.e., MATLAB, etc.) to provide subroutines for the computation of complex matrix operations up to the precision of the floating-point arithmetic. This includes the computation of inverse matrix, exponential matrix, Schur decomposition, etc. Therefore, most of the LL schemes complete the "exact computation" (up to the precision of the floating-point arithmetic) of the function ϕ**.** Clearly, LL schemes of the first class save computer time due to considerably less arithmetic operations are required. On the other hand, the second one provides the "exact" solution of linear ODEs, which might allow these schemes to retain much better the dynamic of the underlying equations with relative larger steps-size. However, this important and complex subject (that has been not considered so far) remains as a open problem that needs further study.

It is also obvious that the dynamical properties of the Local Linear discretization stated in Section 6 hold for the LL schemes mentioned in this section if the approximation to the map ϕ is $o(h)$ and smooth enough (i.e., of class C^2). However, in general, it is not clear when the A-stability of the Local Linear discretization (considered in Section 5) is inherited by the LL schemes mentioned above. Remarkable exceptions are certain schemes of the form (50), whose A-stability is derived from the A-stability of the Padé approximation for the exponential matrix. This, as well as the L-stability of these schemes, is examined in the following theorem.

Theorem 32 *The LL scheme (50) is A-stable if the* (p, q)*-Padé approximation is taken with* $p \leq q \leq p+2$. *Moreover, if* $q = p+1$ *or* $q = p+2$, *then the LL scheme (50) is also L-stable.*

Proof. As in [23] ■

Nevertheless, the trade-off between the computational cost and the preservation of the qualitative and/or geometric features of the underlying dynamical systems by the LL schemes has been poorly evaluated up to now. Therefore, numerical implementations of ϕ with error lower than $O(h^2)$ need further study.

7.2 LLT schemes

When implementing the LLT discretization, that is when a LLT scheme is constructed, the required evaluations of ϕ_γ can be efficiently computed by means of a variety of algorithms.

For instance, by using Theorem 1 in [66], the order γ LLT discretization (17) can be rewritten as

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{v}(t_n, \mathbf{y}_n; h_n), \tag{51}$$

where the $d-$dimensional vector $\mathbf{v}(t_n, \mathbf{y}_n; h_n)$ is defined in the block matrix

$$\left[\begin{array}{cc} - & \mathbf{v}(t_n, \mathbf{y}_n; h_n) \\ \mathbf{0}_{\gamma\times(d+\gamma-1)} & - \end{array} \right] = e^{h_n \mathbf{C}_n}$$

with

$$\mathbf{C}_n = \begin{pmatrix} \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n) & \mathbf{c}_{\gamma-1}(t_n, \mathbf{y}_n) & \mathbf{c}_{\gamma-2}(t_n, \mathbf{y}_n) & \cdots & \mathbf{c}_2(t_n, \mathbf{y}_n) & \mathbf{f}_t(t_n, \mathbf{y}_n) & \mathbf{f}(t_n, \mathbf{y}_n) \\ \mathbf{0}_{1\times d} & 0 & 1 & ... & 0 & 0 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \ddots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 & 0 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 1 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 0 & 1 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{(d+\gamma)\times(d+\gamma)}.$$

Thus, similar to the numerical implementation of expression (40) in the previous subsection, the numerical implementation of ϕ_γ is reduced to the use of a conventional algorithm to compute matrix exponentials. See the previous section for details.

Alternatively, other LLT schemes can be derived. Indeed, by means of the functions ϑ_j recursively defined as

$$\vartheta_j(z) = \begin{cases} (\vartheta_{j-1}(z) - 1/(j-1)!)/z & \text{for } j = 1, 2.. \\ e^z & \text{for } j = 0 \end{cases}$$

for $z \in \mathbb{C}$, the function ϕ_γ can be rewritten as

$$\phi_\gamma(\tau, \xi; \delta) = \sum_{j=0}^{\gamma-1} \delta^{j+1} \vartheta_{j+1}(\delta \mathbf{f}_{\mathbf{x}}(\tau, \xi)) \mathbf{c}_j(\tau, \xi),$$

where

$$\vartheta_j(z) = \begin{cases} (\vartheta_{j-1}(z) - 1/(j-1)!)/z & \text{for } j = 1, 2.. \\ e^z & \text{for } j = 0 \end{cases}$$

and

$$\mathbf{c}_j(\tau,\xi) = \begin{cases} \frac{d^j}{dt^j}\mathbf{f}(\tau,\xi) - \frac{\partial}{\partial \mathbf{x}}\mathbf{f}(\tau,\xi)\frac{d^{j-1}}{dt^{j-1}}\mathbf{f}(\tau,\xi) & \text{for } j \geq 2 \\ \mathbf{f}_t(\tau,\xi) & \text{for } j = 1 \\ \mathbf{f}(\tau,\xi) & \text{for } j = 0 \end{cases}.$$

