

Locally Linearized Runge Kutta method of Dormand and Prince

J.C. Jimenez^{a,b}, A. Sotolongo^c, J.M. Sanchez-Bornot^d

^a*Instituto de Cibernética, Matemática y Física, La Habana, Cuba. e-mail: jcarlos@icimaf.cu*

^b*The Institute of Statistical Mathematics, Tokyo, Japan*

^c*Universidad de la Habana, La Habana, Cuba. e-mail: alina.sotolongo@yahoo.com*

^d*Centro de Neurociencias de Cuba, La Habana, Cuba. e-mail: bornot@gmail.com*

Abstract

In this paper, the effect that produces the local linearization of the embedded Runge-Kutta formulas of Dormand and Prince for initial value problems is studied. For this, embedded Locally Linearized Runge-Kutta formulas are defined and their performance is analyzed by means of exhaustive numerical simulations. For a variety of well-known physical equations with different dynamics, the simulation results show that the locally linearized formulas exhibit significant higher accuracy than the original ones, which implies a substantial reduction of the number of time steps and, consequently, a sensitive reduction of the overall computation cost of their adaptive implementation.

Keywords: Dynamical Systems; Differential equation; Local Linearization; Runge-Kutta; Numerical integrator

1. Introduction

It is well known (see, e.g., [3, 25, 21]) that conventional numerical schemes such as Runge-Kutta, Adams-Bashforth, predictor-corrector and others produce misleading dynamics when integrating Ordinary Differential Equations (ODEs). Typical problems are, for instance, the convergence to spurious steady states, changes in the basis of attraction, appearance of spurious bifurcations, etc. This might yield serious mistakes in the interpretation and analysis of the processes under consideration in practical control engineering or in applied sciences. The essence of such difficulties is that the dynamic of the numerical schemes (considered as discrete dynamical systems) is far richer than that of its continuous counterparts. Contrary to the popular belief, drawbacks of this type may no be solved

by reducing the stepsize of the numerical method. Therefore, it is highly desirable the development of numerical integrators that preserve, as much as possible, the dynamical properties of the underlying dynamical system for all step sizes or relative big ones. In this direction, some modest advances has 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. An example of such integrators are the High Order Local Linearization (HOLL) methods based on Runge-Kutta schemes [4, 5, 13].

HOLL integrators are obtained by splitting, at each time step, the solution of the original ODE in two parts: the solution of a linear ODE plus the solution of an auxiliary ODE. The linear equation is solved by a Local Linearization (LL) scheme [14, 15] in such a way that A-stability is ensured, whereas the solution of the auxiliary one can be approximated by any conventional numerical integrator, preferably a high order explicit scheme. Originally, HOLL methods were introduced as a flexible approach for increasing the order of convergence of the order-2 LL method but, in addition, they can be thought as a strategy for constructing high order A-stable explicit schemes based on conventional explicit integrators. For this reason, if we focus on the conventional integrator involved in a particular HOLL scheme, then it is natural to say that the first one has been locally linearized. In this way, if a Runge Kutta scheme is used to approximate the above mentioned auxiliary ODE, the resulting HOLL scheme are indistinctly called Local Linearization - Runge Kutta (LLRK) scheme or Locally Linearized Runge Kutta (LLRK) scheme.

In [5], general results on the convergence, stability and dynamical properties of the Locally Linearized Runge Kutta method were studied. Specifically, it was demonstrated that: 1) the LLRK approach defines a general class of high order A-stable explicit integrators that preserve the convergence rate of the involved (not A-stable) explicit RK schemes; 2) in contrast with others 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 such as the linearization preserving and the conservation of the exact solution dynamics around hyperbolic equilibrium points and periodic orbits; and 4) because of the flexibility in the numerical implementation of the LLRK discretizations, specific-purpose LLRK schemes can be designed for certain classes of ODEs, e.g., for moderate or large systems of equations. On the other hand, simulation studies carried out in

[4, 5, 22] have shown that, for a variety of test equations, LLRK schemes of order 3 and 4 preserve much better the stability and dynamical properties of the actual solutions than their corresponding conventional RK schemes.

However, the accuracy and computational efficiency of the Local Linearization methods have been much less considered up to now, being the dynamical properties of such schemes the focus of previous studies and the main reason for the development of these methods. The few available results are the following. On an identical time partition [5], the LLRK scheme based on the classical order-4 RK scheme displays better accuracy than the order-5 RK formula of Dormand & Prince [7] in the integration of a variety of ODEs. On different time partitions [22], similar results are obtained by an adaptive implementation of the mentioned LLRK scheme in comparison with the Matlab code ode45, which provides an adaptive implementation of the embedded RK formulas of Dormand & Prince. However, this is achieved at expense of additional evaluations of the vector field, and with larger overall computational time. With this respect, the main drawback of that adaptive LLRK scheme is the absence of a computationally efficient strategy based on embedded formulas.

The main purpose of this work is introducing an adaptive LLRK scheme based on the embedded RK formulas of Dormand & Prince and evaluating, with simulations, its accuracy and computational efficiency in order to study the effect that the local linearization produces on these known RK formulas. The Matlab code developed with this goal is, same as the Matlab code ode45, addressed to low dimensional non stiff initial value problems for medium to low accuracies.

The paper is organized as follows. In the Section 2, a basic introduction on the Local Linearization - Runge Kutta (LLRK) schemes is presented. In the Section 3, the embedded Locally Linearized Runge-Kutta formulas are defined, and an adaptive implementation of them is described. In the last two sections, the results of a variety of exhaustive numerical simulations with well-known test equations are presented and discussed respectively.

2. Notations and preliminaries

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

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

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

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

Let $(t)_h = \{t_n : n = 0, 1, \dots, N\}$ be a time discretization with maximum step-size h defined as a sequence of times that satisfy the conditions $t_0 < t_1 < \dots < t_N = T$ and $\sup_n(h_n) \leq h < 1$, where $h_n = t_{n+1} - t_n$ for $n = 0, \dots, N-1$.

