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Local Linearization–Runge–Kutta methods: A class of A-stable explicit integrators for dynamical systems

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ABSTRACT

A new approach for the construction of high order A-stable explicit integrators for ordinary differential equations (ODEs) is theoretically studied. Basically, the integrators are obtained by splitting, at each time step, the solution of the original equation in two parts: the solution of a linear ordinary differential equation plus the solution of an auxiliary ODE. The first one is solved by a Local Linearization scheme in such a way that A-stability is ensured, while the second one can be approximated by any extant scheme, preferably a high order explicit Runge–Kutta scheme. Results on the convergence and dynamical properties of this new class of schemes are given, as well as some hints for their efficient numerical implementation. An specific scheme of this new class is derived in detail, and its performance is compared with some Matlab codes in the integration of a variety of ODEs representing different types of dynamics.

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1. Introduction

It is well known (see, e.g., [1,2]) that conventional numerical schemes such as Runge–Kutta, Adams–Bashforth, predictor–corrector and others produce misleading dynamics in the integration of Ordinary Differential Equations (ODEs). Typical difficulties 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 the dynamics of the numerical schemes (viewed as discrete dynamical systems) is far richer than that of its continuous counterparts. Contrary to the common belief, drawbacks of this type may not be solved by reducing the step-size of the numerical method. Therefore, the development of numerical integrators that preserve, as much as possible, the dynamical properties of the underlaying dynamical system for all step-sizes or relative big ones is highly desirable. In this direction, some modest advances have been achieved by a number of relative recent integrators of the class of Exponential Methods, which are characterized by the explicit use of exponentials to obtain an approximate solution. In fact, their development has been encouraged because of their capability of preserving a number of geometric and dynamical features of the ODEs at the expense of notably less computational effort than implicit integrators. This has become feasible due to advances in the computation of matrix exponentials (see, e.g., [3–7]) and multiple integrals involving matrix exponentials (see, e.g., [8,9]). Some instances of this type of integrators are the methods known as exponential fitting [10–14], exponential integrating factor [15], exponential integrators [16,17], exponential time

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differencing [18,19], truncated Magnus expansion [20,21], truncated Fer expansion [22] (also named exponential of iterated commutators in [23]), exponential Runge–Kutta [24,25], some schemes based on versions of the variation of constants formula (e.g., [26–30]), local linearization (see, e.g., [31–35]), and high order local linearization methods [36–39].

The present paper deals with the class of high order local linearization integrators called Local Linearization–Runge–Kutta (LLRK) methods, which was recently introduced in [36] as a flexible approach for increasing the order of convergence of the Local Linearization (LL) method while retaining its desired dynamical properties. Essentially, the 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 an LL scheme in such a way that the A-stability is ensured, while the second one is integrated by any high order explicit Runge–Kutta (RK) scheme. Like Implicit–Explicit Runge–Kutta (IMEX RK) and conventional splitting methods (see e.g. [40,41]), the splitting involved in the LLRK approximations 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 ODEs 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, which is solved 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 methods can also be thought of as a flexible approach to construct new A-stable explicit schemes based on standard explicit RK integrators. In comparison with the well known Rosenbrock [42,43] and Exponential Integrators [16,25] the A-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 fulfill both A-stability and order conditions. In contrast, A-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 A-stable LL scheme. Another major difference is that the RK coefficients involved in the LLRK methods are not constrained by any stability condition and they just need satisfy the usual order conditions for RK schemes. Thus, the coefficients in the LLRK methods can be just those of any standard explicit RK scheme. This makes the LLRK approach very flexible and allows for simple numerical implementations on the basis of available subroutines for LL and RK methods.

In [36,44] a number of numerical simulations were carried out in order to illustrate the performance of the LLRK schemes and to compare them with other numerical integrators. With special emphasis, the dynamical properties of the LLRK schemes were considered, as well as their capability for integrating some kinds of stiff ODEs. For these equations, LLRK schemes showed stability similar to that of implicit schemes with the same order of convergence, while demanding much lower computational cost. The simulations also showed that the LLRK schemes exhibit a much better behavior near stationary hyperbolic points and periodic orbits of the continuous systems than other conventional explicit integrators. However, no theoretical support to such findings has been published so far.

The main aim of the present paper is to provide a theoretical study of LLRK integrators. Specifically, the following subjects are considered: rate of convergence, linear stability, preservation of the equilibrium points, and reproduction of the phase portrait of the underlying dynamical system near hyperbolic stationary points and periodic orbits. Furthermore, unlike the majority of the previous papers on exponential integrators, this study is carried out not only for the discretizations but also for the numerical schemes that implement them in practice.

The paper is organized as follows. In Section 2, the formulations of the LL and LLRK methods are briefly reviewed. Sections 3 and 4 deal with the convergence, linear stability and dynamic properties of LLRK discretizations. Section 5 focuses on the preservation of these properties by LLRK numerical schemes. In the last section, a new simulation study is presented in order to compare the performance of an specific order 4 LLRK scheme and some Matlab codes in a variety of ODEs representing different types of dynamics.

2. High order Local Linear discretizations

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

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(t, \mathbf{x}(t)), \quad t \in [t_0, T] \tag{1}$$

$$\mathbf{x}(t_0) = \mathbf{x}_0, \tag{2}$$

where $\mathbf{x}_0 \in \mathcal{D}$ is a given initial value, 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 $\mathcal{D}$.

In what follows, for $h > 0$, $(t)_h$ will denote a partition $t_0 < t_1 < \cdots < t_N = T$ of the time interval $[t_0, T]$ such that

$$\sup_n(h_n) \leq h < 1,$$

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

2.1. Local linear discretization

Suppose that, for each $t_n \in (t)_h$, $\mathbf{y}_n \in \mathcal{D}$ 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 of $\mathbf{f}$ at each time step, the solution of (1)–(2) can be locally approximated on each interval $[t_n, t_{n+1})$ by the solution of the linear ODE

$$\frac{d\mathbf{y}(t)}{dt} = \mathbf{A}_n\mathbf{y}(t) + \mathbf{a}_n(t), \quad t \in [t_n, t_{n+1}) \tag{3}$$

$$\mathbf{y}(t_n) = \mathbf{y}_n, \tag{4}$$

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

$$\mathbf{y}(t) = e^{\mathbf{A}_n(t-t_n)}\left(\mathbf{y}_n + \int_0^{t-t_n} e^{-\mathbf{A}_n u}\mathbf{a}_n(t_n + u)\, du\right). \tag{5}$$

Furthermore, by using the identity

$$\int_0^{\Delta} e^{-\mathbf{A}_n u} du \mathbf{A}_n = -(e^{-\mathbf{A}_n\Delta} - \mathbf{I}), \quad \Delta \geq 0 \tag{6}$$

and simple rules from the integral calculus, the expression (5) can be rewritten as

$$\mathbf{y}(t) = \mathbf{y}_n + \boldsymbol{\phi}(t_n, \mathbf{y}_n; t - t_n), \tag{7}$$

where

$$\begin{aligned}\boldsymbol{\phi}(t_n, \mathbf{y}_n; t - t_n) &= \int_0^{t-t_n} e^{\mathbf{A}_n(t-t_n-u)}(\mathbf{A}_n\mathbf{y}_n + \mathbf{a}_n(t_n + u))\, du \\ &= \int_0^{t-t_n} e^{\mathbf{f}_{\mathbf{x}}(t_n,\mathbf{y}_n)(t-t_n-u)}(\mathbf{f}(t_n, \mathbf{y}_n) + \mathbf{f}_t(t_n, \mathbf{y}_n)\, u) du.\end{aligned} \tag{8}$$

In this way, by setting $\mathbf{y}_0 = \mathbf{x}(t_0)$ and iteratively evaluating the expression (7) at t_{n+1} (for $n = 0, 1, \ldots, N-1$) a sequence of points $\mathbf{y}_{n+1}$ can be obtained as an approximation to the solution of the equations (1)–(2). This is formalized in the following definition.

Definition 1 ([45,34])**.** For a given time discretization $(t)_h$, the Local Linear discretization for the ODE (1)–(2) is defined by the recursive expression

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \boldsymbol{\phi}(t_n, \mathbf{y}_n; h_n), \tag{9}$$

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

The Local Linear discretization (9) is, by construction, A-stable. Furthermore, under quite general conditions, it does not have spurious equilibrium points [33] and preserves the local stability of the exact solution at hyperbolic equilibrium points and periodic orbits [33,46]. On the basis of the recursion (9) (also known as Exponentially fitted Euler, Euler Exponential or piecewise linearized method) a variety of numerical schemes for ODEs have been constructed (see a review in [34,37]). These numerical schemes essentially differ with respect to the numerical algorithm used to compute (8), and so in the dynamical properties that they inherit from the LL discretization. A major limitation of such schemes is their low order of convergence, namely two.

2.2. Local Linear–Runge–Kutta discretizations

A modification of the classical LL method can be done in order to improve its order of convergence while retaining desirable dynamic properties. To do so, note that the solution of the local linear ODE (3)–(4) is an approximation to the solution of the local nonlinear ODE

$$\frac{d\mathbf{z}(t)}{dt} = \mathbf{f}(t, \mathbf{z}(t)), \quad t \in [t_n, t_{n+1})$$

$$\mathbf{z}(t_n) = \mathbf{y}_n,$$

which can be rewritten as

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

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 subsection. From the variation of constants formula, the solution $\mathbf{z}$ of this equation can be written as

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

where

$$\mathbf{y}_{LL}(t; t_n, \mathbf{y}_n) = e^{\mathbf{A}_n(t-t_n)}\left(\mathbf{y}_n + \int_0^{t-t_n} e^{-\mathbf{A}_n u}\mathbf{a}_n(t_n + u)\, du\right) \tag{10}$$

is a solution of the linear equations (3)–(4) and

$$\mathbf{r}(t; t_n, \mathbf{y}_n) = \int_0^{t-t_n} e^{\mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n)(t-t_n-u)}\mathbf{g}(t_n, \mathbf{y}_n; t_n + u, \mathbf{z}(t_n + u))\, du \tag{11}$$

is the remainder term of the LL approximation $\mathbf{y}_{LL}$ to $\mathbf{z}$. Consequently, if $\mathbf{r}_\kappa$ is an approximation to $\mathbf{r}$ of order $\kappa > 2$, then $\mathbf{y}(t) = \mathbf{y}_{LL}(t; t_n, \mathbf{y}_n) + \mathbf{r}_\kappa(t; t_n, \mathbf{y}_n)$ should provide a better estimate to $\mathbf{z}(t)$ than the LL approximation $\mathbf{y}(t) = \mathbf{y}_{LL}(t; t_n, \mathbf{y}_n)$ for all $t \in [t_n, t_{n+1})$. This motivates the definition of the following high order local linear discretization.

Definition 2 (*[38]*)**.** For a given time discretization $(t)_h$, an order γ Local Linear discretization for the ODE (1)–(2) is defined by the recursive expression

$$\mathbf{y}_{n+1} = \mathbf{y}_{LL}(t_n + h_n; t_n, \mathbf{y}_n) + \mathbf{r}_\kappa(t_n + h_n; t_n, \mathbf{y}_n), \tag{12}$$

starting with $\mathbf{y}_0 = \mathbf{x}_0$, where $\mathbf{r}_\kappa$ is an approximation to the remainder term (11) such that $\|\mathbf{x}(t_n) - \mathbf{y}_n\| = O(h^\gamma)$ with $\gamma > 2$, for all $t_n \in (t)_h$.

Depending on the way in which the remainder term $\mathbf{r}$ is approximated, two classes of high order LL discretizations have been proposed. In the first one, $\mathbf{g}$ is approximated by a polynomial. For instance, by means of a truncated Taylor expansion [37] or a Hermite interpolation polynomial [39], resulting in the so-called Local Linearization—Taylor schemes and the Linearized Exponential Adams schemes, respectively. The second one is based on approximating $\mathbf{r}$ by means of a standard integrator that solves an auxiliary ODE. This is called the Local Linearization—Runge–Kutta (LLRK) methods when a Runge–Kutta integrator is used for this purpose [36]. A computational advantage of the latter class is that it does not require calculation of high order derivatives of the vector field $\mathbf{f}$.

Specifically, the LLRK methods are derived as follows. By taking derivatives with respect to t in (11), it is obtained that $\mathbf{r}(t; t_n, \mathbf{y}_n)$ satisfies the differential equation

$$\frac{d\mathbf{u}(t)}{dt} = \mathbf{q}(t_n, \mathbf{y}_n; t, \mathbf{u}(t)), \quad t \in [t_n, t_{n+1}), \tag{13}$$
$$\mathbf{u}(t_n) = \mathbf{0}, \tag{14}$$

with vector field

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

which can also be written as

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

where $\boldsymbol{\phi}$ is the vector function (8) that defines the LL discretization (9). Thus, an approximation $\mathbf{r}_\kappa$ to $\mathbf{r}$ can be obtained by solving the ODE (13)–(14) through any conventional numerical integrator. Namely, if $\mathbf{u}_{n+1} = \mathbf{u}_n + \boldsymbol{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{u}_n; h_n)$ is some one-step numerical scheme for this equation, then $\mathbf{r}_\kappa(t_n + h_n; t_n, \mathbf{y}_n) = \boldsymbol{\Lambda}^{\mathbf{y}_n}(t_n, \mathbf{0}; h_n)$.