In this way, similar to the LL schemes derived from expression (42) in the previous subsection, LLT schemes based on Taylor, Padé or Krylov approximation could be obtained just by directly applying these approximations to either $\vartheta_j(\delta\mathbf{f}_{\mathbf{x}}(\tau,\xi))$ or $\vartheta_j(\delta\mathbf{f}_{\mathbf{x}}(\tau,\xi))\,\mathbf{c}_j(\tau,\xi)$. See also [3] for a recursive evaluation of ϑ_j based on an extension of the matrix exponential scaling and squaring method.

In general, a LLT scheme will preserve the order γ of the LLT discretization if the needed evaluations of ϕ_γ are carried out with an error of order γ. This is formalized in the following theorem.

Theorem 33 *Denote by $\widetilde{\phi}_\gamma$ a numerical implementation of ϕ_γ, and by*

$$\widetilde{\mathbf{y}}(t) = \widetilde{\mathbf{y}}_{n_t} + \widetilde{\phi}_\gamma(t_{n_t}, \widetilde{\mathbf{y}}_{n_t}; t - t_{n_t})$$

a numerical implementation of the LLT approximation (17) for all $t \in [t_0, T]$. If $\widetilde{\phi}_\gamma$ is a locally Lipschitz function with respect to its second argument and condition

$$\left\| \phi_\gamma(t_{n_t}, \xi; t - t_{n_t}) - \widetilde{\phi}_\gamma(t_{n_t}, \xi; t - t_{n_t}) \right\| \leq C h^{r+1} \tag{52}$$

for all $\xi \in \mathbb{R}^d$, then

$$\sup_{t_0 \leq t \leq T} \|\mathbf{x}(t) - \widetilde{\mathbf{y}}(t)\| \leq M h^{\min\{\gamma, r\}},$$

where C and M are positive constants.

Proof. (sketch) Since

$$\begin{aligned} \left\| \mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - \widetilde{\phi}_\gamma(t_n, \mathbf{x}(t_n); h_n) \right\| \quad \leq \quad & \|\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - \phi_\gamma(t_n, \mathbf{x}(t_n); h_n)\| \\ & + \left\| \phi_\gamma(t_{n_t}, \mathbf{x}(t_n); t - t_{n_t}) - \widetilde{\phi}_\gamma(t_{n_t}, \mathbf{x}(t_n); t - t_{n_t}) \right\|, \end{aligned}$$

condition (52) and Theorem 10 imply that

$$\left\| \mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - \widetilde{\phi}_\gamma(t_n, \mathbf{x}(t_n); h_n) \right\| \leq M h^{\min\{\gamma, r\}},$$

where M is a positive constant. The proof is complete by using Theorem 3.6 in [29]. ■

As an example let us consider the Padé approximation combined with the "scaling and squaring" strategy to compute the exponential matrix in expression (51) for the LLT discretization. To do so note that, according to that expression, the function ϕ can be written as

$$\phi(t_n, \widetilde{\mathbf{y}}_n; h_n) = \mathbf{L} e^{\widetilde{\mathbf{C}}_n h_n} \mathbf{r},$$

with matrices

$$\widetilde{\mathbf{C}}_n = \begin{pmatrix} \mathbf{f}_{\mathbf{x}}(t_n,\widetilde{\mathbf{y}}_n) & \mathbf{c}_{\gamma-1}(t_n,\widetilde{\mathbf{y}}_n) & \mathbf{c}_{\gamma-2}(t_n,\widetilde{\mathbf{y}}_n) & \cdots & \mathbf{c}_2(t_n,\widetilde{\mathbf{y}}_n) & \mathbf{f}_t\,(t_n,\widetilde{\mathbf{y}}_n) & \mathbf{f}(t_n,\widetilde{\mathbf{y}}_n) \\ \mathbf{0}_{1\times d} & 0 & 1 & ... & 0 & 0 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \ddots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 & 0 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 1 & 0 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 0 & 1 \\ \mathbf{0}_{1\times d} & 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{(d+\gamma)\times(d+\gamma)},$$

$\mathbf{L} = \left[\begin{array}{cc} \mathbf{I}_d & \mathbf{0}_{d\times\gamma} \end{array}\right]$ and $\mathbf{r}^{\intercal} = \left[\begin{array}{cc} \mathbf{0}_{1\times(d+\gamma-1)} & 1 \end{array}\right]$.