For a given (t_n, \mathbf{y}_n) , let $\mathbf{v}_{n+1} = \mathbf{y}_n + \Lambda_1(t_n, \mathbf{y}_n; h_n)$ be an order- γ_1 approximation to solution of the linear ODE

$$\frac{d\mathbf{z}_1(t)}{dt} = \mathbf{B}_n \mathbf{z}_1(t) + \mathbf{b}_n(t), \quad t \in [t_n, t_{n+1}], \quad (3)$$

$$\mathbf{z}_1(t_n) = \mathbf{y}_n \quad (4)$$

at t_{n+1} , and let $\mathbf{w}_{n+1} = \Lambda_2^{y_n}(t_n, \mathbf{0}; h_n)$ be an order- γ_2 Runge-Kutta scheme approximating the solution of the nonlinear ODE

$$\frac{d\mathbf{z}_2(t)}{dt} = \mathbf{q}(t_n, \mathbf{y}_n; t, \mathbf{z}_2(t)), \quad t \in [t_n, t_{n+1}], \quad (5)$$

$$\mathbf{z}_2(t_n) = \mathbf{0} \quad (6)$$

at t_{n+1} , where $\mathbf{B}_n = \mathbf{f}_x(t_n, \mathbf{y}_n)$ is a $d \times d$ constant matrix, and

$$\mathbf{b}_n(t) = \mathbf{f}_t(t_n, \mathbf{y}_n)(t - t_n) + \mathbf{f}(t_n, \mathbf{y}_n) - \mathbf{B}_n \mathbf{y}_n$$

and

$$\begin{aligned} \mathbf{q}(t_n, \mathbf{y}_n; s, \xi) &= \mathbf{f}(s, \mathbf{y}_n + \Lambda_1(t_n, \mathbf{y}_n; s - t_n) + \xi) - \mathbf{f}_x(t_n, \mathbf{y}_n) \Lambda_1(t_n, \mathbf{y}_n; s - t_n) \\ &\quad - \mathbf{f}_t(t_n, \mathbf{y}_n)(s - t_n) - \mathbf{f}(t_n, \mathbf{y}_n) \end{aligned}$$

are d -dimensional vectors. Here, \mathbf{f}_x and \mathbf{f}_t denote the partial derivatives respect to \mathbf{x} and t , respectively. Note that the vector field of the equation (5) not only depends on the point (t_n, \mathbf{y}_n) but also of the numerical flow used to approximate $\mathbf{z}_1(t)$.

Definition 1. ([4, 13, 5]) A Local Linearization - Runge Kutta (LLRK) scheme for the ODE (1)-(2) is defined by the recursive expression

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Lambda_1(t_n, \mathbf{y}_n; h_n) + \Lambda_2^{y_n}(t_n, \mathbf{0}; h_n) \quad (7)$$

for all $t_n \in (t)_h$, starting with $\mathbf{y}_0 = \mathbf{x}_0$.

Local truncation error, rate of convergence and various dynamical properties of the general class of Local Linearization - Runge Kutta schemes (7) has been studied in [5].

According to the Definition 1, a variety of LLRK schemes can be derived. In previous works [4, 5], the Local Linearization scheme based on Padé approximations [14, 15] has been used to integrate the linear ODE (3)-(4), whereas the so called *four order classical* Runge-Kutta scheme [2] has been applied to integrate the nonlinear ODE (5)-(6). This yields the order-4 LLRK scheme

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{u}_4 + \frac{h_n}{6}(2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4), \quad (8)$$

where

$$\mathbf{u}_j = \mathbf{L}(\mathbf{P}_{6,6}(2^{-\kappa_j}\mathbf{D}_n c_j h_n))^{2^{\kappa_j}} \mathbf{r}$$

and

$$\mathbf{k}_j = \mathbf{f}(t_n + c_j h_n, \mathbf{y}_n + \mathbf{u}_j + c_j h_n \mathbf{k}_{j-1}) - \mathbf{f}(t_n, \mathbf{y}_n) - \mathbf{f}_x(t_n, \mathbf{y}_n) \mathbf{u}_j - \mathbf{f}_t(t_n, \mathbf{y}_n) c_j h_n,$$

with $\mathbf{k}_1 \equiv \mathbf{0}$ and $c = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$. Here, $\mathbf{P}_{p,q}(\cdot)$ denotes the (p, q) -Padé approximation for exponential matrices [18], and κ_j the smallest integer number such that $\|2^{-\kappa_j}\mathbf{D}_n c_j h_n\| \leq \frac{1}{2}$. The matrices \mathbf{D}_n , \mathbf{L} and \mathbf{r} are defined as

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

$\mathbf{L} = \begin{bmatrix} \mathbf{I}_d & \mathbf{0}_{d \times 2} \end{bmatrix}$ and $\mathbf{r}^\top = \begin{bmatrix} \mathbf{0}_{1 \times (d+1)} & 1 \end{bmatrix}$ for non-autonomous ODEs; and as

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

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

On an identical time partition [5], LLRK formula (8) displays better accuracy than the order-5 RK formula of Dormand & Prince in the integration of a variety of ODEs. On different time partitions [22], similar results are obtained by an adaptive implementation of LLRK formula (8) in comparison with the Matlab ode45 code, which provides an adaptive implementation of the embedded RK formulas of Dormand & Prince. However, this is achieved at expense of additional

evaluations of the vector field \mathbf{f} , and with larger overall computational time. This cost can be sensitively reduced by using the $(2, 2)$ -Padé approximations instead of the order $(6, 6)$ one used in formula (8), preserving the order of convergence and without significant loss of accuracy [22].

Local truncation error, rate of convergence, A-stability and various dynamical properties of the LLRK schemes based on Padé approximations has also been studied in [5].

For a precise comparison of the Local Linearization - Runge Kutta method with well-known integration methods such as Rosenbrock, Exponential Integrators, Splitting Methods and others, the interested reader might read [5] or [13].