In particular, we will focus on the approximation $\mathbf{r}_\kappa$ obtained by means of an explicit RK scheme of order κ. Consider an s-stage explicit RK scheme with coefficients $\mathbf{c} = [c_i]$, $\mathbf{A} = \left[a_{ij}\right]$, $\mathbf{b} = \left[b_j\right]$ applied to Eqs. (13)–(14), i.e., the approximation defined by the map

$$\boldsymbol{\rho}(t_n, \mathbf{y}_n; h_n) = h_n \sum_{j=1}^{s} b_j\mathbf{k}_j, \tag{15}$$

where

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

This suggests the following definition.

Definition 3 (*[37]*)**.** An order γ *Local Linear–Runge–Kutta (LLRK) discretization*is an order γ Local Linear discretization of the form (12), where the approximation $\mathbf{r}_\kappa$ to the remainder term (11) is defined by the *Runge–Kutta* formula (15).

3. Convergence and linear stability

In order to study the rate of convergence of the LLRK discretizations, three useful lemmas will be stated first.

Lemma 4. *Let* $\mathbf{u}_{n+1} = \mathbf{u}_n + \Lambda^{\mathbf{y}_n}(t_n, \mathbf{u}_n; h_n)$ *be an approximate solution of the auxiliary equation (13)–(14) at* $t = t_{n+1} \in (t)_h$ *given by an order* γ *numerical integrator, and* $\mathbf{y}_{n+1}$ *the discretization*

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

where

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

with $\mathbf{y}_0 = \mathbf{x}_0$. *Then the local truncation error* L_{n+1} *satisfies*

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

for all $t_n, t_{n+1} \in (t)_h$. *Moreover, if* F *satisfies the local Lipschitz condition*

$$\left\|F(s, \boldsymbol{\xi}_2; h) - F(s, \boldsymbol{\xi}_1; h)\right\| \leq B_\epsilon \left\|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right\|, \quad \text{with } B_\epsilon > 0 \text{ and } \boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \epsilon(\boldsymbol{\xi}) \subset \mathcal{D}, \tag{16}$$

where $\epsilon(\boldsymbol{\xi})$ *is a neighborhood of* $\boldsymbol{\xi}$ *for each* $\boldsymbol{\xi} \subset \mathcal{D}$, *then for* h *small enough there exists a positive constant* $C_2(\mathbf{x}_0)$ *depending only on* $\mathbf{x}_0$ *such that*

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{y}_{n+1}\| \leq C_2(\mathbf{x}_0) h^\gamma$$

for all $t_{n+1} \in (t)_h$.

Proof. Taking into account that

$$\mathbf{x}(t_{n+1}; \mathbf{x}_0) = \mathbf{y}_{LL}(t_n + h_n; t_n, \mathbf{x}(t_n; \mathbf{x}_0)) + \mathbf{r}(t_n + h_n; t_n, \mathbf{x}(t_n; \mathbf{x}_0)),$$

where $\mathbf{y}_{LL}$ and $\mathbf{r}$ are defined as in (10) and (11), respectively, it is obtained that

$$L_{n+1} = \left\|\mathbf{r}(t_n + h_n; t_n, \mathbf{x}(t_n; \mathbf{x}_0)) - \Lambda^{\mathbf{x}(t_n;\mathbf{x}_0)}(t_n, \mathbf{0}; h_n)\right\|,$$

where L_{n+1} denotes the local truncation error of the discretization under consideration. Since $\mathbf{r}(t_n + h_n; t_n, \mathbf{x}(t_n; \mathbf{x}_0))$ is the exact solution of the equation (13)–(14) with $\mathbf{y}_n = \mathbf{x}(t_n; \mathbf{x}_0)$ at t_{n+1} and $\mathbf{u}_{n+1} = \mathbf{u}_n + \Lambda^{\mathbf{x}(t_n;\mathbf{x}_0)}(t_n, \mathbf{u}_n; h_n)$ is the approximate solution of that equation at t_{n+1} given by an order γ numerical integrator, there exists a positive constant $C_1(\mathbf{x}_0)$ such that

$$\left\|\mathbf{r}(t_n + h_n; t_n, \mathbf{x}(t_n; \mathbf{x}_0)) - \Lambda^{\mathbf{x}(t_n;\mathbf{x}_0)}(t_n, \mathbf{0}; h_n)\right\| \leq C_1(\mathbf{x}_0) h_n^{\gamma+1},$$

which provides the stated bound for L_{n+1}.

On the other hand, since the compact set $\mathcal{X} = \{\mathbf{x}(t; \mathbf{x}_0) : t \in [t_0, T]\}$ is contained in the open set $\mathcal{D} \subset \mathbb{R}^d$, there exists $\varepsilon > 0$ such that the compact set

$$\mathcal{A}_\varepsilon = \left\{\xi \in \mathbb{R}^d : \min_{\mathbf{x}(t;\mathbf{x}_0) \in \mathcal{X}} \|\xi - \mathbf{x}(t; \mathbf{x}_0)\| \leq \varepsilon\right\}$$

is contained in $\mathcal{D}$. Since F satisfies the local Lipschitz condition (16), Lemma 2 in [47, pp. 92] implies the existence of a positive constant L such that

$$\left\|F(s, \boldsymbol{\xi}_2; h) - F(s, \boldsymbol{\xi}_1; h)\right\| \leq L \left\|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right\| \tag{17}$$

for all $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \mathcal{A}_\varepsilon$. Hence, the stated estimate $\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{y}_{n+1}\| \leq C_2(\mathbf{x}_0) h^\gamma$ for the global error straightforwardly follows from the Lipschitz condition (17) and Theorem 3.6 in [48], where $C_2(\mathbf{x}_0)$ is a positive constant. Finally, in order to guarantee that $\mathbf{y}_{n+1} \in \mathcal{A}_\varepsilon$ for all $n = 0, \ldots, N-1$, and so that the LLRK discretization is well-defined, it is sufficient that $0 < h < \delta$, where δ is chosen in such a way that $C_2(\mathbf{x}_0)\delta^\gamma \leq \varepsilon$. □

Note that this lemma requires of an order γ numerical integrator for the auxiliary equation (13)–(14). For this, certain conditions on the vector field $\mathbf{q}$ of this equation have to be assumed (usually, Lipschitz and smoothness conditions). The next two lemmas show that the function $\boldsymbol{\phi}$, and so the vector field $\mathbf{q}$, inherits such conditions from the vector field $\mathbf{f}$.

Lemma 5. *Let* $\boldsymbol{\varphi}(.; h) = \frac{1}{h}\boldsymbol{\phi}(.; h)$. *Suppose that*

$$\boldsymbol{f} \in \mathcal{C}^{p+1,q+1}([t_0, T] \times \mathcal{D}, \mathbb{R}^d),$$

where $p, q \in \mathbb{N}$. *Then* $\boldsymbol{\varphi} \in \mathcal{C}^{p,q,r}([t_0, T] \times \mathcal{D} \times \mathbb{R}_+, \mathbb{R}^d)$ *for all* $r \in \mathbb{N}$.

Proof. Let ϑ_j be the analytical function recursively defined by

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

for $z \in \mathbb{C}$. Since

$$\vartheta_j(s\mathbf{M}) = \frac{1}{(j-1)!s^j}\int_0^s e^{(s-u)\mathbf{M}}u^{j-1}du,$$

for all $s \in \mathbb{R}_+$ and $\mathbf{M} \in \mathbb{R}^d \times \mathbb{R}^d$ (see for instance [4]), the function $\boldsymbol{\varphi}$ can be written as

$$\boldsymbol{\varphi}(\tau, \boldsymbol{\xi}; \delta) = \vartheta_1(\delta \mathbf{f}_{\mathbf{x}}(\tau, \boldsymbol{\xi}))\,\mathbf{f}(\tau, \boldsymbol{\xi}) + \vartheta_2(\delta \mathbf{f}_{\mathbf{x}}(\tau, \boldsymbol{\xi}))\,\mathbf{f}_t(\tau, \boldsymbol{\xi})\,\delta$$

for all $\tau \in \mathbb{R}$, $\boldsymbol{\xi} \in \mathbb{R}^d$ and $\delta \geq 0$. Thus, from the analyticity of ϑ_j and the continuity of $\mathbf{f}$ the proof is completed. □

Lemma 6. *Let* $\mathbf{f}$ *and* $\mathbf{q}$ *be the vector fields of the ODEs (1)–(2) and (13)–(14), respectively.*

(i) There exists $\varepsilon > 0$ such that the compact set

$$\mathcal{A}_\varepsilon = \left\{\mathbf{z} \in \mathbb{R}^d : \min_{t\in[t_0,T]} \|\mathbf{x}(t) - \mathbf{z}\| \leq \varepsilon\right\}$$

is contained in $\mathcal{D}$. Moreover, there exists a compact set $\mathcal{K}_\varepsilon$ included into an open neighborhood of $\mathbf{0}$ and a $\delta_\varepsilon > 0$, such that

$$\mathbf{x}(t) + \boldsymbol{\phi}(t, \mathbf{x}(t); \delta) + \boldsymbol{\xi} \in \mathcal{A}_\varepsilon,$$

for all $\delta \in [0, \delta_\varepsilon]$, $\boldsymbol{\xi} \in \mathcal{K}_\varepsilon$ and $t \in [t_0, T]$.

(ii) If $\mathbf{f}$ and its first partial derivatives are bounded on $[t_0, T] \times \mathcal{D}$, and $\mathbf{f}(t, .)$ is a locally Lipschitz function on $\mathcal{D}$ with Lipschitz constant independent of t, then there exists a positive constant P such that

$$\left\|\mathbf{q}(t, \mathbf{x}(t); t+\delta, \boldsymbol{\xi}_2) - \boldsymbol{q}(t, \mathbf{x}(t); t+\delta, \boldsymbol{\xi}_1)\right\| \leq P\left\|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right\|$$

for all $\delta \in [0, \delta_\varepsilon]$, $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \mathcal{K}_\varepsilon$ and $t \in [t_0, T]$.

(iii) If $\mathbf{f} \in \mathcal{C}^p\left([t_0, T] \times \mathcal{D}, \mathbb{R}^d\right)$ for some $p \in \mathbb{N}$, then $\mathbf{q}(t, \mathbf{x}(t); \cdot) \in \mathcal{C}^p([t, t+\delta_\varepsilon] \times \mathcal{K}_\varepsilon, \mathbb{R}^d)$ for all $t \in [t_0, T]$.

Proof. The first part of assertion (i) follows from the fact that $\mathcal{X} = \{\mathbf{x}(t) : t \in [t_0, T]\}$ is a compact set contained into the open set $\mathcal{D}$, whereas its second part results from the continuity of $\boldsymbol{\phi}$ on $[t_0, T] \times \mathcal{A}_\varepsilon \times [0, \delta_\varepsilon]$ stated by Lemma 5. Assertion (ii) is a straightforward consequence of Lemma 2 in [47, pp. 92]. Assertion (iii) follows from the definition of the vector field $\mathbf{q}$ and Lemma 5. □

The next theorem characterizes the convergence rate of LLRK discretizations. For this purpose, for all $t_n \in (t)_h$, denote by

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_n\boldsymbol{\varphi}_\gamma(t_n, \mathbf{y}_n; h_n) \tag{18}$$

the LL discretization defined in (12), taking $\mathbf{r}_\kappa$ as an order γ RK scheme of the form (15). That is,

$$\boldsymbol{\varphi}_\gamma(t_n, \mathbf{y}_n; h_n) = \frac{1}{h_n}\{\boldsymbol{\phi}(t_n, \mathbf{y}_n; h_n) + \boldsymbol{\rho}(t_n, \mathbf{y}_n; h_n)\},$$

where $\boldsymbol{\phi}$ is defined by (8).

Theorem 7. *Suppose that*

$$\mathbf{f} \in \mathcal{C}^{\gamma+1}([t_0, T] \times \mathcal{D}, \mathbb{R}^d). \tag{19}$$

Then

$$\left\|\mathbf{x}(t_n + h; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - h\boldsymbol{\varphi}_\gamma(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h)\right\| \leq C_1(\mathbf{x}_0)h^{\gamma+1},$$

and the LLRK discretization (18) satisfies

$$\|\mathbf{x}(t_{n+1}; \mathbf{x}_0) - \mathbf{y}_{n+1}\| \leq C_2(\mathbf{x}_0)h^\gamma,$$

for all $t_n, t_{n+1} \in (t)_h$, *where* $C_1(\mathbf{x}_0)$ *and* $C_2(\mathbf{x}_0)$ *are positive constants depending only on* $\mathbf{x}_0$.