Theorem 34 *Let* $\widetilde{\phi}_\gamma\,(t_n,\widetilde{\mathbf{y}}_n;h_n) = \mathbf{L}\,(\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{C}}_n h_n))^{2^{k_n}}\ \mathbf{r}$, *where* $\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{C}}_n h_n)$ *is the* (p,q)*-Padé approximation of* $e^{2^{-k_n}\widetilde{\mathbf{C}}_n h_n}$, k_n *is the smallest integer number such that* $\left\|2^{-k_n}\widetilde{\mathbf{C}}_n h_n\right\| \leq \frac{1}{2}$, *and matrices* $\widetilde{\mathbf{C}}_n$, $\mathbf{L}$, $\mathbf{r}$ *defined as above. Then, under the assumptions of Theorem 10, the global error of the LLT scheme*

$$\widetilde{\mathbf{y}}_{t_{n+1}} = \widetilde{\mathbf{y}}_{t_n} + \widetilde{\phi}_\gamma\,(t_n,\widetilde{\mathbf{y}}_n;h_n) \tag{53}$$

is given by

$$\|\mathbf{x}(t_n) - \widetilde{\mathbf{y}}(t_n)\| \leq M h^{\min\{\gamma,p+q\}}$$

for all $t_n \in (t)_h$, *where* M *is a positive constant.*

Proof. Similar to the proof of Theorem 30. ■

The next theorem deals with the stability of some LLT schemes for linear equations.

Theorem 35 *LLT schemes (53) are A-stable if the* (p,q)*-Padé approximation is taken with* $p \leq q \leq p+2$. *Moreover, if* $q = p+1$ *or* $q = p+2$, *then such LLT schemes (53) are also L-stable.*

Proof. Consider the scalar test equation (28). By similar arguments to those in the proof of Theorem 13, the LLT scheme (53) applied to this autonomous equation reduces to the LL scheme (50). This and Theorem 13 imply the A-stability and the L-stability of the LLT scheme (53). ■

Finally, note that the dynamical properties of an order γ LLT discretization, as stated in Section 6, also hold for its numerical implementations if the approximation to the map $\phi+\rho$ is $o(h^{\gamma-1})$ and smooth enough (i.e., of class C^γ). In particular, these conditions are satisfied by the implementation introduced above, namely, those given by (53).

7.3 LLRK schemes

When implementing the LLRK discretization

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \phi(t_n,\mathbf{y}_n;h_n) + \rho(t_n,\mathbf{y}_n;h_n), \tag{54}$$

that is, when a LLRK scheme is constructed, the required evaluations of the expression $\mathbf{y}_n + \phi(t_n,\mathbf{y}_n;\cdot)$ at $t_{n+1}-t_n$ and $c_i\,(t_{n+1}-t_n)$ may be computed by different algorithms. In subsection 7.1 a number of them were presented, which yield the following two basic kinds of LLRK schemes:

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_{n+1} + \widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; h_n) + \widetilde{\rho}(t_n, \widetilde{\mathbf{y}}_n; h_n),$$

and

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{z}}(t_n + h_n; t_n, \widetilde{\mathbf{y}}_n) + \widetilde{\rho}(t_n, \widetilde{\mathbf{y}}_n; h_n),$$

where $\widetilde{\phi}$ is a numerical implementation of ϕ, $\widetilde{\mathbf{z}}$ is a numerical solution of the linear ODE

$$\begin{aligned} \frac{d\mathbf{z}(t)}{dt} &= \mathbf{B}_n \mathbf{z}(t) + \mathbf{b}_n(t), \quad t \in [t_n, t_{n+1}], & (55) \\ \mathbf{z}(t_n) &= \widetilde{\mathbf{y}}_n, & (56) \end{aligned}$$

and $\widetilde{\rho}$ is the map of the Runge-Kutta scheme applied to the ODE

$$\begin{aligned} \frac{d\mathbf{v}(t)}{dt} &= \widetilde{\mathbf{q}}(t_n, \mathbf{z}(t_n); t, \mathbf{v}(t)), \quad t \in [t_n, t_{n+1}], & (57) \\ \mathbf{v}(t_n) &= \mathbf{0}, & (58) \end{aligned}$$