3. Numerical scheme

3.1. Embedded Locally Linearized Runge-Kutta formulas

In view of the Definition 1, new integration formulas can be obtained as follows. Similarly to the LLRK scheme (8), the Local Linearization scheme based on Padé approximations [14, 15] is used for integrating the linear ODE (3)-(4) but, instead of the classical order-4 RK scheme, the embedded Runge-Kutta formulas of Dormand & Prince [7] is now applied to integrate the nonlinear ODE (5)-(6). This yields the embedded Locally Linearized Runge-Kutta formulas

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{u}_s + h_n \sum_{j=1}^s b_j \mathbf{k}_j \quad \text{and} \quad \hat{\mathbf{y}}_{n+1} = \mathbf{y}_n + \mathbf{u}_s + h_n \sum_{j=1}^s \hat{b}_j \mathbf{k}_j, \quad (9)$$

where $s = 7$ is the number of the stages,

$$\mathbf{u}_j = \mathbf{L}(\mathbf{P}_{p,q}(2^{-\kappa_j} \mathbf{D}_n c_j h_n))^{2^{\kappa_j}} \mathbf{r} \quad (10)$$

and

$$\mathbf{k}_j = \mathbf{f}(t_n + c_j h_n, \mathbf{y}_n + \mathbf{u}_j + h_n \sum_{i=1}^{s-1} a_{j,i} \mathbf{k}_i) - \mathbf{f}(t_n, \mathbf{y}_n) - \mathbf{f}_{\mathbf{x}}(t_n, \mathbf{y}_n) \mathbf{u}_j - \mathbf{f}_t(t_n, \mathbf{y}_n) c_j h_n,$$

with $\mathbf{k}_1 \equiv \mathbf{0}$ and Runge-Kutta coefficients $a_{j,i}$, b_j , \hat{b}_j and c_j defined in the Table 1. Here, $\mathbf{P}_{p,q}(\cdot)$ denotes the (p, q) -Padé approximation for exponential matrices with $p + q > 4$. The number κ_j and the matrices \mathbf{D}_n , \mathbf{L} and \mathbf{r} are defined as in the previous section.

0							
$\frac{1}{5}$	$\frac{1}{5}$						
$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$					
$\frac{4}{5}$	$\frac{44}{45}$	$-\frac{56}{15}$	$\frac{32}{9}$				
$\frac{8}{9}$	$\frac{19372}{6561}$	$-\frac{25360}{2187}$	$\frac{64448}{6561}$	$-\frac{212}{729}$			
1	$\frac{9017}{3168}$	$-\frac{355}{33}$	$\frac{46732}{5247}$	$\frac{49}{176}$	$-\frac{5103}{18656}$		
1	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	
y	$\frac{35}{384}$	0	$\frac{500}{1113}$	$\frac{125}{192}$	$-\frac{2187}{6784}$	$\frac{11}{84}$	0
\hat{y}	$\frac{5179}{57600}$	0	$\frac{7571}{16695}$	$\frac{393}{640}$	$-\frac{92097}{339200}$	$\frac{187}{2100}$	$\frac{1}{40}$

Table 1: Coefficients tableau for the embedded formulas.

The local truncation error, the rate of convergence and the A-stability of the LLRK formulas (9) will be consider in what follows. With this purpose, these formulas are rewritten as

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h_n \boldsymbol{\varphi}(t_n, \mathbf{y}_n; h_n) \quad \text{and} \quad \hat{\mathbf{y}}_{n+1} = \mathbf{y}_n + h_n \hat{\boldsymbol{\varphi}}(t_n, \mathbf{y}_n; h_n),$$

and the following additional notations are introduced. Let \mathcal{D} be an open subset of \mathbb{R}^d , \mathcal{M} an upper bound for $\|\mathbf{f}_{\mathbf{x}}\|$ on $[t_0, T] \times \mathcal{D}$, and \mathcal{L} the Lipschitz constant of the function $q(t, x(t); \cdot)$ (which exists for all $t \in [t_0, T]$ because Lemma 6 in [5] under regular conditions for \mathbf{f}). Denote by L_{n+1} the local truncation error of the Local Linearization scheme $\mathbf{y}_{n+1} = \mathbf{y}_n + u_4$ when it is applied to the linear equation (3)-(4), for which the inequality

$$L_{n+1} \leq Ch^{p+q+1}$$

holds with positive constant C [15]. Further, denote by L_{n+1}^1 and L_{n+1}^2 the local truncation errors of the classical embedded Runge-Kutta formulas of Dormand and Prince when they are applied to the nonlinear equation (5)-(6), for which the inequalities

$$L_{n+1}^1 \leq C_1 h^6 \quad \text{and} \quad L_{n+1}^2 \leq C_2 h^5$$

hold with positive constants C_1 and C_2 [7, 8].

Theorem 1. *Let \mathbf{x} be the solution of the ODE (1)-(2) with vector field \mathbf{f} six times continuously differentiable on $[t_0, T] \times \mathcal{D}$. Then, the embedded Locally Linearized Runge-Kutta formulas (9) have local truncation errors*

$$\|\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - h_n \boldsymbol{\varphi}(t_n, \mathbf{x}(t_n); h_n)\| \leq K h_n^{p+q+1} + C_1 h_n^6$$

and

$$\|\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) - h_n \widehat{\boldsymbol{\varphi}}(t_n, \mathbf{x}(t_n); h_n)\| \leq K h_n^{p+q+1} + C_2 h_n^5;$$

and global errors

$$\|\mathbf{x}(t_{n+1}) - \mathbf{y}_{n+1}\| \leq M_1 h^{\min\{p+q, 5\}}$$

and

$$\|\mathbf{x}(t_{n+1}) - \widehat{\mathbf{y}}_{n+1}\| \leq M_2 h^{\min\{p+q, 4\}}$$

for all $t_{n+1} \in (t)_h$ and h small enough, where $K = C(1 + \frac{\mathcal{M}}{\mathcal{L}}(e^{\mathcal{L}} - 1))$ is a positive constant, and M_1 and M_2 as well. In addition, the embedded Locally Linearized Runge-Kutta formulas (9) are A-stable if in the involved (p, q) -Padé approximation the inequality $p \leq q \leq p + 2$ holds.

Proof. The local truncation errors and the global errors are a straightforward consequence of Theorem 15 in [5], whereas the A-stability is a direct result of Theorem 17 in [5]. \square

Clearly, according to this result, the Locally Linearized Runge-Kutta formulas (9) preserve the convergence rate of the classical embedded Runge-Kutta formulas of Dormand and Prince if the inequality $p + q > 4$ holds. Further, note that these Locally Linearized formulas not only preserve the stability of the linear ODEs when $p \leq q \leq p + 2$, but they are also able to "exactly" (up to the precision of the floating-point arithmetic) integrate this class of equations when $p + q = 12$ (for the numerical precision of the current personal computers [18]).