Proof. By Theorem 3.1 in [48], the local truncation error of the order γ explicit RK scheme (15) for Eqs. (13)–(14) with $\mathbf{y}_n = \mathbf{x}(t_n; \mathbf{x}_0)$ is

$$\|\mathbf{u}(t_n + h) - \boldsymbol{\rho}(t_n, \mathbf{x}(t_n; \mathbf{x}_0); h)\| \leq C(\mathbf{x}_0)h^{\gamma+1}, \tag{20}$$

where

$$C(\mathbf{x}_0) = \frac{1}{(\gamma+1)!}\max_{\theta\in[0,1]}\left\|\frac{d^{\gamma+1}}{dt^{\gamma+1}}\mathbf{u}(t_n + \theta h)\right\| + \frac{1}{\gamma!}\sum_{i=1}^{s}|b_i|\max_{\theta\in[0,1]}\left\|\frac{d^\gamma}{dt^\gamma}\mathbf{k}_i(\theta h)\right\|$$

with

$$\mathbf{k}_i(\theta h) = \mathbf{q}\left(t_n, \mathbf{x}(t_n; \mathbf{x}_0), t_n + c_i\theta h, \theta h \sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j(\theta h)\right).$$

By taking into account that the solution $\mathbf{r}$ of (13)–(14) is the remainder term of the LL approximation and by setting $\mathbf{y}_n = \mathbf{x}(t_n; \mathbf{x}_0)$ in (13), it follows that

$$\mathbf{u}(t_n + \theta h) = \mathbf{x}(t_n + \theta h; \mathbf{x}_0) - \mathbf{x}(t_n; \mathbf{x}_0) - \boldsymbol{\phi}(t_n, \mathbf{x}(t_n; \mathbf{x}_0); \theta h), \tag{21}$$

and so

$$\left\| \frac{d^{\gamma+1}}{dt^{\gamma+1}}\mathbf{u}(t_n + \theta h) \right\| = \left\| \frac{d^{\gamma}}{dt^{\gamma}}\mathbf{q}(t_n, \mathbf{x}(t_n; \mathbf{x}_0); t_n + \theta h, \mathbf{u}(t_n + \theta h)) \right\|,$$

where the derivative in the right term of the last expression is with respect to the last two arguments of the function $\mathbf{q}$. Condition (19), assertion (iii) of Lemma 6 and expression (21) imply that $\mathbf{q}(., \mathbf{x}(., \mathbf{x}_0); ., \mathbf{u}(.)) \in \mathcal{C}^{\gamma}([t_0, T], \mathbb{R}^d)$. Hence, there exists a constant M such that

$$\max_{\theta\in[0,1], t_n\in[t_0,T]} \left\| \frac{d^{\gamma+1}}{dt^{\gamma+1}}\mathbf{u}(t_n + \theta h) \right\| \leq M.$$

Likewise, condition (19) and Lemma 6 imply that

$$\max_{\theta\in[0,1], t_n\in[t_0,T]} \left\| \frac{d^{\gamma}}{dt^{\gamma}}\mathbf{k}_i(\theta h) \right\| \leq M.$$

Therefore, $C(\mathbf{x}_0)$ in (20) is bounded as a function of $\mathbf{x}_0 \in \mathcal{D}$.

In addition, Lemma 5 and Lemma 3.5 in [48] combined with assertion (iii) of Lemma 6 imply that $\boldsymbol{\phi}$ and $\boldsymbol{\rho}$ satisfy the local Lipschitz condition (16), and so does the function

$$\boldsymbol{\varphi}_{\gamma}(t_n, \mathbf{y}_n; h) = \frac{1}{h}\{\boldsymbol{\phi}(t_n, \mathbf{y}_n; h) + \boldsymbol{\rho}(t_n, \mathbf{y}_n; h)\}$$

as well. This and Lemma 4 complete the proof. □

Note that the Lipschitz and smoothness conditions in Lemma 4 and Theorem 7 are the usual ones required to derive the convergence of numerical integrators (see, e.g., Theorems 3.1 and 3.6 in [48]). These conditions directly imply that smoothness of the solution of the ODE in a bounded domain (see, e.g., Theorem 1 pp. 79 and Remark 1 pp. 83 in [47]). In this way, to ensure the convergence of the LLRK integrators, the involved RK coefficients are not constrained by any stability condition and they just need to satisfy the usual order conditions for RK schemes. This is a major difference with the Rosenbrock and Exponential Integrators and makes the LLRK methods more flexible and simple. Further note that, like these integrators, the LLRK are trivially A-stable.

4. Steady states

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

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}(t)), \quad t \in [t_0, T], \tag{22}$$

$$\mathbf{x}(t_0) = \mathbf{x}_0 \in \mathbb{R}^d, \tag{23}$$

and those of their LLRK discretizations is considered. For the sake of simplicity, a uniform time partition $h_n = h$ is adopted.

It will be convenient to rewrite the order γ LLRK discretization in the form

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\boldsymbol{\varphi}_{\gamma}(\mathbf{y}_n, h), \tag{24}$$

where

$$\boldsymbol{\varphi}_{\gamma}(\boldsymbol{\xi}, \delta) = \Phi(\boldsymbol{\xi}, \delta)\mathbf{f}(\boldsymbol{\xi}) + \sum_{i=1}^{s} b_i\mathbf{k}_i(\boldsymbol{\xi}, \delta), \tag{25}$$

with

$$\Phi(\boldsymbol{\xi}, \delta) = \frac{1}{\delta}\int_0^{\delta} e^{\mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi})u}du, \tag{26}$$

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

and

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

For later reference, the following Lemma states some useful properties of the functions $\boldsymbol{\varphi}_\gamma$ on neighborhoods of invariant sets of ODEs.

Lemma 8. *Let $\Sigma \subset \mathbb{R}^d$ be an invariant set for the flow of Eq. (22). 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 (22)–(23) fulfills the condition*

$$\mathbf{x}(t;\mathbf{x}_0) \subset \Omega \quad \text{for all initial point } \mathbf{x}_0 \in \mathcal{K} \text{ and } t \in [t_0, T], \tag{27}$$

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

$$\mathbf{f} \in \mathcal{C}^{\gamma+1}(\Omega, \mathbb{R}^d). \tag{28}$$

Further, let

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

be the order γ LLRK discretization defined by (24). Then

(i) $\boldsymbol{\varphi}_\gamma \to \mathbf{f}$ *and* $\partial\boldsymbol{\varphi}_\gamma/\partial\mathbf{y}_n \to \mathbf{f}_{\mathbf{x}}$ *as* $h \to 0$ *uniformly in* $\mathcal{K}$,
(ii) $\left\|(\mathbf{x}(t_0+h;\mathbf{x}_0)-\mathbf{x}_0)/h - \boldsymbol{\varphi}_\gamma(\mathbf{x}_0,h)\right\| = O(h^\gamma)$ *uniformly for* $\mathbf{x}_0 \in \mathcal{K}$.

Proof. According to Lemma 5 in [33], $\mathbf{f} \in \mathcal{C}^{\gamma+1}(\Omega)$ implies that $\Phi f \to \mathbf{f}$ and $\partial(\Phi f)/\partial\xi \to \mathbf{f}_{\mathbf{x}}$ as $h \to 0$ uniformly in $\mathcal{K}$.

On the other hand, $\mathbf{k}_i(\boldsymbol{\xi}, 0) = \mathbf{0}$, for all $\boldsymbol{\xi} \in \Omega$ and $i = 1, \ldots, s$. Besides, since

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

where

$$\begin{aligned}\frac{\partial\mathbf{q}}{\partial\boldsymbol{\xi}}(\boldsymbol{\xi};\delta,\mathbf{u}) = {} & \mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi}+\delta\Phi(\boldsymbol{\xi},\delta)\mathbf{f}(\boldsymbol{\xi})+\mathbf{u})\frac{\partial}{\partial\boldsymbol{\xi}}(\boldsymbol{\xi}+\delta\Phi(\boldsymbol{\xi},\delta)\mathbf{f}(\boldsymbol{\xi})+\mathbf{u}) \\ & -\delta\frac{\partial}{\partial\boldsymbol{\xi}}(\mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi})\Phi(\boldsymbol{\xi},\delta)\mathbf{f}(\boldsymbol{\xi})) - \mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi}) + \mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi}+\delta\Phi(\boldsymbol{\xi},\delta)\mathbf{f}(\boldsymbol{\xi})+\mathbf{u})\frac{\partial\mathbf{u}}{\partial\boldsymbol{\xi}}\end{aligned}$$

with

$$\mathbf{u} = \delta\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j(\boldsymbol{\xi},\delta) \quad \text{and} \quad \frac{\partial\mathbf{u}}{\partial\boldsymbol{\xi}} = \delta\sum_{j=1}^{i-1} a_{ij}\frac{\partial}{\partial\boldsymbol{\xi}}\mathbf{k}_j(\boldsymbol{\xi},\delta),$$

$\partial\mathbf{k}_i(\boldsymbol{\xi},0)/\partial\boldsymbol{\xi} = \mathbf{0}$ for all $i = 1, \ldots, s$. Thus, since each $\mathbf{k}_i$ and $\partial\mathbf{k}_i/\partial\boldsymbol{\xi}$ are continuous functions on $\Omega \times [0,1]$, it holds that $\mathbf{k}_i \to \mathbf{0}$ and $\partial\mathbf{k}_i/\partial\boldsymbol{\xi} \to \mathbf{0}$ as $h \to 0$ uniformly in the compact set $\mathcal{K}$. Thus, assertion (i) holds.

From Theorem 7 we have

$$\left\|(\mathbf{x}(t_0+h;\mathbf{x}_0)-\mathbf{x}_0)/h - \boldsymbol{\varphi}_\gamma(\mathbf{x}_0,h)\right\| \le C(\mathbf{x}_0)h^\gamma,$$

where

$$C(\mathbf{x}_0) = \frac{1}{(\gamma+1)!}\max_{\theta\in[0,1]}\left\|\frac{d^{\gamma+1}}{dt^{\gamma+1}}\mathbf{u}(t_0+\theta h)\right\| + \frac{1}{\gamma!}\sum_{i=1}^{s}|b_i|\max_{\theta\in[0,1]}\left\|\frac{d^\gamma}{dt^\gamma}\mathbf{k}_i(\theta h)\right\|$$

is a positive constant depending of $\mathbf{x}_0$,

$$\mathbf{k}_i(\theta h) = \mathbf{q}\left(\mathbf{x}(t_0;\mathbf{x}_0); c_i\theta h, \theta h\sum_{j=1}^{i-1} a_{ij}\mathbf{k}_j(\theta h)\right), \quad i = 1, \ldots, s$$

and $\mathbf{u}(t_0+\theta h) = \mathbf{x}(t_0+\theta h;\mathbf{x}_0) - \mathbf{x}(t_0;\mathbf{x}_0) - \boldsymbol{\phi}(t_0, \mathbf{x}(t_0;\mathbf{x}_0); \theta h)$.

Clearly,

$$\begin{aligned}\left\|\frac{d^{\gamma+1}}{dt^{\gamma+1}}\mathbf{u}(s)\right\| &= \left\|\frac{d^{\gamma+1}}{dt^{\gamma+1}}(\mathbf{x}(s;\mathbf{x}_0) - \mathbf{x}(t_0;\mathbf{x}_0) - \boldsymbol{\phi}(t_0,\mathbf{x}(t_0;\mathbf{x}_0); s-t_0))\right\| \\ &\le \left\|\frac{d^\gamma}{dt^\gamma}\mathbf{f}(\mathbf{x}(s;\mathbf{x}_0))\right\| + \left\|\frac{d^{\gamma+1}}{dt^{\gamma+1}}\boldsymbol{\phi}(t_0,\mathbf{x}(t_0;\mathbf{x}_0); s-t_0)\right\|\end{aligned}$$

for all $s \in [t_0, t_0 + h]$. Since $\mathbf{x}(t; \mathbf{x}_0) \in \Omega$ for all $t \in [t_0, T]$ and $\mathbf{x}_0 \in \mathcal{K} \subset \Omega$, there exists a compact set $\mathcal{A}_h$ depending on h such that $\mathcal{K} \subset \mathcal{A}_h \subset \Omega$ and $\mathbf{x}(s; \mathbf{x}_0) \in \mathcal{A}_h$ for all $s \in [t_0, t_0 + h]$ and $\mathbf{x}_0 \in \mathcal{K}$. In addition, since condition $\mathbf{f} \in \mathcal{C}^{\gamma+1}(\Omega, \mathbb{R}^d)$ implies that there exists a constant M such that

$$\sup_{\xi \in \mathcal{A}_h} \left\| \frac{d^\gamma}{dt^\gamma} \mathbf{f}(\xi) \right\| \leq M,$$

it is obtained that

$$\max_{\theta \in [0,1], \mathbf{x}_0 \in \mathcal{K}} \left\| \frac{d^\gamma}{dt^\gamma} \mathbf{f}(\mathbf{x}(t_0 + \theta h; \mathbf{x}_0)) \right\| \leq \sup_{\xi \in \mathcal{A}_h} \left\| \frac{d^\gamma}{dt^\gamma} \mathbf{f}(\xi) \right\| \leq M.$$