with vector field

$$\widetilde{\mathbf{q}}(t_n, \widetilde{\mathbf{y}}_n; s, \xi) = \mathbf{f}(s, \widetilde{\mathbf{y}}_n + \widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; s - t_n) + \xi) - \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n)\widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; s - t_n) - \mathbf{f}_t(t_n, \widetilde{\mathbf{y}}_n)(s - t_n) - \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n),$$

for the first kind of LLRK scheme, or

$$\widetilde{\mathbf{q}}(t_n, \widetilde{\mathbf{y}}_n; s, \xi) = \mathbf{f}(s, \widetilde{\mathbf{z}}(s; t_n, \widetilde{\mathbf{y}}_n) + \xi) - \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n)(\widetilde{\mathbf{z}}(s; t_n, \widetilde{\mathbf{y}}_n) - \widetilde{\mathbf{y}}_n) - \mathbf{f}_t(t_n, \widetilde{\mathbf{y}}_n)(s - t_n) - \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n)$$

for the second one. In equation (55), $\mathbf{B}_n = \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n)$ is a $d \times d$ constant matrix and $\mathbf{b}_n(t) = \mathbf{f}_t(t_n, \widetilde{\mathbf{y}}_n)(t - t_n) + \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n) - \mathbf{B}_n \widetilde{\mathbf{y}}_n$ is a d-dimensional linear vector function.

Clearly, a LLRK scheme will preserve the order γ of the underlaying LLRK discretization only if $\widetilde{\phi}$ is a suitable approximation to ϕ. This requirement is considered in what follows.

Theorem 36 *Let* $\mathbf{x}$ *be the solution of the ODE (1)-(2) with vector field* $\mathbf{f}$ *satisfing the condition (27). With* $t_n, t_{n+1} \in (t)_h$*, let* $\widetilde{\mathbf{z}}_{n+1} = \widetilde{\mathbf{z}}_n + h_n \mathbf{\Lambda}_1(t_n, \widetilde{\mathbf{z}}_n; h_n)$ *and* $\widetilde{\mathbf{v}}_{n+1} = \widetilde{\mathbf{v}}_n + h_n \mathbf{\Lambda}_2^{\widetilde{\mathbf{z}}_n}(t_n, \widetilde{\mathbf{v}}_n; h_n)$ *be one-step explicit integrators of the ODEs (55)-(56) and (57)-(58), respectively. Suppose that these integrators have order of convergence* r *and* p*, respectively. Further, assume that* $\mathbf{\Lambda}_1$ *and* $\mathbf{\Lambda}_2^{\widetilde{\mathbf{z}}_n}$ *satisfy the local Lipschitz condition in their second argument. Then, for* h *small enough, the numerical scheme*

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + h_n \mathbf{\Lambda}_1(t_n, \widetilde{\mathbf{y}}_n; h_n) + h_n \mathbf{\Lambda}_2^{\widetilde{\mathbf{y}}_n}(t_n, \mathbf{0}; h_n)$$

satisfies that

$$\|\mathbf{x}(t_{n+1}) - \widetilde{\mathbf{y}}_{n+1}\| \leq C h^{\min\{r,p\}}$$

for $t_{n+1} \in (t)_h$*, where* C *is a positive constant.*

Proof. As in [23]. ■

As an example, consider the computation of the function ϕ by the same algorithm of the LL scheme (50), that is, by the Padé approximation combined with the "scaling and squaring" strategy to compute exponential matrices.

Proposition 37 *Let* $\widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) = \mathbf{L}\ \left(\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{D}}_n h_n)\right)^{2^{k_n}}\ \mathbf{r}$, *where* $\mathbf{P}_{p,q}(2^{-k_n}\widetilde{\mathbf{D}}_n h_n)$ *is the* (p,q)*-Padé approximation of* $e^{2^{-k_n}\widetilde{\mathbf{D}}_n h_n}$, k_n *is the smallest integer number such that* $\left\|2^{-k_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$, *and* $\widetilde{\mathbf{D}}_n$, $\mathbf{L}$, $\mathbf{r}$ *are matrices defined as in (49). Further, let* $\widetilde{\rho}$ *be the numerical solution of the ODE (57)-(58) given by an order* γ *explicit Runge-Kutta scheme. Then, under the assumptions of Theorem 12, the global error of the LLRK scheme*

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) + \widetilde{\rho}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) \tag{59}$$

in the integration of the ODE (1)-(2) is given by

$$\|\mathbf{x}(t_n) - \widetilde{\mathbf{y}}_n\| \leq M h^{\min\{\gamma, p+q\}}$$

for all $t_n \in (t)_h$, *where* M *is a positive constant.*

Proof. As in [23]. ■

The next theorem deals with the stability of some LLRK schemes for linear equations.