In addition, and trivially, the embedded Locally Linearized Runge-Kutta formulas (9) inherit the dynamical properties derived in [5] for the general class of Local Linearization - Runge Kutta methods.

3.2. Adaptive strategy

In order to write a code that automatically adjust the stepsizes for achieving a prescribed tolerance of the local error at each step, an adequate adaptive strategy is necessary. At glance, the automatic stepsize control for the embedded RK formulas of Dormand & Prince seems to fit well for the embedded LLRK formulas

(9). In what follows, the adaptive strategy of the Matlab code ode45 for these formulas is described.

Once the values for the relative and absolute tolerances $RTol$ and $ATol$, and for the maximum and minimum stepsizes h_{\max} and h_{\min} are set, the basic steps of the algorithm are:

1. Estimation of the initial stepsize

$$h_0 = \min\{h_{\max}, \max\{h_{\min}, \Delta\}\}$$

where

$$\Delta = \begin{cases} \frac{1}{r_h} & \text{if } h_{\max} \cdot r_h > 1 \\ h_{\max} & \text{otherwise} \end{cases}$$

with

$$r_h = \frac{1}{0.8 \cdot RTol^{1/5}} \max_{i=1 \dots d} \left\{ \frac{\mathbf{f}^i(\mathbf{y}_0)}{\max\{|\mathbf{y}_0^i|, tr\}} \right\}$$

and $tr = \frac{ATol}{RTol}$. Initialize $fail = 0$.

2. Evaluation of the embedded formula (9)
3. Estimation of the error

$$error = \left\| \frac{\mathbf{y}_{n+1} - \widehat{\mathbf{y}}_{n+1}}{\max_{i=1, \dots, d} \{|\mathbf{y}_n^i|, |\mathbf{y}_{n+1}^i|, tr\}} \right\|_{\infty}$$

4. Estimation of a new stepsize

$$h_{new} = \min\{h_{\max}, \max\{h_{\min}, \Delta\}\}$$

where

$$\Delta = \begin{cases} 0.8 \cdot \left(\frac{RTol}{error}\right)^{1/5} \cdot h & \text{if } error \leq RTol \\ \max\{0.1, 0.8 \cdot \left(\frac{RTol}{error}\right)^{1/5}\} \cdot h & \text{if } error > RTol \text{ and } fail = 0 \\ 0.5 \cdot h & \text{if } error > RTol \text{ and } fail = 1 \end{cases}$$

5. Validation of y_{n+1} : if $error \leq RTol$, then accept y_{n+1} as an approximation to \mathbf{x} at $t_{n+1} = t_n + h$. Otherwise, return to 2 with $h_n = h_{new}$ and $fail = 1$.
6. Control of the final step: if $t_n + h = T$, stop. If $t_n + h + h_{new} > T$, then redefine $h_{new} = T - (t_n + h)$.
7. Return to 2 with $n = n + 1$, $h_n = h_{new}$, and $fail = 0$.

j/i	1	2	3	4
1	1	$-183/64$	$37/12$	$-145/128$
2	0	0	0	0
3	0	$1500/371$	$-1000/159$	$1000/371$
4	0	$-125/32$	$125/12$	$-375/64$
5	0	$9477/3392$	$-729/106$	$25515/6784$
6	0	$-11/7$	$11/3$	$-55/28$
7	0	$3/2$	-4	$5/2$

Table 2: Values of the coefficient $\alpha_{i,j}$ involved in the continuous LLRK formula (11) .

3.3. Continuous formula

Continuous formulas of RK methods are usually defined for computing the solutions on a dense set of time instants with minimum computational cost. Typically [8], they are constructing by means of a polynomial interpolation of the RK formulas between two consecutive times $t_n, t_{n+1} \in (t)_h$.

By a simple combination of the LLRK formulas (9) with the continuous formulas of the Dormand & Prince RK method [8] for (5)-(6), a continuous 7-stage LLRK formula can be defined as

$$\mathbf{y}(t_n + \theta h_n) = \mathbf{y}_n + \mathbf{u}(\theta h_n) + h_n \sum_{j=1}^7 b_j(t_n + \theta h_n) \mathbf{k}_j, \quad 0 < \theta < 1, \quad (11)$$

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

$$\mathbf{u}(\theta h_n) = \mathbf{L}(\mathbf{P}_{p,q}(2^{-\kappa_j} \mathbf{D}_n \theta h_n))^{2^{\kappa_j}} \mathbf{r} \quad (12)$$

is a d -dimensional vector, and

$$b_j(\delta) = \sum_{i=1}^4 \alpha_{i,j} \delta^i$$

is a polynomial with coefficients $\alpha_{i,j}$. Here, the function \mathbf{k}_j , the matrices \mathbf{D}_n , \mathbf{L} and \mathbf{r} , and the number κ_j are defined as in (9), as well as the (p, q) -Padé approximation $\mathbf{P}_{p,q}$. The coefficients $\alpha_{i,j}$, defined in Table 2, coincide with those of the continuous RK formula implemented in the Matlab code ode45.

3.4. LLDP45 code

This subsection describes a Matlab2007b(32bits) implementation of the adaptive scheme described above, which will be denoted as LLDP45 code.

In order to make a fair comparison between the linearized and the nonlinearized RK formulas, the LLDP45 code is an exact copy of the ode45 one with the exception of the program lines corresponding to the embedded and continuous formulas of Dormand and Prince, which are replaced by the formulas (9) and (11) respectively. We recall that the code ode45 implements the adaptive strategy of the subsection 3.2 for the embedded RK formulas of Dormand & Prince, which is considered by many authors the most recommendable code to be applied as first try for most problems [19].