Taking into account that $\boldsymbol{\phi}$ and $\mathbf{k}_i$ are functions of $\mathbf{f}$, we can similarly proceed to find a bound $B > 0$ independent of θ, $\mathbf{x}_0$ for $\left\| \frac{d^{\gamma+1}}{dt^{\gamma+1}} \boldsymbol{\phi}(t_0, \mathbf{x}(t_0; \mathbf{x}_0); s - t_0) \right\|$ and $\left\| \frac{d^\gamma}{dt^\gamma} \mathbf{k}_i(\theta h) \right\|$. Hence, we conclude that $C(\mathbf{x}_0)$ is bounded on $\mathcal{K}$ by a constant independent of $\mathbf{x}_0$, and so (ii) follows. □

4.1. Fixed points and linearization preserving

Theorem 9. *Suppose that the vector field* $\mathbf{f}$ *of Eq. (22) and its derivatives up to order* γ *are defined and bounded on* $\mathbb{R}^d$*. Then, all equilibrium points of the given ODE (22) are fixed points of any LLRK discretization.*

Proof. Let $\boldsymbol{\varphi}_\gamma$, Φ and $\mathbf{k}_i$ be the functions defined in expression (25). If $\boldsymbol{\xi}$ is an equilibrium point of (22), then $\mathbf{f}(\boldsymbol{\xi}) = \mathbf{0}$ and so $\Phi(\boldsymbol{\xi}, h)\mathbf{f}(\boldsymbol{\xi}) = \mathbf{0}$ and $\mathbf{k}_i(\boldsymbol{\xi}, h) = \mathbf{0}$ for all h and $i = 1, \ldots, s$. Thus, $\boldsymbol{\varphi}_\gamma(\boldsymbol{\xi}, h) = \mathbf{0}$ for all h, which implies that $\boldsymbol{\xi}$ is a fixed point of the LLRK discretization (24). □

A numerical integrator $\mathbf{u}_{n+1} = \mathbf{u}_n + \Lambda(t_n, \mathbf{u}_n; h_n)$ is linearization preserving at an equilibrium point $\boldsymbol{\xi}$ of the ODE (22) if from the Taylor series expansion of $\Lambda(t_n, \cdot; h_n)$ around $\boldsymbol{\xi}$ it is obtained that

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

Furthermore, an integrator is said to be linearization preserving if it is linearization preserving at all equilibrium points of the ODE [46].

This property ensures that the integrator correctly captures all eigenvalues of the linearized system at every equilibrium point of an ODE, which guarantees the exact preservation (in type and parameters) of a number of local bifurcations of the underlying equation [46]. 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.

In [46] the linearization preserving property of the LL discretization (9) was demonstrated. This property is also inherited by LLRK discretizations as it is shown by the next theorem.

Theorem 10. *Let the vector field* $\mathbf{f}$ *of Eq. (22) and its derivatives up to order* 2 *be functions defined and bounded on* $\mathbb{R}^d$*. Then, LLRK discretizations are linearization preserving.*

Proof. Let $\boldsymbol{\xi}$ be an arbitrary equilibrium point of the ODE (22) and let the initial condition $\mathbf{y}_n$ be in the neighborhood of $\boldsymbol{\xi}$.

Let us consider the Taylor expansion of $\mathbf{f}$ around $\boldsymbol{\xi}$

$$\mathbf{f}(\mathbf{y}_n) = \mathbf{f}_\mathbf{x}(\boldsymbol{\xi})(\mathbf{y}_n - \boldsymbol{\xi}) + O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2)$$

and the LL discretization

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

where Φ defined as in (26) is, according to assertion (i) of Lemma 1 in [33], a Lipschitz function. By combining this Taylor expansion with both the identity (6) and the Lipschitz inequality $\|\Phi(\mathbf{y}_n, h) - \Phi(\boldsymbol{\xi}, h)\| \leq \lambda \|\mathbf{y}_n - \boldsymbol{\xi}\|$ it is obtained

$$h\Phi(\boldsymbol{\xi}, h)\mathbf{f}(\mathbf{y}_n) = (e^{h\mathbf{f}_\mathbf{x}(\boldsymbol{\xi})} - \mathbf{I})(\mathbf{y}_n - \boldsymbol{\xi}) + O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2) \tag{29}$$

and

$$\|(\Phi(\mathbf{y}_n, h) - \Phi(\boldsymbol{\xi}, h))\mathbf{f}(\mathbf{y}_n)\| \leq C \|\mathbf{y}_n - \boldsymbol{\xi}\|^2, \tag{30}$$

respectively, where C is a positive constant.

Now, consider the LLRK discretization

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

with $\boldsymbol{\varphi}_\gamma$ defined as in (25). From the Taylor formula with a Lagrange remainder it is obtained that

$$\begin{aligned}\|\mathbf{q}(\mathbf{y}_n; h, \mathbf{u})\| &= \|\mathbf{f}(\mathbf{y}_n + \Phi(\mathbf{y}_n, h)\mathbf{f}(\mathbf{y}_n)h + \mathbf{u}) - \mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)\Phi(\mathbf{y}_n, h)\mathbf{f}(\mathbf{y}_n)h - \mathbf{f}(\mathbf{y}_n)\| \\ &\leq M\|\Phi(\mathbf{y}_n, h)\mathbf{f}(\mathbf{y}_n)h + \mathbf{u}\|^2 + \|\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)\|\,\|\mathbf{u}\|,\end{aligned}$$

where the positive constant M is a bound for $\|\mathbf{f}_{\mathbf{xx}}\|$ on a compact subset $\mathcal{K} \subset \mathbb{R}^d$ such that $\mathbf{y}_n, \mathbf{y}_{n+1}, \boldsymbol{\xi} \in \mathcal{K}$. By using (29) and (30) it follows that

$$\|\mathbf{q}(\mathbf{y}_n; h, \mathbf{u})\| \leq 2M\|\mathbf{u}\|^2 + \|\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)\|\,\|\mathbf{u}\| + O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2).$$

From the last inequality and taking into account that $\mathbf{k}_1 = \mathbf{0}$, it is obtained that $\|\mathbf{k}_2\| \leq O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2)$. Furthermore, by induction, it is obtained that $\|\mathbf{k}_i\| \leq O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2)$ for all $i = 1, 2, \ldots, s$. From this, (25) and (29) it follows that

$$h\boldsymbol{\varphi}_\gamma(\mathbf{y}_n, h) = (e^{h\mathbf{f}_{\mathbf{x}}(\boldsymbol{\xi})} - \mathbf{I})(\mathbf{y}_n - \boldsymbol{\xi}) + O(\|\mathbf{y}_n - \boldsymbol{\xi}\|^2),$$

which implies that the LLRK discretization is linearization preserving. □

The next two subsections deal with a more precise analysis of the dynamical behavior of the LLRK discretizations in the neighborhood of some steady states.

4.2. Phase portrait near equilibrium points

Let $\mathbf{0}$ be a hyperbolic equilibrium point of Eq. (22). 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 11. *Suppose that the conditions (27)–(28) of Lemma 8 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 LLRK discretization (24) at $\mathbf{0}$ are of the form*

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

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

$$\sup\{\|\mathbf{x}(t_n; \mathbf{x}_0) - \mathbf{y}_n(\mathbf{z}_0)\| : \mathbf{x}(t; \mathbf{x}_0) \in \mathcal{K}_\varepsilon \quad \text{for } t \in [t_0, t_n]\} \leq Ch^\gamma. \tag{31}$$

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 fulfills (31), where the supremum is taken over all n satisfying $\mathbf{y}_j(\mathbf{z}_0) \in \mathcal{K}_\varepsilon$, $j = 0, \ldots, n$.

Proof. Since Ω is a neighborhood of the invariant set $\mathbf{0}$, there exists a constant $\varepsilon > 0$ and a compact set $\mathcal{K}_\varepsilon = \{\boldsymbol{\xi} \in \mathbb{R}^d : \|\boldsymbol{\xi}\| \leq \varepsilon\} \subset \Omega$ such that Lemma 8 holds with $\mathcal{K} = \mathcal{K}_\varepsilon$. Furthermore, by assertion (i) of Theorem 9, $\mathbf{f}(\boldsymbol{\xi}) = \mathbf{0}$ implies $\boldsymbol{\varphi}_\gamma(\boldsymbol{\xi}, h) = \mathbf{0}$ for all h. Thus, the hypotheses of Theorem 3.1 in [49] hold for the LLRK discretizations, which completes the prove. □

Theorem 11 shows that the phase portrait of a continuous dynamical system near a hyperbolic equilibrium point is correctly reproduced by LLRK discretizations for sufficiently small step-sizes. It states that any trajectory of the dynamical system can be correctly approximated by a trajectory of the LLRK discretization if the discrete initial value is conveniently adjusted. It also affirms that any trajectory of an LLRK discretization approximates some trajectory of the continuous system with a suitable selection of the starting point. In both cases, these results are valid for sufficiently small step-sizes and as long as the trajectories stay within some neighborhood of the equilibrium point. Moreover, the theorem ensures that the local stable and unstable manifolds of an LLRK discretization at the equilibrium point converge to those of the continuous system as the step-size goes to zero.

4.3. Phase portraits near periodic orbits

Suppose that Eq. (22) 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 12. *Let the assumptions (27)–(28) of Lemma 8 hold on a neighborhood of $\overline{\Omega}$. Then there exist $h_0 > 0$ and an open neighborhood U of Γ such that the order γ LLRK discretization*

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

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

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

and

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

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

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

Proof. Since Lemma 8 holds on a neighborhood of $\overline{\Omega}$, it also holds on Ω. In addition, Lemmas 5 and 6 imply that $\boldsymbol{\varphi}_\gamma \in \mathcal{C}^2(\overline{\Omega} \times [0, h_0])$, so $\partial\boldsymbol{\varphi}_\gamma/\partial\mathbf{y}_n$ is Lipschitz on Ω uniformly in h. Thus, the hypotheses of Theorem 2.1 in [50] hold for the LLRK discretizations of order $\gamma > 2$, which completes the proof. □

Theorem 12 affirms that, for h sufficiently small, the LLRK discretizations have a closed invariant curve Γ_h, i.e., $(1 + h\boldsymbol{\varphi}(.; h))(\Gamma_h) = \Gamma_h$, which converges to the periodic orbit Γ of the continuous system.

The next theorem deals with the behavior of the discrete trajectories of LLRK discretizations near the invariant curve Γ_h when the ODE (22) 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,

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

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

Theorem 13. *Let* Γ *be a stable closed orbit of equation* (22)*. Then, under the assumptions of Theorem* 12*, there exist* h_0, α, β, C *and* $\rho > 0$ *such that for* $h \leq h_0$ *and* $dist(\mathbf{x}_0, \Gamma_h) \leq \rho$ *the following holds:*

$$dist(\mathbf{y}_n(\mathbf{x}_0), \Gamma_h) \leq C \exp(-\alpha t_n) dist(\mathbf{x}_0, \Gamma_h)$$

and

$$dist(\mathbf{y}_n(\mathbf{x}_0), w(\mathbf{x}_0)) \leq C(h^{\gamma} + \min\{h^{\gamma} \exp(\beta t_n), \exp(-\alpha t_n)\})$$

for $n \geq 0$*. 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,*

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

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

Proof. It can be proved in a similar way as Theorem 12, but using Theorem 3.2 in [50] instead of Theorem 2.1. □

This theorem states the stability of the invariant curve Γ_h and the convergence of the trajectories of an LLRK discretization to the continuous trajectories of the underlying ODE when the discretization starts at a point close enough to the stable periodic orbit Γ.

5. A-stable explicit LLRK schemes

This section deals with practical issues of the LLRK methods, that is, with the so-called Local Linearization—Runge–Kutta schemes.

Roughly speaking, every numerical implementation of an LLRK discretization will be called the LLRK scheme. More precisely, they are defined as follows.

Definition 14. For an order γ LLRK discretization

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_n\boldsymbol{\varphi}_\gamma(t_n, \mathbf{y}_n; h_n), \tag{32}$$

as defined in (18), any recursion of the form

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + h_n\widetilde{\boldsymbol{\varphi}}_\gamma(t_n, \widetilde{\mathbf{y}}_n; h_n), \quad \text{with } \widetilde{\mathbf{y}}_0 = \mathbf{y}_0,$$

where $\widetilde{\boldsymbol{\varphi}}_\gamma$ denotes some numerical algorithm to compute $\boldsymbol{\varphi}_\gamma$, is called an LLRK scheme.