Theorem 38 *LLRK schemes of the form (59) are A-stable if the* (p,q)*-Pad é approximation is taken with* $p \leq q \leq p+2$. *Moreover, if* $q = p+1$ *or* $q = p+2$, *then such LLRK schemes are also L-stable.*

Proof. As in [23]. ■

From an implementation viewpoint, further simplifications for LLRK schemes can be achieved in order to reduce the computational budget of the algorithms. For instance, if all the Runge-Kutta coefficients c_i have a minimum common multiple κ then, LLRK scheme (59) can be implemented in terms of a few powers of the same matrix exponential $e^{\kappa h_n \widetilde{\mathbf{D}}_n}$. To illustrate this, let us consider the so-called *classical four order Runge-Kutta scheme* (pp. 181 in [9]) with coefficients $c = \left[\begin{array}{cccc} 0 & \frac{1}{2} & \frac{1}{2} & 1 \end{array}\right]$. This yields the following efficient LLRK4 scheme

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) + \widetilde{\rho}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right), \tag{60}$$

where

$$\widetilde{\rho}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) = \frac{h_n}{6}(2\widetilde{\mathbf{k}}_2 + 2\widetilde{\mathbf{k}}_3 + \widetilde{\mathbf{k}}_4),$$

with

$$\begin{aligned} \widetilde{\mathbf{k}}_i \ &= \ \mathbf{f}\left(t_n + c_i h_n, \widetilde{\mathbf{y}}_n + \widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; t_n + c_i h_n) + c_i h_n \widetilde{\mathbf{k}}_{i-1}\right) - \mathbf{f}\left(t_n, \widetilde{\mathbf{y}}_n\right) \\ &\quad -\mathbf{f}_{\mathbf{x}}\left(t_n, \widetilde{\mathbf{y}}_n\right) \widetilde{\phi}\left(t_n, \widetilde{\mathbf{y}}_n; t_n + c_i h_n\right) \ - \mathbf{f}_t\left(t_n, \widetilde{\mathbf{y}}_n\right) c_i h_n \end{aligned}$$

$\widetilde{\mathbf{k}}_1 \equiv \mathbf{0}$, $\widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; t_n + \frac{h_n}{2}) = \mathbf{LAr}$, $\widetilde{\phi}(t_n, \widetilde{\mathbf{y}}_n; t_n + h_n) = \mathbf{LA}^2\mathbf{r}$, $\mathbf{A} = (\mathbf{P}_{q-1,q}(2^{-k_n}\widetilde{\mathbf{D}}_n h_n))^{2^{k_n}}$, and

$$\widetilde{\mathbf{D}}_n = \begin{bmatrix} \mathbf{f}_{\mathbf{x}}(t_n, \widetilde{\mathbf{y}}_n) & \mathbf{f}_t(t_n, \widetilde{\mathbf{y}}_n) & \mathbf{f}(t_n, \widetilde{\mathbf{y}}_n) \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{(d+2)\times(d+2)}.$$

Finally, observe that the dynamical properties of an order γ LLRK discretization, as stated in Section 6, are inherited for its numerical implementations if the approximation to the map $\phi+\rho$ is $o(h^{\gamma-1})$ and smooth enough (i.e., of class C^γ). In particular, these conditions are satisfied by the implementations introduced above, namely, those given by (59).

8 Numerical simulations

In [44, 20, 21, 22] a number of numerical simulations were carried out in order to illustrate the performance of the LL schemes and compare them to other numerical integrators. With special emphasis, the simulations illustrate the dynamical properties of the LL scheme, as well as, their capability for integrating stiff ODEs. The simulations show that the LL schemes (50), (53) and (60) exhibit a much better behavior near stationary hyperbolic points and periodic orbits of the continuous systems than other conventional explicit integrators. In the integration of stiff ODEs, these LL schemes show a stability similar to that of implicit schemes, but with low computational cost (comparable to conventional explicit schemes).

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