Note that, the embedded LLRK formulas (9) require the computation of six Padé approximations $\mathbf{P}_{p,q}$ at each integration step, which increases the computational cost of the original embedded RK formulas. Nevertheless, this number of Padé approximations can be reduced by taking in to account that: a) $(\mathbf{P}_{p,q}(2^{-\kappa}\mathbf{D}_n c_j h_n))^{2^\kappa}$ gives an approximation to exponential matrix $\mathbf{e}^{\mathbf{D}_n c_j h_n}$; and b) the flow property of the exponential operator. Indeed, this can be carried out in two steps:

1. approximating $\mathbf{e}^{\mathbf{D}_n h_n/90}$ by the matrix $\mathbf{M}_{1/90} = (\mathbf{P}_{p,q}(2^{-\kappa}\mathbf{D}_n h_n/90))^{2^\kappa}$, where κ is the smallest integer number such that $\|2^{-\kappa}\mathbf{D}_n h_n/90\| \leq \frac{1}{2}$; and
2. the successive computation of the matrices

$$\begin{aligned}
 \mathbf{M}_{2/90} &= \mathbf{M}_{1/90}\mathbf{M}_{1/90} & \mathbf{M}_{4/90} &= \mathbf{M}_{2/90}\mathbf{M}_{2/90} \\
 \mathbf{M}_{8/90} &= \mathbf{M}_{4/90}\mathbf{M}_{4/90} & \mathbf{M}_{16/90} &= \mathbf{M}_{8/90}\mathbf{M}_{8/90} \\
 \mathbf{M}_{32/90} &= \mathbf{M}_{16/90}\mathbf{M}_{16/90} & \mathbf{M}_{80/90} &= \mathbf{M}_{32/90}\mathbf{M}_{16/90}\mathbf{M}_{32/90} \\
 \mathbf{M}_{1/10} &= \mathbf{M}_{8/90}\mathbf{M}_{1/90} & \mathbf{M}_{1/5} &= \mathbf{M}_{1/10}\mathbf{M}_{1/10} \\
 \mathbf{M}_{2/5} &= \mathbf{M}_{1/5}\mathbf{M}_{1/5} & \mathbf{M}_{4/5} &= \mathbf{M}_{2/5}\mathbf{M}_{2/5} \\
 \mathbf{M}_{3/10} &= \mathbf{M}_{1/10}\mathbf{M}_{1/5} & \mathbf{M}_1 &= \mathbf{M}_{4/5}\mathbf{M}_{1/5}.
 \end{aligned}$$

Consequently, the matrix \mathbf{M}_{c_j} corresponding to each RK coefficient c_j provides an approximation to $\mathbf{e}^{\mathbf{D}_n c_j h_n}$, for all $j = 1, \dots, 6$. In this way, at each integration step, the code LLDP45 performs six evaluation of \mathbf{f} (same than the ode45 code), one Jacobian matrix and one matrix exponential.

The matrix $\mathbf{M}_{1/90}$ is computed by means of the function "expmf", which provides a C++ implementation of the classical (p, q) -Padé approximations algorithm for exponential matrices with scaling and squaring strategy [18], and $p = q = 3$.

4. Numerical simulations

In this section, the performance of the LLDP45 and ode45 codes is compared by means of numerical simulations. To do so, a variety of ODEs and simulation types were selected. For all of them, the Relative Error

$$RE = \max_{i=1,\dots,d; t_j \in (t)_h} \left| \frac{\mathbf{x}^i(t_j) - \mathbf{y}^i(t_j)}{\mathbf{x}^i(t_j)} \right| \quad (13)$$

between the "exact" solution \mathbf{x} and its approximation \mathbf{y} is evaluated.

The simulations with the code ode45 were carried out with a wide range of tolerances: crude with $RTol = 10^{-3}$ and $ATol = 10^{-6}$, mild with $RTol = 10^{-6}$ and $ATol = 10^{-9}$, and refined with $RTol = 10^{-9}$ and $ATol = 10^{-12}$. The Matlab code ode15s with refined tolerance $RTol = 10^{-13}$ and $ATol = 10^{-13}$ was used to compute the "exact" solution \mathbf{x} in all simulations.

4.1. Test examples

The first four examples have the semi-linear form

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} + \mathbf{g}(\mathbf{x}), \quad (14)$$

where \mathbf{A} is a square matrix and \mathbf{g} is a function of \mathbf{x} . The vector field of the first two examples have Jacobian with eigenvalues on or near the imaginary axis, which made these equations difficult to be integrated by conventional schemes [19]. The other two are also hard for conventional explicit schemes since they are examples of stiff equations [19]. Example 4 has an additional complexity for a number of integrators that do not update the Jacobian of the vector field at each integration step [19, 12]: the Jacobian of the linear term has positive eigenvalues, which results a problem for the integration in a neighborhood of the stable equilibrium point $\mathbf{x} = 1$.

Example 1. *Periodic linear* [5]

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

with

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

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

Example 2. *Periodic linear plus nonlinear term* [5]

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

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

Example 3. *Stiff linear* [5]

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

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

Example 4. *Stiff linear plus nonlinear term* [5]

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

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

The following examples are well known nonlinear test equations. This include highly oscillatory, non stiff and mild stiff equations.

Example 5. *Fermi–Pasta–Ulam equation defined by the Hamiltonian system* [10]

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \sum_{i=1}^3 (\mathbf{p}_{2i-1}^2 + \mathbf{p}_{2i}^2) + \frac{w^2}{4} \sum_{i=1}^3 (\mathbf{q}_{2i} - \mathbf{q}_{2i-1})^2 + \sum_{i=0}^3 (\mathbf{q}_{2i+1} - \mathbf{q}_{2i})^2$$

with $w = 50$, initial conditions $1, 1, 1/w, 1$ for the four first variables and zero for the remainder eight, and $[t_0, T] = [0, 15]$.

Example 6. *Brusselator equation* [8]:

$$\begin{aligned} \frac{dx_1}{dt} &= 1 + x_1^2 x_2 - 4x_1 \\ \frac{dx_2}{dt} &= 3x_1 - x_1^2 x_2, \end{aligned}$$

where $(x_1(t_0), x_2(t_0)) = (1.5, 3)$ and $[t_0, T] = [0, 20]$.

Example 7. *Rigid body equation [8]:*

$$\begin{aligned}\frac{dx_1}{dt} &= x_2 x_3 \\ \frac{dx_2}{dt} &= -x_1 x_3 \\ \frac{dx_3}{dt} &= -0.51 x_1 x_2\end{aligned}$$

with $(x_1(t_0), x_2(t_0), x_3(t_0)) = (0, 1, 1)$ over $[t_0, T] = [0, 12]$.