When implementing the LLRK discretization (32), that is, when an LLRK scheme is constructed, the required evaluations of the expression $\mathbf{y}_n+\boldsymbol{\phi}(t_n,\mathbf{y}_n;.)$ at $t_{n+1}-t_n$ and $c_i(t_{n+1}-t_n)$ may be computed by different algorithms. In [37,34] a number of them were reviewed, which yield the following two basic kinds of LLRK schemes:

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

and

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

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

$$\frac{d\mathbf{z}(t)}{dt}=\mathbf{B}_n\mathbf{z}(t)+\mathbf{b}_n(t),\quad t\in[t_n,t_{n+1}], \tag{33}$$

$$\mathbf{z}(t_n)=\widetilde{\mathbf{y}}_n, \tag{34}$$

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

$$\frac{d\mathbf{v}(t)}{dt}=\widetilde{\mathbf{q}}(t_n,\mathbf{z}(t_n);t,\mathbf{v}(t)),\quad t\in[t_n,t_{n+1}], \tag{35}$$

$$\mathbf{v}(t_n)=\mathbf{0}, \tag{36}$$

with vector field

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

for the first kind of LLRK scheme, or

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

for the second one. In Eq. (33), $\mathbf{B}_n=\mathbf{f}_{\mathbf{x}}(t_n,\widetilde{\mathbf{y}}_n)$ is a $d\times d$ constant matrix and $\mathbf{b}_n(t)=\mathbf{f}_t(t_n,\widetilde{\mathbf{y}}_n)(t-t_n)+\mathbf{f}(t_n,\widetilde{\mathbf{y}}_n)-\boldsymbol{B}_n\widetilde{\mathbf{y}}_n$ is a d-dimensional linear vector function.

Obviously, an LLRK scheme will preserve the order γ of the underlaying LLRK discretization only if $\widetilde{\boldsymbol{\phi}}$ is a suitable approximation to $\boldsymbol{\phi}$. This requirement is considered in the next theorem.

Theorem 15. *Let* $\mathbf{x}$ *be the solution of the ODE (1)–(2) with vector field* $\mathbf{f}$ *satisfying the condition (19). With* t_n, $t_{n+1}\in(t)_h$, *let* $\widetilde{\mathbf{z}}_{n+1}=\widetilde{\mathbf{z}}_n+h_n\Lambda_1(t_n,\widetilde{\mathbf{z}}_n;h_n)$ *and* $\widetilde{\mathbf{v}}_{n+1}=\widetilde{\mathbf{v}}_n+h_n\Lambda_2^{\widetilde{\mathbf{z}}_n}(t_n,\widetilde{\mathbf{v}}_n;h_n)$ *be one-step explicit integrators of the ODEs (33)–(34) and (35)–(36), respectively. Suppose that these integrators have order of convergence* r *and* p, *respectively. Further, assume that* Λ_1 *and* $\Lambda_2^{\widetilde{\mathbf{z}}_n}$ *fulfill the local Lipschitz condition (16). Then, for* h *small enough, the numerical scheme*

$$\widetilde{\mathbf{y}}_{n+1}=\widetilde{\mathbf{y}}_n+h_n\Lambda_1(t_n,\widetilde{\mathbf{y}}_n;h_n)+h_n\Lambda_2^{\widetilde{\mathbf{y}}_n}(t_n,\mathbf{0};h_n)$$

satisfies that

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

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

Proof. Let $\mathcal{X}=\{\mathbf{x}(t):t\in[t_0,T]\}$. Since $\mathcal{X}$ is a compact set contained in the open set $\mathcal{D}\subset\mathbb{R}^d$, there exists $\varepsilon>0$ such that the compact set

$$\mathcal{A}_\varepsilon=\left\{\xi\in\mathbb{R}^d:\min_{\mathbf{x}(t)\in\mathcal{X}}\|\xi-\mathbf{x}(t)\|\le\varepsilon\right\}$$

is contained in $\mathcal{D}$.

First, set $\widetilde{\mathbf{y}}_n=\mathbf{x}(t_n)$ in Eqs. (33)–(34) and (35)–(36). Since $\mathbf{x}(t_{n+1})=\mathbf{y}_{LL}(t_n+h_n;t_n,\mathbf{x}(t_n))+\mathbf{r}(t_n+h_n;t_n,\mathbf{x}(t_n))$, it is obtained that

$$\begin{aligned}\left\|\mathbf{x}(t_{n+1})-\mathbf{x}(t_n)-h_n\Lambda_1(t_n,\mathbf{x}(t_n);h_n)-h_n\Lambda_2^{\mathbf{x}(t_n)}(t_n,\mathbf{0};h_n)\right\|&\le\|\boldsymbol{\phi}(t_n,\mathbf{x}(t_n);h_n)-h_n\Lambda_1(t_n,\mathbf{x}(t_n);h_n)\|\\&\quad+\|\mathbf{r}(t_n+h_n;t_n,\mathbf{x}(t_n))-\mathbf{v}(t_{n+1})\|\\&\quad+\left\|\mathbf{v}(t_{n+1})-h_n\Lambda_2^{\mathbf{x}(t_n)}(t_n,\mathbf{0};h_n)\right\|,\end{aligned} \tag{37}$$

where $\mathbf{v}(t_{n+1})$ is the solution of equation (35)–(36) at $t=t_{n+1}$.

By definition, $\mathbf{r}(t_n+h_n;t_n,\mathbf{x}(t_n))$ is a solution of the differential equation

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

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

evaluated at $t = t_{n+1}$. Thus, by applying the "fundamental lemma" (see, e.g., Theorem 10.2 in [48]), it is obtained that

$$\|\mathbf{r}(t; t_n, \mathbf{x}(t_n)) - \mathbf{v}(t)\| \leq \frac{\epsilon}{P}(e^{P(t-t_n)} - 1) \tag{38}$$

for $t \in [t_n, t_{n+1}]$, where

$$\begin{aligned}\epsilon &= \sup_{t\in[t_n,t_{n+1}]} \|\mathbf{q}(t_n, \mathbf{x}(t_n); t, \mathbf{u}(t)) - \widetilde{\mathbf{q}}(t_n, \mathbf{x}(t_n); t, \mathbf{u}(t))\| \\ &\leq M\|\boldsymbol{\phi}(t_n, \mathbf{x}(t_n); h_n) - h_n\Lambda_1(t_n, \mathbf{x}(t_n); h_n)\|,\end{aligned}$$

$M = 2\sup_{t\in[t_0,T],\xi\in\mathcal{A}_\varepsilon}\|\mathbf{f}_{\mathbf{x}}(t,\xi)\|$, and P is the Lipschitz constant of the function $\mathbf{q}(t_n, \mathbf{x}(t_n); \cdot)$ (which exists by Lemma 6).

Furthermore,

$$\|\boldsymbol{\phi}(t_n, \mathbf{x}(t_n); h_n) - h_n\Lambda_1(t_n, \mathbf{x}(t_n); h_n)\| = \|\mathbf{z}(t_{n+1}) - \mathbf{z}(t_n) - h_n\Lambda_1(t_n, \mathbf{z}(t_n); h_n)\|, \tag{39}$$

since $\mathbf{z}(t_{n+1}) = \mathbf{x}(t_n) + \boldsymbol{\phi}(t_n, \mathbf{x}(t_n); h_n)$ is the solution (33)–(34) with $\widetilde{\mathbf{y}}_n = \mathbf{x}(t_n)$ at $t = t_{n+1}$. On the other hand,

$$\|\mathbf{z}(t_{n+1}) - \mathbf{z}(t_n) - h_n\Lambda_1(t_n, \mathbf{z}(t_n); h_n)\| \leq c_1 h^{r+1} \tag{40}$$

and

$$\left\|\mathbf{v}(t_{n+1}) - h_n\Lambda_2^{\mathbf{x}(t_n)}(t_n, \mathbf{0}; h_n)\right\| \leq c_2 h^{p+1} \tag{41}$$

hold, since $\widetilde{\mathbf{z}}_{n+1} = \widetilde{\mathbf{z}}_n + h_n\Lambda_1(t_n, \widetilde{\mathbf{z}}_n; h_n)$ and $\widetilde{\mathbf{v}}_{n+1} = \widetilde{\mathbf{v}}_n + h_n\Lambda_2^{\widetilde{\mathbf{z}}_n}(t_n, \widetilde{\mathbf{v}}_n; h_n)$ are order r and p integrators, respectively. Here, c_1 and c_2 are positive constants independent of h.

From the inequalities (37)–(41), the one-step integrator

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + h_n\Lambda_1(t_n, \widetilde{\mathbf{y}}_n; h_n) + h_n\Lambda_2^{\widetilde{\mathbf{y}}_n}(t_n, \mathbf{0}; h_n)$$

has local truncation error

$$\left\|\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - h_n\Lambda_1(t_n, \mathbf{x}(t_n); h_n) - h_n\Lambda_2^{\mathbf{x}(t_n)}(t_n, \mathbf{0}; h_n)\right\| \leq ch^{\min\{r,p\}+1},$$

where $c = c_1 + c_2 + c_1M(e^P - 1)/P$ is a positive constant. In addition, since $\Lambda_1 + \Lambda_2^{\mathbf{x}(t_n)}$ with fixed t_n, h_n is a local Lipschitz function on $\mathcal{D}$, Lemma 2 in [47, pp. 92] implies that $\Lambda_1 + \Lambda_2^{\mathbf{x}(t_n)}$ is a Lipschitz function on $\mathcal{A}_\varepsilon \subset \mathcal{D}$. Thus, the stated estimate $\|\mathbf{x}(t_{n+1}) - \widetilde{\mathbf{y}}_{n+1}\| \leq Ch^{\min\{r,p\}}$ for the global error of the LLRK scheme $\widetilde{\mathbf{y}}_{n+1}$ straightforwardly follows from Theorem 3.6 in [48], where C is a positive constant. Finally, in order to guarantee that $\mathbf{y}_{n+1} \in \mathcal{A}_\varepsilon$ for all $n = 0, \ldots, N-1$, and so that the LLRK scheme is well-defined, it is sufficient that $0 < h < \delta$, where δ is chosen in such a way that $C\delta^{\min\{r,p\}} \leq \varepsilon$. □

As an example, consider the computation of the function $\boldsymbol{\phi}$ through a Padé approximation combined with the "scaling and squaring" strategy for exponential matrices [51]. To do so, note that $\boldsymbol{\phi}$ can be written as [52,34]

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

where

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

$\mathbf{L} = \begin{bmatrix}\mathbf{I}_d & \mathbf{0}_{d\times 2}\end{bmatrix}$ and $\mathbf{r}^\intercal = \begin{bmatrix}\mathbf{0}_{1\times(d+1)} & 1\end{bmatrix}$ in the case of non-autonomous ODEs; and

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

$\mathbf{L} = \begin{bmatrix}\mathbf{I}_d & \mathbf{0}_{d\times 1}\end{bmatrix}$ and $\mathbf{r}^\intercal = \begin{bmatrix}\mathbf{0}_{1\times d} & 1\end{bmatrix}$ for autonomous equations.

Proposition 16. *Set* $\widetilde{\boldsymbol{\phi}}(t_n, \widetilde{\mathbf{y}}_n; h_n) = \mathbf{L}(\mathbf{P}_{p,q}(2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n))^{2^{\kappa_n}}\mathbf{r}$, *where* $\mathbf{P}_{p,q}(2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n)$ *is the* (p, q)*-Pad é approximation of* $e^{2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n}$, κ_n *is the smallest integer number such that* $\left\|2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$, *and the matrices* $\widetilde{\mathbf{D}}_n$, $\mathbf{L}$, $\mathbf{r}$ *are defined as above. Further, let* $\widetilde{\boldsymbol{\rho}}$ *be the numerical solution of the ODE (35)–(36) given by an order* γ *explicit Runge–Kutta scheme. Then, under the assumptions of Theorem 7, the global error of the LLRK scheme*

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\boldsymbol{\phi}}(t_n, \widetilde{\mathbf{y}}_n; h_n) + \widetilde{\boldsymbol{\rho}}(t_n, \widetilde{\mathbf{y}}_n; h_n) \tag{42}$$

for the integration of the ODE (1)–(2) is given by

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

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

Proof. Let $\mathcal{K} \subset \mathcal{D}$ be a compact set. Since $\mathbf{P}_{p,q}$ is an analytical function on the unit circle, it is also a Lipschitz function on this region. This and condition $\left\|2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$ for all $t_n \in (t)_h$ imply that there exists a positive constant L such that

$$\left\|\widetilde{\boldsymbol{\phi}}\left(t_n, \boldsymbol{\xi}_2; h_n\right) - \widetilde{\boldsymbol{\phi}}\left(t_n, \boldsymbol{\xi}_1; h_n\right)\right\| \leq L\left\|\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1\right\|$$

for all $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \in \mathcal{K}$ and $t_n \in (t)_h$. On the other hand, Lemma 4.1 in [53] implies that there exists a positive constant M such that

$$\left\|\mathbf{z}(t_{n+1}) - \mathbf{z}(t_n) - \widetilde{\boldsymbol{\phi}}\left(t_n, \mathbf{z}(t_n); h_n\right)\right\| \leq Mh^{p+q+1}$$

for all $t_n \in (t)_h$, where $\mathbf{z}$ is the solution of the linear ODE (33)–(34).

In addition, since $\widetilde{\boldsymbol{\rho}}$ is an order γ approximation to the solution of (35)–(36) that satisfies the condition (16), the hypotheses of Theorem 15 hold, which completes the proof. □

The next theorem presents a way to define a class of A-stable LLRK schemes on the basis of Padé approximations to matrix exponentials.

Theorem 17. *LLRK schemes of the form (42) 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. Consider the scalar test equation

$$dx(t) = \lambda x(t)\, dt,$$

where λ is a complex number with non-positive real part.

An LLRK scheme of the form (42) applied to this autonomous equation results in the recurrence

$$\begin{aligned}\widetilde{y}_{n+1} &= \widetilde{y}_n + \widetilde{\boldsymbol{\phi}}\left(t_n, \widetilde{y}_n; h_n\right) \\ &= \widetilde{y}_n + \mathbf{L}\left(\mathbf{P}_{p,q}(\mathbf{M})\right)^{2^{\kappa_n}}\mathbf{r},\end{aligned} \tag{43}$$

where $\mathbf{M} = 2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n$ and

$$\widetilde{\mathbf{D}}_n = \begin{bmatrix}\lambda & \lambda\widetilde{y}_n \\ 0 & 0\end{bmatrix}.$$

Here,

$$\mathbf{P}_{p,q}(z) = \frac{\mathbf{N}_{p,q}(z)}{\mathbf{D}_{p,q}(z)}$$

denotes the (p, q)-Padé approximation to e^z, where

$$\mathbf{N}_{p,q}(z) = 1 + \frac{p}{q+p}z + \frac{p(p-1)}{(q+p)(q+p-1)}\frac{z^2}{2!} + \cdots + \frac{p(p-1)\ldots 1}{(q+p)\ldots(q+1)}\frac{z^p}{p!},$$

and $\mathbf{D}_{p,q}(z) = \mathbf{N}_{q,p}(-z)$.

Since

$$(\mathbf{M})^j = \begin{bmatrix}\left(2^{-\kappa_n}h_n\lambda\right)^j & \left(2^{-\kappa_n}h_n\lambda\right)^j\widetilde{y}_n \\ 0 & 0\end{bmatrix},$$

it can be shown that

$$\mathbf{N}_{p,q}(\mathbf{M}) = \begin{bmatrix}\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right) & \left(\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right) - 1\right)\widetilde{y}_n \\ 0 & 1\end{bmatrix}.$$

Likewise,

$$\mathbf{D}_{p,q}(\mathbf{M}) = \begin{bmatrix}\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right) & \left(\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right) - 1\right)\widetilde{y}_n \\ 0 & 1\end{bmatrix}.$$

Hence,

$$\mathbf{D}_{p,q}^{-1}(\mathbf{M}) = \begin{bmatrix}\left(\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)\right)^{-1} & -\dfrac{\left(\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right) - 1\right)}{\left(\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)\right)}\widetilde{y}_n \\ 0 & 1\end{bmatrix}.$$

Therefore,

$$\mathbf{P}_{p,q}(\mathbf{M}) = \mathbf{N}_{p,q}(\mathbf{M})\mathbf{D}_{p,q}^{-1}(\mathbf{M}) = \begin{bmatrix} \dfrac{\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}{\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)} & \left(\dfrac{\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}{\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)} - 1\right)\widetilde{y}_n \\ 0 & 1 \end{bmatrix},$$

and so

$$\left(\mathbf{P}_{p,q}(\mathbf{M})\right)^{2^{\kappa_n}} = \begin{bmatrix} \left(\dfrac{\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}{\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}\right)^{2^{\kappa_n}} & \left(\left(\dfrac{\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}{\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}\right)^{2^{\kappa_n}} - 1\right)\widetilde{y}_n \\ 0 & 1 \end{bmatrix}.$$

By substituting the above expression in (43) it is obtained that

$$\widetilde{y}_{n+1} = R(\lambda)\widetilde{y}_n,$$

where

$$R(\lambda) = \left(\frac{\mathbf{N}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}{\mathbf{D}_{p,q}\left(2^{-\kappa_n}h_n\lambda\right)}\right)^{2^{\kappa_n}}.$$

Since $\Re(2^{-\kappa_n}h_n\lambda) \leq 0$, Theorem 353A, pp. 238 in [54] implies that $|R(\lambda)| \leq 1$ for $p \leq q \leq p+2$. That is, for these values of p and q the LLRK scheme (42) is A-stable. The proof concludes by noting that, for $q = p+1$ or $q = p+2$, $R(z) = 0$ when $z \to \infty$. □

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 the LLRK scheme (42) 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 *four order classical Runge–Kutta scheme* (see, e.g., pp. 180 in [54]) with coefficients $c = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$. This yields the following efficient order 4 LLRK scheme

$$\widetilde{\mathbf{y}}_{n+1} = \widetilde{\mathbf{y}}_n + \widetilde{\boldsymbol{\phi}}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right) + \widetilde{\boldsymbol{\rho}}\left(t_n, \widetilde{\mathbf{y}}_n; h_n\right), \tag{44}$$

where

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

with

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

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

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

and κ_n is the smallest integer number such that $\left\|2^{-\kappa_n}\widetilde{\mathbf{D}}_n h_n\right\| \leq \frac{1}{2}$.

Note that the dynamical properties of an order γ LLRK discretization, as stated in Section 4, are inherited by its numerical implementations if the approximation to the map $\boldsymbol{\phi} + \boldsymbol{\rho}$ is $o(h^{\gamma-1})$ and smooth enough (i.e., of class C^γ). In particular, these conditions are satisfied by the implementations just introduced, namely, those given by (42). This provides theoretical support to the simulation study presented in [36,44], which reports satisfactory dynamical behavior of LLRK schemes in the neighborhood of invariant sets of ODEs.

Finally note that, as an example, this section has focused on a specific kind of LLRK scheme, namely, the A-stable scheme (44) that combines the A-stable Padé algorithm to compute the $\boldsymbol{\varphi}_\gamma$ with the 4 order classical Runge–Kutta scheme to compute the solution of the auxiliary equation (35)–(36). However, because of the flexibility in the numerical implementation of the LLRK methods, specific schemes can be designed for certain classes of ODEs, i.e., LLRK schemes based on L-stable Padé algorithm and Rosenbrock schemes for stiff equations; or LLRK schemes based on the Krylov algorithm in case of high dimensional ODEs, etc. For all of them the results of this section also apply.

Table 1
Values of ξ_h and r_h computed by the LL2, RK45 and LLRK4 schemes in the integration of the system (45)–(46), for different values of h.

Step-size	Scheme					
	LL2		RK45		LLRK4	
h	ξ_h	r_h	ξ_h	r_h	ξ_h	r_h
2^{-1}	0.71911		0.70377		0.56615	
2^{-2}	0.69688	1.931	0.53673	3.00	0.58441	5.142
2^{-3}	0.61727	2.190	0.59859	4.18	0.59032	2.384
2^{-4}	0.59639	2.145	0.59088	7.23	0.59049	3.354
2^{-5}	0.59182	2.056	0.590458	6.93	0.590459	3.901
2^{-6}	0.59079	2.027	0.59045593	6.39	0.5904561	3.973
2^{-7}	0.59054	2.014	0.5904559168	5.98	0.590455917	3.989
2^{-8}	0.59048		0.5904559165		0.590455916	

6. Numerical simulations

In this section, the performance of the LLRK4 scheme (44) is illustrated by means of numerical simulations. To do so, a variety of ODEs were selected. All simulations were carried out in Matlab2007b, and the Matlab function "expm" was used in all computations involving exponential matrices.

The first example is taken from [49] to illustrate the dynamical behavior of the LLRK4 scheme in the neighborhood of hyperbolic stationary points. For comparative purposes, the order 2 Local Linearization scheme of [33], and a straightforward non-adaptive implementation of the order 5 Runge–Kutta formula of Dormand and Prince [55] (used in Matlab2007b) are considered too. They will be denoted by LL2 and RK45, respectively.

Example 1.

$$\frac{d\mathbf{x}_1}{dt} = -2\mathbf{x}_1 + \mathbf{x}_2 + 1 - \mu f\left(\mathbf{x}_1, \lambda\right), \tag{45}$$

$$\frac{d\mathbf{x}_2}{dt} = \mathbf{x}_1 - 2\mathbf{x}_2 + 1 - \mu f\left(\mathbf{x}_2, \lambda\right), \tag{46}$$

where $f\left(u, \lambda\right) = u\left(1 + u + \lambda u^2\right)^{-1}$.

For $\mu = 15$, $\lambda = 57$, this system has two stable stationary points and one unstable stationary point in the region $0 \leq x_1, x_2 \leq 1$. There is a nontrivial stable manifold for the unstable point which separates the basins of attraction for the two stable points.

Fig. 1(a) presents the phase portrait obtained by the LLRK4 scheme with a very small step-size $\left(h = 2^{-13}\right)$, which can be regarded as the exact solution for comparative purposes. The stable manifold M_s of the unstable point was found by bisection. Fig. 1(b), (c) and (d) show the phase portraits obtained, respectively, by the LL2, the RK45 and the LLRK 4 schemes with step-size $h = 2^{-2}$ fixed. It can be observed that the RK45 discretization fails to reproduce correctly the phase portrait of the underlying system near one of the point attractors. On the contrary, the exact phase portrait is adequately approximated near both point attractors by the LL2 and LLRK4 schemes, the latter being much more accurate. Other significant differences in the integration of this equation appear near to the stable manifold M_s. Changes in the intersection point $(0, \xi_h)$ of the approximate stable manifold M_s^h with the x_2-axis are shown in Table 1 for the considered schemes. The values of ξ_h were calculated by a bisection method and the estimated order of convergence was calculated as

$$r_h = \frac{1}{\ln 2} \ln\left(\frac{\xi_h - \xi_{h/2}}{\xi_{h/2} - \xi_{h/4}}\right).$$

For $h < 2^{-4}$, the reported values of r_h for the schemes LL2 and LLRK 4 are in agreement with the expected asymptotic behavior $\xi_h = \xi_0 + Ch^r + O(h^{r+1})$ stated by Theorem 11 and Theorem 3 in [33], respectively, but not with that stated by Theorem 3.1 in [49] for the RK45, i.e., $r_h \approx 5$. This means that the LL2 and LLRK4 schemes provide better approximations to the stable and unstable manifolds on bigger neighborhoods of the equilibrium points, which is obviously a favorable result for them. These results show too that the LLRK4 scheme preserves much better the basins of attraction of the ODE (45)–(46) than the RK45 and LL2 schemes.

In what follows, we compare the accuracy of the LLRK4 scheme with those of the LL2 scheme, and the Matlab2007b codes ode45 and ode15*s* in the integration of a variety of ODEs. We recall that the code ode45 is a variable step-size implementation of the explicit Runge–Kutta (4, 5) pair of Dormand and Prince [55], which is considered for many authors the most recommendable scheme to apply as a first try for most problems. On the other hand, the code ode15*s* is a quasi-constant step-size implementation in terms of backward differences of the Klopfenstein–Shampine family of numerical differentiation formulas of orders 1–5, which is designed for stiff problems when the ode45 fails to provide the desired result [43].

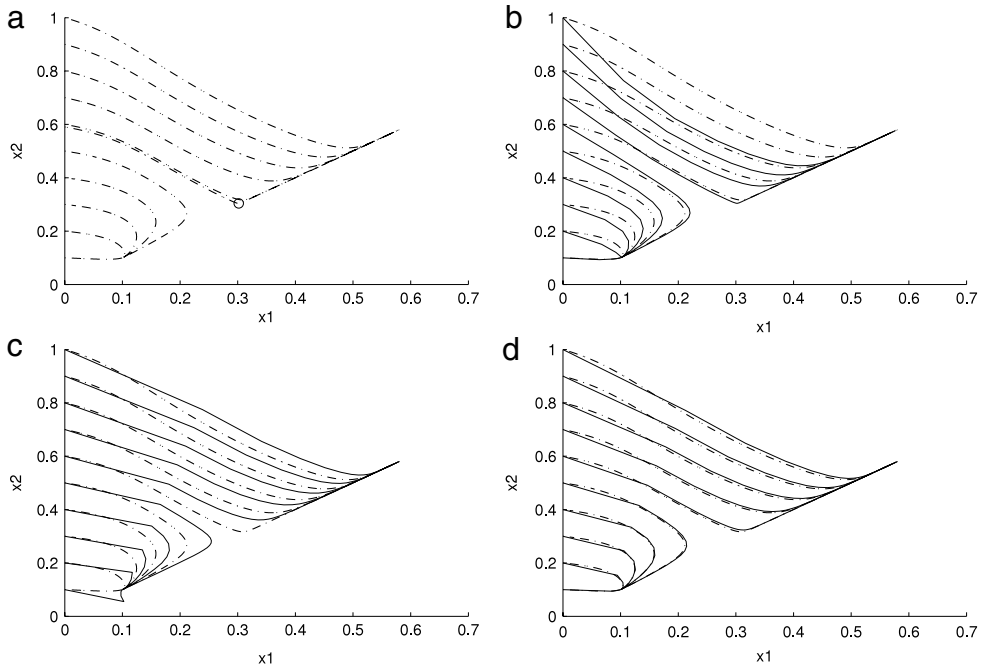

Fig. 1. Phase portrait of the system (45)–(46) computed with fixed step-size h by (a) LLRK4 scheme with $h = 10^{-13}$ (dashed line). The unstable point is pointed out with "o"; (b) LL2 scheme, with $h = 2^{-2}$; (c) RK45 scheme, with $h = 2^{-2}$; and (d) LLRK4 scheme, with $h = 2^{-2}$. In all cases the solid lines represent the solution computed with $h = 2^{-2}$.