Example 8. *Chemical reaction [19]:*

$$\begin{aligned}\frac{dx_1}{dt} &= 1.3(x_3 - x_1) + 10400k(x_1)x_2 \\ \frac{dx_2}{dt} &= 1880(x_4 - x_2(1 + k(x_1))) \\ \frac{dx_3}{dt} &= 1752 - 269x_3 + 267x_1 \\ \frac{dx_4}{dt} &= 0.1 + 320x_2 - 321x_4\end{aligned}$$

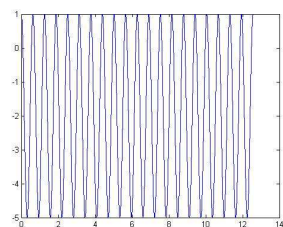
where $k(x_1) = e^{(20.7 - \frac{1500}{x_1})}$. With initial condition $(50, 0, 600, 0.1)$ over $[t_0, T] = [0, 1]$, this is mild stiff equation.

Example 9. *Van der Pol equation [9]:*

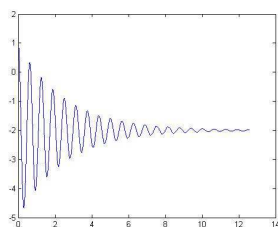
$$\begin{aligned}\frac{dx_1}{dt} &= x_2 \\ \frac{dx_2}{dt} &= \varepsilon(1 - x_2^2)x_1 + x_2\end{aligned}$$

with $(x_1(t_0), x_2(t_0)) = (2, 0)$. With $\varepsilon = 1$ and $\varepsilon = 10^2$, this is a non stiff and a mild stiff equation on the intervals $[t_0, T] = [0, 20]$ and $[t_0, T] = [0, 300]$, respectively.

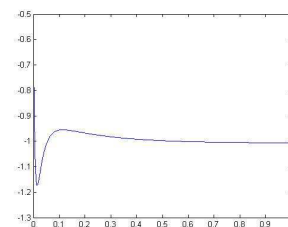
As illustration, Figure 1 shows the first component of the solution of each example, which will be consecutively named as *PerLin*, *PerNoLin*, *StiffLin*, *StiffNoLin*, *fpu*, *bruss*, *rigid*, *chm*, *vdpl* and *vdpl100*.



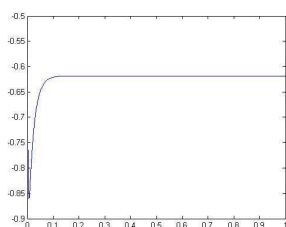
PerLin



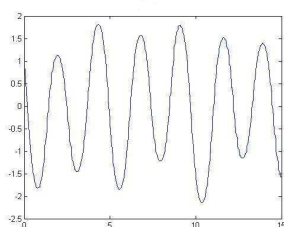
PerNoLin



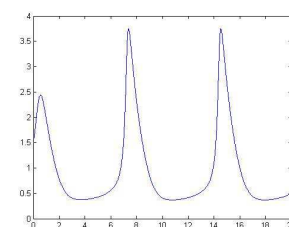
StiffLin



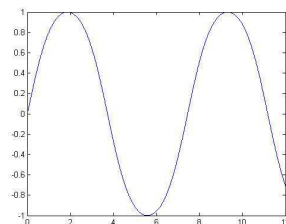
StiffNoLin



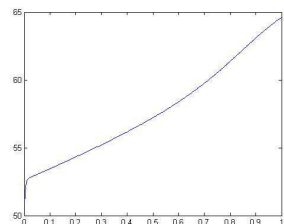
fpu



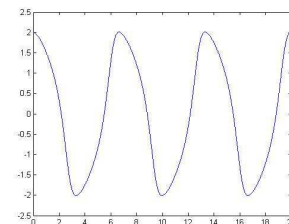
bruss



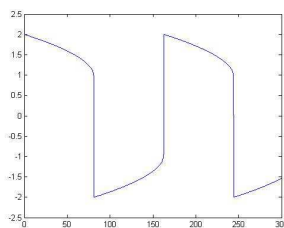
rigid



chm



vdp1



vdp100

Figure 1: Path of the first components of the solution in each example.

4.2. Simulation A: integration over same time partition

This simulation is designed to compare the accuracy of the order-5 formulas of the codes LLDP45 and ode45 over identical time partitions. First, the ode45 code integrates all the examples with the crude tolerances $RTol = 10^{-3}$ and $ATol = 10^{-6}$. This defined, for each example, a time partition $(t)_h$ over which the order-5 formula of the LLDP45 code is evaluated as well. That is, the formula

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \mathbf{u}_s + h_n \sum_{j=1}^s b_j \mathbf{k}_j \quad (15)$$

with $\mathbf{u}_j = \mathbf{L}(\mathbf{P}_{3,3}(2^{-\kappa_j} \mathbf{D}_n c_j h_n))^{2^{\kappa_j}} \mathbf{r}$ for the LLDP45 code. Tables 3 and 4 present, respectively, the Relative Error (13) of the order-5 formula of each code in the integration of the four semilinear and six nonlinear examples defined above. The number of accepted time steps is shown as well. This comparison is repeated twice but with the mild and refined tolerances $RTol = 10^{-6}, ATol = 10^{-9}$ and $RTol = 10^{-9}, ATol = 10^{-12}$. The results are also shown in Tables 3 and 4.

Example	Tol	Time steps	Relative Error DP formulas	Relative Error LLDP formulas
PerLin	Crude	147	1.01	2.0×10^{-6}
	Mild	598	2.6×10^{-2}	3.2×10^{-7}
	Refined	2394	2.7×10^{-5}	1.3×10^{-6}
PerNoLin	Crude	105	1.3×10^{-2}	4.9×10^{-5}
	Mild	411	2.6×10^{-5}	6.9×10^{-8}
	Refined	1634	1.2×10^{-7}	1.4×10^{-9}
StiffLin	Crude	60	1.1×10^{-3}	2.7×10^{-12}
	Mild	78	1.1×10^{-6}	2.7×10^{-12}
	Refined	173	8.0×10^{-10}	2.7×10^{-12}
StiffNoLin	Crude	104	1.4×10^{-2}	9.7×10^{-5}
	Mild	133	1.5×10^{-5}	6.8×10^{-8}
	Refined	294	1.4×10^{-8}	1.3×10^{-8}

Table 3: Relative error of the order-5 formula of each code when integrate the semilinear examples over identical time partition.