Table 2
Accuracy of the LL2, LLRK4, ode45 and ode15*s* schemes in the integration of Examples 2–7. With the symbol * is denoted the Matlab code used to set the time partition $(t)_h$ in each example. NS denotes the number of steps required for each scheme to compute the solution on $(t)_h$.

Example	Scheme	Relative tolerance	Absolute tolerance	NS	Relative error
2 : Periodic linear	*ode*15*s**	10^{-3}	10^{-6}	334	0.19
	*ode*45	5×10^{-6}	5×10^{-9}	340	8.2×10^{-5}
	*LL*2	–	–	334	1.6×10^{-12}
	*LLRK*4	–	–	334	1.6×10^{-12}
3 : Periodic linear plus nonlinear part	*ode*15*s**	10^{-3}	10^{-6}	287	0.30
	*ode*45	6×10^{-6}	6×10^{-9}	289	1.3×10^{-4}
	*LL*2	–	–	287	3.1×10^{-2}
	*LLRK*4	–	–	287	1.1×10^{-5}
4 : Stiff linear	*ode*15*s**	10^{-3}	10^{-6}	66	6.7×10^{-2}
	*ode*45	5×10^{-4}	5×10^{-7}	66	5.3×10^{-3}
	*LL*2	–	–	66	1.8×10^{-10}
	*LLRK*4	–	–	66	1.8×10^{-10}
5 : Stiff linear plus nonlinear part	*ode*15*s**	10^{-2}	10^{-4}	49	0.31
	*ode*45	10^{-1}	10^{-3}	104	0.37
	*LL*2	–	–	49	0.43
	*LLRK*4	–	–	49	4.3×10^{-5}
6 : Nonlinear (no stiff)	*ode*15*s*	10^{-2}	10^{-5}	103	0.35
	*ode*45*	10^{-3}	10^{-6}	47	0.08
	*LL*2	–	–	47	4.19
	*LLRK*4	–	–	47	0.25
7 : Nonlinear (moderate stiff)	*ode*15*s*	1.5×10^{-9}	1.5×10^{-12}	2281	1.2×10^{-3}
	*ode*45*	10^{-7}	10^{-10}	2285	1.6×10^{-3}
	*LL*2	–	–	2285	400
	*LLRK*4	–	–	2285	6.9×10^{-3}

In order to compare the (non-adaptive) LL schemes with the adaptive Matlab codes, the following procedure was carried out. First, one of the Matlab codes is used to compute the solution with fixed values of relative (RT) and absolute (AT) tolerance. Then, the resulting integration steps $(t)_h$ are set as input in the other schemes for obtaining solutions at the same integration steps. Second, the Matlab code ode15*s* is used to compute on $(t)_h$ a very accurate solution $\mathbf{z}$

with $RT = RA = 10^{-13}$. Third, the approximate solution $\mathbf{y}$ of the ODE is computed for each scheme on $(t)_h$, and the relative error

$$RE = \max_{i=1,\ldots,d;\, t_j \in (t)_h} \left| \frac{\mathbf{z}_i(t_j) - \mathbf{y}_i(t_j)}{\mathbf{z}_i(t_j)} \right|$$

is evaluated.

The following four examples are of the form

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{f}(\mathbf{x}), \tag{47}$$

where $\mathbf{A}$ is a square constant matrix, and $\mathbf{f}$ is a nonlinear function of $\mathbf{x}$. The vector field of the first two ones has Jacobians with eigenvalues on or near to the imaginary axis, which makes these oscillators difficult to be integrated by a number of conventional integrators [56,43]. The other two are also hard for conventional explicit schemes since they are examples of stiff equations [43]. Example 5 has an additional complexity for a number of integrators that do not update the Jacobians of the vector field at each integration step [43,57]: the Jacobian of the linear term has positive eigenvalues, which results in a problem for the integration in a neighborhood of the stable equilibrium point $\mathbf{x} = 1$.

Example 2. Periodic linear:

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}(\mathbf{x} + 2),$$

with

$$\mathbf{A} = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix},$$

$\mathbf{x}_1(t_0) = -2.5, \mathbf{x}_2(t_0) = -1.5$, and $[t_0, T] = [0, 4\pi]$.

Example 3. Periodic linear plus nonlinear part:

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}(\mathbf{x} + 2) + 0.1\mathbf{x}^2,$$

where the matrix $\mathbf{A}$ is defined as in the previous example, $\mathbf{x}(t_0) = 1$, and $[t_0, T] = [0, 4\pi]$.

Example 4. Stiff equation:

$$\frac{d\mathbf{x}}{dt} = -100\mathbf{H}(\boldsymbol{x} + \mathbf{1}),$$

where $\mathbf{H}$ is the 12-dimensional Hilbert matrix (with conditioned number 1.69×10^{16}), $\mathbf{x}_i(t_0) = 1$, and $[t_0, T] = [0, 1]$.

Example 5. Stiff linear plus nonlinear part:

$$\frac{d\mathbf{x}}{dt} = 100\mathbf{H}(\mathbf{x} - \mathbf{1}) + 100(\mathbf{x} - \mathbf{1})^2 - 60(\mathbf{x}^3 - \mathbf{1}),$$

where $\mathbf{H}$ is the 12-dimensional Hilbert matrix, $\mathbf{x}_i(t_0) = -0.5$, and $[t_0, T] = [0, 1]$.

The results of the integration of these equations for each scheme are shown in Table 2. For illustration, Fig. 2 shows the path of the variable $\mathbf{x}_1$ and its approximation $\mathbf{y}_1$ obtained by the LLRK4 scheme in the integration of these equations. Remarkably, in all the examples, the relative error of the solution obtained by the LLRK4 scheme is much lower that those of the LL2, ode45 and ode15*s* with the same or lower number of steps. These results are easily comprehensible for five reasons: (1) the dynamics of these equations strongly depend on the linear part of their vector fields; (2) the LL2 and LLRK4 schemes preserve the stability of the linear systems for all step-sizes, which is not so for conventional explicit integrators; (3) the LL2 and LLRK4 schemes are able to "exactly" (up to the precision of the floating-point arithmetic) integrate linear ODEs, which is a property not satisfied by conventional explicit and implicit schemes; (4) the LL2 and LLRK4 schemes update the exact Jacobian of the vector field at each integration step, which is not done by most of the conventional schemes; and (5) the LLRK4 has a higher order of convergence than the LL2 scheme. Further, note that although the LLRK4 scheme is not designed for the integration of stiff ODEs in general (because the auxiliary equation (35)–(36) might "inherit" the stiffness of the original one) it is clear that, by construction, it is suitable for equations with stiffness confined to the linear part. An example are the classes of stiff linear and semilinear equations represented in Examples 2 and 3. This is so, because at each integration step the stiff linear term is locally removed from the vector field of the auxiliary equation (35) and, in this way, the stiff linear part is well integrated by the (A-stable) LL scheme and the resulting non-stiff equation (35) can be well integrated by the explicit RK scheme.

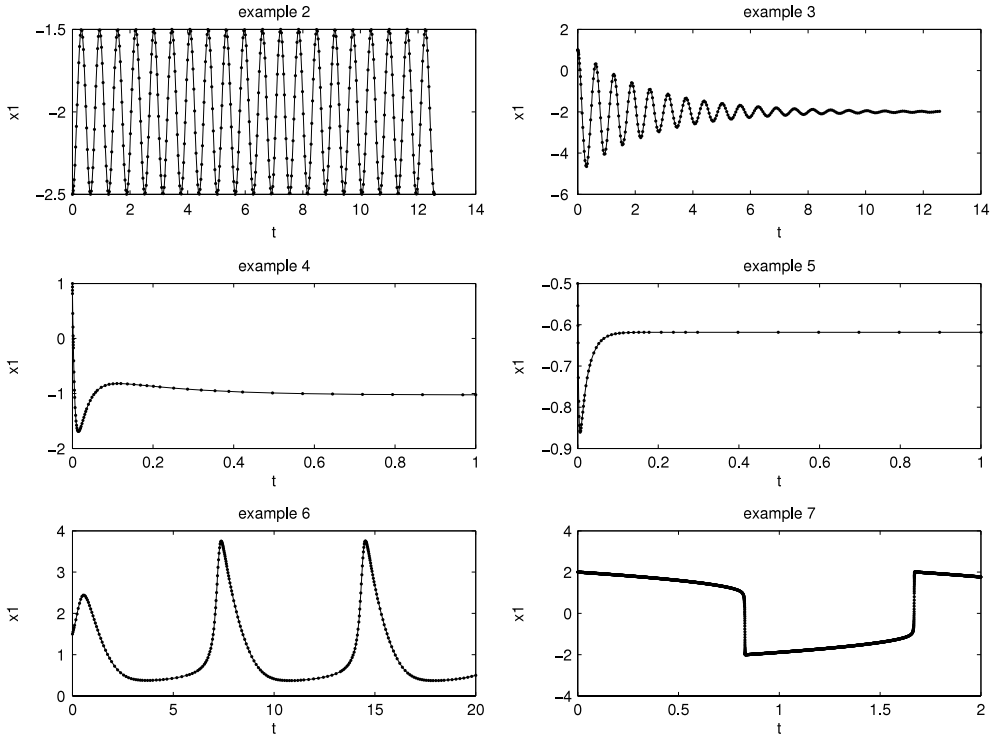

Fig. 2. Path of the variables $\mathbf{x}_1$ (solid line) and its approximation $\mathbf{y}_1$ (dots) obtained by the LLRK4 scheme in the integration of the ODEs of Examples 2–7. The time partition $(t)_h$ used in each case for $\mathbf{y}_1$ is specified in Table 2. The "exact" path of $\mathbf{x}_1$ is computed with the Matlab code ode15*s* with $RT = RA = 10^{-13}$ on a very thin partition.

The following two examples are well known nonlinear oscillators.

Example 6. Non-stiff nonlinear:

$$\frac{d\mathbf{x}_1}{dt} = 1 + \mathbf{x}_1^2\mathbf{x}_2 - 4\mathbf{x}_1,$$
$$\frac{d\mathbf{x}_2}{dt} = 3\mathbf{x}_1 - \mathbf{x}_1^2\mathbf{x}_2$$

where $\mathbf{x}_1(t_0) = 1.5$, $\mathbf{x}_2(t_0) = 3$, and $[t_0, T] = [0, 20]$. This equation, known as the Brusselator equation, is a typical test equation of non-stiff nonlinear problems (see, e.g., [48]).

Example 7. Mild-stiff nonlinear:

$$\frac{d\mathbf{x}_1}{dt} = \mathbf{x}_2,$$
$$\frac{d\mathbf{x}_2}{dt} = \varepsilon((1 - \mathbf{x}_2^2)\mathbf{x}_1 + \mathbf{x}_2),$$

where $\varepsilon = 10^3$, $\mathbf{x}_1(t_0) = 2$, $\mathbf{x}_2(t_0) = 0$, and $[t_0, T] = [0, 2]$. This equation, known as the Van der Pol equation, is a typical test equation of stiff nonlinear problems (see, e.g., [58]).

The results of the integration of the last two equations for each scheme are also shown in Table 2 and Fig. 2. For these equations, the relative error of the solutions obtained by the LLRK4 scheme is much lower that those of the LL2, but quite similar to those of the codes ode45 and ode15*s* (which have higher order of convergence). This indicates that the LLRK4 scheme is also appropriate for integrating non-stiff and mild-stiff nonlinear problems as well.

In summary, results of Table 2 clearly indicate that the non-adaptive implementation of the LLRK4 scheme provides similar or much better accuracy than the Matlab codes with equal or lower numbers of steps in the integration of a variety of equations. This suggests that adaptive implementations of the LLRK discretizations might achieve similar accuracy than the Matlab codes with lower or much lower numbers of steps, a subject that has already been studied in [59,60].

Finally, we want to point out that equations of the type (47) frequently arise from the discretization of nonlinear partial differential equations. In such a case, mild or high dimensional ODEs of that form are obtained and, as it is obvious, LLRK

schemes like (44) based on Padé approximations are not appropriate. Nevertheless, because of the flexibility of the high order Local Linearization approach described in Section 2, feasible high order LL schemes can be designed for this purpose too. For instance, by taking into account that

$$\boldsymbol{\phi}\left(t_n, \mathbf{y}_n; \frac{h_n}{2}\right) = \boldsymbol{\varphi}\left(\frac{h_n}{2}\mathbf{f}_{\mathbf{x}}(\mathbf{y}_n)\right)\mathbf{f}(\mathbf{y}_n),$$

where $\boldsymbol{\varphi}(z) = (e^z - 1)/z$, the LLRK4 scheme (44) can be easily modified to define an order 4 LLRK scheme for high dimensional ODEs. Indeed, such a scheme can be defined by the same expression (44), but replacing the formulas of $\widetilde{\boldsymbol{\phi}}(t_n, \widetilde{\mathbf{y}}_n; \frac{h_n}{2})$ and $\widetilde{\boldsymbol{\phi}}(t_n, \widetilde{\mathbf{y}}_n; h_n)$ by

$$\widetilde{\boldsymbol{\phi}}\left(t_n, \widetilde{\mathbf{y}}_n; \frac{h_n}{2}\right) = \widetilde{\boldsymbol{\varphi}}\left(\frac{h_n}{2}\mathbf{f}_{\mathbf{x}}(\widetilde{\mathbf{y}}_n)\right)\mathbf{f}(\widetilde{\mathbf{y}}_n)$$

and

$$\widetilde{\boldsymbol{\phi}}(t_n, \widetilde{\mathbf{y}}_n; h_n) = \left(\frac{h_n}{4}\mathbf{f}_{\mathbf{x}}(\widetilde{\mathbf{y}}_n)\widetilde{\boldsymbol{\varphi}}\left(\frac{h_n}{2}\mathbf{f}_{\mathbf{x}}(\widetilde{\mathbf{y}}_n)\right) + \mathbf{I}\right)\widetilde{\boldsymbol{\phi}}\left(t_n, \widetilde{\mathbf{y}}_n; \frac{h_n}{2}\right),$$

respectively, where $\widetilde{\boldsymbol{\varphi}}$ denotes the approximation to $\boldsymbol{\varphi}$ provided by the Krylov subspace method (see, e.g., [16]). Then, a comparison with exponential-type integrators designed for high dimensional equations of the form (47) can be carried out, but this subject is outside the scope of this paper.

7. Conclusions

In summary, this paper has shown the following: (1) the LLRK approach defines a general class of high order A-stable explicit integrators; (2) in contrast with other A-stable explicit methods (such as Rosenbrock or the Exponential integrators), the RK coefficients involved in the LLRK integrators are not constrained by any stability condition and they just need to satisfy the usual, well-known order conditions of RK schemes, which makes the LLRK approach more flexible and simple; (3) LLRK integrators have a number of convenient dynamical properties as the linearization preserving and the conservation of the exact solution dynamics around hyperbolic equilibrium points and periodic orbits; (4) unlike the majority of the previous published works on exponential integrators, the above mentioned convergence, stability and dynamical properties are studied not only for the discretizations but also for the numerical schemes that implement them in practice; (5) because of the flexibility in the numerical implementation of the LLRK methods, specific-purpose schemes can be designed for certain classes of ODEs, e.g., for stiff equations, high dimensional systems of equations, etc.; and (6) the order 4 LLRK formula considered in this paper provides similar or much better accuracy than the order 5 Matlab codes with equal or lower numbers of steps in the integration of a variety of equations, as well as much better reproduction of the dynamics of the underlying equation near stationary hyperbolic points.

Finally, it is worth pointing out that theoretical properties of the LLRK methods studied here strongly support the results of the numerical experiments carried out by the authors in previous works [36,44], in which the performance of other LLRK schemes is compared with that of existing explicit and implicit schemes.

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References

[1] J.H.E. Cartwright, O. Piro, The dynamics of Runge–Kutta methods, Int. J. Bifurcation and Chaos 2 (1992) 427–449.
[2] I. Stewart, Numerical methods: Warning-handle with care!, Nature 355 (1992) 16–17.
[3] M. Hochbruck, C. Lubich, On Krylov subspace approximations to the matrix exponential operator, SIAM Numer. Anal. 34 (1997) 1911–1925.
[4] R.B. Sidje, EXPOKIT: software package for computing matrix exponentials, AMC Trans. Math. Software 24 (1998) 130–156.
[5] L. Dieci, A. Papini, Padé approximations for the exponential of a block triangular matrix, Linear Algebra Appl. 308 (2000) 183–202.
[6] E. Celledoni, A. Iserles, Methods for the approximation of matrix exponentials in a Lie-algebraic setting, IMA J. Numer. Anal. 21 (2001) 463–488.
[7] N.J. Higham, The scaling and squaring method for the matrix exponential revisited, SIAM J. Matrix Anal. Appl. 26 (2005) 1179–1193.
[8] F. Carbonell, J.C. Jimenez, L.M. Pedroso, Computing multiple integrals involving matrix exponentials, J. Comput. Appl. Math. 213 (2008) 300–305.
[9] C.F Van Loan, Computing integrals involving the matrix exponential, IEEE Trans. Automat. Control AC-23 (1978) 395–404.
[10] W. Liniger, R.A. Willoughby, Efficient integration methods for stiff systems of ordinary differential equations, SIAM J. Numer. Anal. 7 (1970) 47–66.
[11] J. Carroll, A matricial exponentially fitted scheme for the numerical solution of stiff initial-value problems, Comput. Math. Appl. 26 (1993) 57–64.
[12] D. Voss, A fifth-order exponentially fitted formula, SIAM J. Numer. Anal. 25 (1988) 670–678.
[13] J.R. Cash, On the exponential fitting of composite, multiderivative linear multistep methods, SIAM J. Numer. Anal. 18 (1981) 808–821.
[14] A. Iserles, A-stability and dominating pairs, Math. Comp. 32 (1978) 19–33.
[15] J.D. Lawson, Generalized Runge–Kutta processes for stable systems with large Lipschitz constants, SIAM J. Numer. Anal. 4 (1967) 372–380.
[16] M. Hochbruck, C. Lubich, H. Selhofer, Exponential integrators for large systems of differential equations, SIAM J. Sci. Comput. 19 (1998) 1552–1574.
[17] M. Hochbruck, A. Ostermann, Exponential integrators, Acta Numer. 19 (2010) 209–286.
[18] S.M. Cox, P.C. Matthews, Exponential time differencing for stiff systems, J. Comput. Phys. 176 (2002) 430–455.
[19] A. Kassam, L.N. Trefethen, Fourth-order time stepping for stiff PDEs, SIAM J. Scient. Comput. 26 (2005) 1214–1233.
[20] A. Iserles, A. Marthinsen, S.P. Nørset, On the implementation of the method of Magnus series for linear differential equations, BIT 39 (1999) 281–304.

[21] S. Blanes, F. Casas, J. Ros, Improved high order integrators based on the Magnus expansion, BIT 40 (2000) 434–450.
[22] A. Zanna, Collocation and relaxed collocation for the FER and the Magnus expansions, SIAM J. Numer. Anal. 36 (1999) 1145–1182.
[23] A. Iserles, Solving linear ordinary differential equations by exponentials of iterated commutators, Numer. Math. 45 (1984) 183–199.
[24] M. Hochbruck, A. Ostermann, Explicit exponential Runge–Kutta methods for semilinear parabolic problems, SIAM J. Numer. Anal. 43 (2005) 1069–1090.
[25] M. Hochbruck, A. Ostermann, Exponential Runge–Kutta methods for parabolic problems, Appl. Numer. Math. 53 (2005) 323–339.
[26] S.P. Norsett, An A-stable modification of the Adams–Bashforth method, in: Conference on the Numerical Solution of Differential Equations, Dunde, Scotland, Springer, Berlin, 1969, pp. 214–219.
[27] R.K. Jain, Some A-stable methods for stiff ordinary differential equations, Math. Comp. 26 (1972) 71–77.
[28] A. Iserles, Quadrature methods for stiff ordinary differential systems, Math. Comp. 36 (1981) 171–182.
[29] B.V. Pavlov, O.E. Rodionova, The method of local linearization in the numerical solution of stiff systems of ordinary differential equations, U.S.S.R. Comput. Maths. Math. Phys. 27 (1987) 30–38.
[30] R.A. Friesner, L.S. Tuckerman, B.C. Dornblaser, T.V. Russo, A method for exponential propagation of large systems of stiff nonlinear differential equations, J. Sci. Comput. 4 (1989) 327–354.
[31] D.A. Pope, An exponential method of numerical integration of ordinary differential equations, Comm. AGM 6 (1963) 491–493.
[32] J.I. Ramos, C.M. Garcia-Lopez, Piecewise-linearized methods for initial-value problems, Appl. Math. Comput. 82 (1997) 273–302.
[33] J.C. Jimenez, R. Biscay, C. Mora, L.M. Rodriguez, Dynamic properties of the Local Linearization method for initial-value problems, Appl. Math. Comput. 126 (2002) 63–81.
[34] J.C. Jimenez, F. Carbonell, Rate of convergence of local linearization schemes for initial-value problems, Appl. Math. Comput. 171 (2005) 1282–1295.
[35] E.J. Carr, T.J. Moroney, I.W. Turner, Efficient simulation of unsaturated flow using exponential time integration, Appl. Math. Comput. 217 (2011) 6587–6596.
[36] H. de la Cruz, R.J. Biscay, F. Carbonell, J.C. Jimenez, T. Ozaki, Local linearization—Runge Kutta (LLRK) methods for solving ordinary differential equations, in: Lecture Note in Computer Sciences, vol. 3991, Springer-Verlag, 2006, pp. 132–139.
[37] H. de la Cruz, R.J. Biscay, F. Carbonell, T. Ozaki, J.C. Jimenez, A higher order Local Linearization method for solving ordinary differential equations, Appl. Math. Comput. 185 (2007) 197–212.
[38] J.C. Jimenez, Local Linearization methods for the numerical integration of ordinary differential equations: An overview. Preprint 2009035, International Center for Theoretical Physics, Trieste, June 2009. http://users.ictp.it/~pub_off/preprints-sources/2009/IC2009035P.pdf.
[39] M. Hochbruck, A. Ostermann, Exponential multistep methods of Adams-type, BIT 51 (2011) 889–908.
[40] R.I. McLachlan, G.R.W. Quispel, Splitting methods, Acta Numer. 11 (2002) 341–434.
[41] U.M. Ascher, S.J. Ruth, R.J. Spiteri, Implicit–explicit Runge–Kutta methods for time-dependent partial differential equations, Appl. Numer. Math. 25 (1997) 151–167.
[42] T.D. Bui, Some A-stable and L-stable methods for the numerical integration of stiff ordinary differential equations, J. ACM 26 (1979) 483–493.
[43] L.F. Shampine, M.W. Reichelt, The Matlab ODE suite, SIAM J. Scient. Comput. 18 (1997) 11–22.
[44] H. de la Cruz, High order local linearization methods for the integration of ordinary and stochastic differential equations, In: Ph. D. Dissertation, 2007.
[45] J.C. Jimenez, R.J Biscay, Approximation of continuous time stochastic processes by the local linearization method revisited, Stoch. Anal. Appl. 20 (2002) 105–121.
[46] R.I. McLachlan, G.R.W Quispel, P.S.P. Tse, Linearization-preserving self-adjoint and symplectic integrators, BIT 49 (2009) 177–197.
[47] L. Perko, Differential Equations and Dynamical Systems, Springer, New York, 2001.
[48] E. Hairer, S.P. Norsett, G. Wanner, Solving Ordinary Differential Equations I, second ed., Springer-Verlag, Berlin, 1993.
[49] W.J. Beyn, On the numerical approximation of phase portraits near stationary points, SIAM J. Numer. Anal. 24 (1987) 1095–1113.
[50] W.J. Beyn, On invariant closed curves for one-step methods, Numer. Math. 51 (1987) 103–122.
[51] G.H. Golub, C.F. Van Loan, Matrix Computations, second ed., The Johns Hopkins University Press, 1989.
[52] J.C. Jimenez, A simple algebraic expression to evaluate the local linearization schemes for stochastic differential equations, Appl. Math. Lett. 15 (2002) 775–780.
[53] J.C. Jimenez, H. de la Cruz, Convergence rate of strong Local Linearization schemes for stochastic differential equations with additive noise, BIT 52 (2012) 357–382.
[54] J.C. Butcher, Numerical Methods for Ordinary Differential Equations, second ed., John Wiley, 2008.
[55] J.R. Dormand, P.J. Prince, A family of embedded Runge–Kutta formulae, J. Comput. Appl. Math. 6 (1980) 19–26.
[56] P.W. Gaffney, A performance evaluation of some FORTRAN subroutines for the solution of stiff oscillatory ordinary differential equations, ACM Trans. Math. Software 10 (1984) 58–72.
[57] M. Hochbruck, A. Ostermann, J. Schweitzer, Exponential Rosenbrock type methods, SIAM J. Numer. Anal. 47 (2009) 786–803.
[58] E. Hairer, G. Wanner, Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems, third ed., Springer-Verlag, Berlin, 1996.
[59] A. Sotolongo, Study of some adaptive Local Linearization codes for ODEs. B.S. Dissertation, Havana University, July 2011.
[60] J.C. Jimenez, A. Sotolongo, J.M. Sanchez-Bornot, Locally Linearized Runge–Kutta method of Dormand and Prince, Res. Memo. No. 1152, The Institute of Statistical Mathematics, Tokyo, arXiv:1209.1415 [math.NA].