Note that, in general, the ode45 code is able to adequately integrate the test equations with the tree specified tolerances. Exceptions are the highly oscillatory *fpu* equation and the moderate stiff equation *vpd100* at crude tolerances, for which the relative error is high or unacceptable, respectively. Observe that, the order-5 locally linearized formula (15) is able to integrate the first equation with an adequate relative error, but fail to integrate the second one on the time partition generated by the ode45 code. In this last case, the Padé algorithm fails to compute

the exponential matrix at some point of the mentioned time partition and, because of that, the place corresponding to this information in Table 4 is empty.

Example	Tol	Time steps	Relative Error DP formulas	Relative Error LLDP formulas
fpu	Crude	964	1.9×10^2	1.5×10^{-2}
	Mild	4474	8.1	2.9×10^{-3}
	Refined	19190	1.7×10^{-2}	1.7×10^{-2}
rigid	Crude	19	2.7×10^{-2}	1.5×10^{-3}
	Mild	66	7.5×10^{-5}	4.0×10^{-6}
	Refined	256	2.0×10^{-7}	1.8×10^{-8}
chm	Crude	679	1.1×10^{-3}	5.5×10^{-7}
	Mild	723	1.1×10^{-6}	2.5×10^{-7}
	Refined	1520	1.2×10^{-8}	1.2×10^{-8}
bruss	Crude	46	7.7×10^{-2}	2.4×10^{-2}
	Mild	148	8.7×10^{-6}	3.5×10^{-7}
	Refined	558	1.5×10^{-8}	1.2×10^{-9}
vdp1	Crude	59	2.0	0.14
	Mild	204	2.8×10^{-4}	1.5×10^{-5}
	Refined	785	5.6×10^{-7}	3.1×10^{-8}
vdp100	Crude	16916	1.9×10^4	—
	Mild	17516	0.42	9.2×10^{-2}
	Refined	31254	1.2×10^{-3}	8.1×10^{-4}

Table 4: Relative error of the order-5 formula of each code when integrate the nonlinear examples over identical time partition.

4.3. Simulation B: integration with same tolerance

This simulation is designed to compare the performance the codes LLDP45 and ode45 with the same tolerances. As a difference with Simulation A, here each codes use a different time partition defined by their own adaptive strategy.

Tables 5 and 6 summarize the results of each code in the integration of each example for the three sets of tolerances specified above. The column "Time" in these tables presents the relative overall time of each numerical scheme with respect to that of the ode45 code on the whole interval $[t_0, T]$. This overall time ratio works as simple indicator to compare the total computational cost of each code. In addition, the tables show the number of accepted and failed steps, the number of evaluations of \mathbf{f} and \mathbf{f}_x , and the number of exponential matrices computed in the integration of each example.

Example	Code	Tol	Time steps	Failed steps	f	$\exp(f_x)$	Time	Relative Error
PerLin	ode45	Crude	147	0	883	0	1	10.2
		Mild	598	0	3589	0	1	2.6×10^{-2}
		Refined	2394	0	14365	0	1	2.7×10^{-5}
	LLDP45	Crude	14	0	85	14	0.27	2.0×10^{-9}
		Mild	14	0	85	14	0.08	3.0×10^{-9}
		Refined	15	0	91	15	0.01	2.0×10^{-9}
PerNoLin	ode45	Crude	105	0	631	0	1	1.3×10^{-2}
		Mild	411	0	2467	0	1	2.6×10^{-5}
		Refined	1634	0	9805	0	1	1.2×10^{-7}
	LLDP45	Crude	42	0	253	42	0.74	2.2×10^{-3}
		Mild	137	0	823	137	0.62	3.6×10^{-6}
		Refined	534	0	3205	534	0.57	2.1×10^{-9}
StiffLin	ode45	Crude	60	6	397	0	1	1.1×10^{-3}
		Mild	78	1	475	0	1	1.1×10^{-6}
		Refined	172	6	1069	0	1	8.0×10^{-10}
	LLDP45	Crude	14	0	85	14	0.33	2.5×10^{-12}
		Mild	14	0	85	14	0.34	2.3×10^{-12}
		Refined	15	0	91	15	0.15	2.3×10^{-12}
StiffNoLin	ode45	Crude	104	4	649	0	1	1.4×10^{-2}
		Mild	133	5	829	0	1	1.5×10^{-5}
		Refined	294	2	1777	0	1	1.4×10^{-8}
	LLDP45	Crude	21	0	127	21	0.32	8.0×10^{-4}
		Mild	43	0	259	43	0.53	1.6×10^{-6}
		Refined	132	2	805	134	0.68	9.2×10^{-9}

Table 5: Code performance in the integration of the semilinear examples with the same tolerances.

4.4. Simulation C: integration with similar accuracy

In this type of simulation, the tolerances $RTol$ and $ATol$ of the LLDP45 code is changed until its relative error in the integration of each example achieves similar value to that corresponding to the code ode45. This simulation is carried out three times, changing the tolerances of the ode45 from the crude values to the refined values specified above. Tables 7 and 8 summarize the performance of each code in the integration of each example. As in the previous two tables, this includes the relative overall time, number of accepted and failed steps, the number of evaluations of \mathbf{f} and \mathbf{f}_x , and the number of exponential matrices computed in the integration of each example.

Example	Code	Tol	Time steps	Failed steps	f	$\exp(f_x)$	Time	Relative Error
fpu	ode45	Crude	964	2	5797	0	1	1.9×10^{-2}
		Mild	4474	60	27205	0	1	8.1
		Refined	19190	45	115411	0	1	1.7×10^{-2}
	LLDP45	Crude	377	48	2551	425	0.81	17.4
		Mild	1496	125	9727	1621	0.67	2.0×10^{-2}
		Refined	6021	86	36643	6107	0.49	1.7×10^{-2}
rigid	ode45	Crude	19	2	127	0	1	2.7×10^{-2}
		Mild	66	4	421	0	1	7.5×10^{-5}
		Refined	256	1	1543	0	1	2.0×10^{-7}
	LLDP45	Crude	16	0	97	16	1.18	3.3×10^{-3}
		Mild	53	5	349	58	1.55	8.6×10^{-6}
		Refined	201	0	1207	201	1.48	3.1×10^{-8}
chm	ode45	Crude	679	47	4357	0	1	1.1×10^{-3}
		Mild	723	16	4435	0	1	1.1×10^{-6}
		Refined	1521	1	9133	0	1	1.2×10^{-8}
	LLDP45	Crude	152	1	919	153	0.43	8.4×10^{-4}
		Mild	357	2	2155	359	1.05	9.2×10^{-7}
		Refined	859	57	5497	916	1.18	1.2×10^{-8}
bruss	ode45	Crude	46	12	349	0	1	7.7×10^{-2}
		Mild	148	13	967	0	1	8.7×10^{-6}
		Refined	558	4	3373	0	1	1.5×10^{-8}
	LLDP45	Crude	36	7	259	43	1.32	6.2×10^{-3}
		Mild	105	14	715	119	1.47	5.4×10^{-6}
		Refined	396	11	2443	407	1.38	4.8×10^{-9}
vdp1	ode45	Crude	59	10	415	0	1	2.24
		Mild	204	32	1417	0	1	2.8×10^{-4}
		Refined	785	19	4825	0	1	5.7×10^{-7}
	LLDP45	Crude	44	10	325	54	1.23	1.95
		Mild	162	38	1201	200	1.45	5.8×10^{-5}
		Refined	609	12	3727	621	1.24	1.4×10^{-7}
vdp100	ode45	Crude	16916	1074	107941	0	1	1.9×10^4
		Mild	17516	1540	114337	0	1	0.41
		Refined	31253	9	187573	0	1	1.2×10^{-3}
	LLDP45	Crude	3866	120	23917	3986	0.35	16.1
		Mild	7893	19	47473	7912	0.69	2.1×10^{-3}
		Refined	19887	568	122731	20455	1.02	5.6×10^{-4}

Table 6: Code performance in the integration of the nonlinear examples with the same tolerances.

Example	Code	Tol	Time steps	Failed steps	f	$\exp(f_x)$	Time	Relative Error
PerLin	ode45	Crude	147	0	883	0	1	10.1
		Mild	598	0	3589	0	1	2.6×10^{-2}
		Refined	2394	0	14365	0	1	2.7×10^{-5}
	LLDP45	$100 \times$ Crude	13	0	79	13	0.23	2.0×10^{-9}
		$100 \times$ Crude	13	0	79	13	0.06	2.0×10^{-9}
		$100 \times$ Crude	13	0	79	13	0.01	2.0×10^{-9}
PerNoLin	ode45	Crude	105	0	361	0	1	1.2×10^{-2}
		Mild	411	0	2467	0	1	2.6×10^{-5}
		Refined	1634	0	9805	0	1	1.2×10^{-7}
	LLDP45	$7.5 \times$ Crude	32	0	193	32	0.55	1.2×10^{-2}
		$7 \times$ Mild	95	0	571	95	0.44	1.5×10^{-5}
		$80 \times$ Refined	224	0	1345	224	0.24	1.2×10^{-7}
StiffLin	ode45	Crude	60	6	397	0	1	1.1×10^{-3}
		Mild	78	1	475	0	1	1.1×10^{-6}
		Refined	172	6	1069	0	1	8.0×10^{-10}
	LLDP45	$100 \times$ Crude	13	0	79	13	0.35	2.6×10^{-12}
		$100 \times$ Crude	13	0	79	13	0.28	2.6×10^{-12}
		$100 \times$ Crude	13	0	79	13	0.12	2.6×10^{-12}
StiffNoLin	ode45	Crude	104	4	649	0	1	1.4×10^{-2}
		Mild	133	5	829	0	1	1.5×10^{-5}
		Refined	294	2	1777	0	1	1.4×10^{-8}
	LLDP45	$9 \times$ Crude	24	2	157	26	0.38	1.3×10^{-2}
		$40 \times$ Mild	28	0	169	28	0.35	1.1×10^{-5}
		$8.45 \times$ Refined	90	0	541	90	0.46	1.0×10^{-8}

Table 7: Code performance in the integration of the semilinear examples with similar accuracy.

4.5. Simulation D: evaluation of the dense output

This simulation is designed to compare the accuracy of the continuous formulas of the codes LLDP45 and ode45 over their dense output. For this, both codes are applied first to each example with the same crude tolerances $RTol = 10^{-3}$ and $ATol = 10^{-6}$ but, the relative error of each code is now computed on its respective dense output instead on the time partition $(t)_h$ defined by the adaptive strategy. Tables 9 and 10 present these relative errors. The number of accepted time steps and dense output times are also shown. This comparison is repeated twice but with the mild and refined tolerances $RTol = 10^{-6}, ATol = 10^{-9}$ and $RTol = 10^{-9}, ATol = 10^{-12}$. The results are also shown in Tables 9 and 10.

Example	Code	Tol	Time steps	Failed steps	f	$\exp(f_x)$	Time	Relative Error
fpu	ode45	Crude	964	2	5797	0	1	1.9×10^{-2}
		Mild	4474	60	27205	0	1	8.1
		Refined	19190	45	115411	0	1	1.7×10^{-2}
	LLDP45	$10 \times$ Crude	242	29	1627	271	0.49	1.0×10^{-2}
		$100 \times$ Mild	567	39	3637	606	0.26	5.2
		$10 \times$ Refined	3783	107	23341	3890	0.37	1.1×10^{-2}
rigid	ode45	Crude	19	2	127	0	1	2.7×10^{-2}
		Mild	66	4	421	0	1	7.5×10^{-5}
		Refined	256	1	1543	0	1	2.0×10^{-7}
	LLDP45	$30 \times$ Crude	15	0	91	15	1.14	1.8×10^{-2}
		$22 \times$ Mild	30	2	193	32	0.93	3.3×10^{-5}
		$19.7 \times$ Refined	111	1	673	112	0.83	1.3×10^{-7}
chm	ode45	Crude	679	47	4357	0	1	1.1×10^{-3}
		Mild	723	16	4435	0	1	1.1×10^{-6}
		Refined	1521	1	9133	0	1	1.3×10^{-8}
	LLDP45	$1.5 \times$ Crude	146	1	883	147	0.41	1.1×10^{-3}
		$1.4 \times$ Mild	341	2	2059	343	1.00	1.0×10^{-6}
		$2.0 \times$ Refined	789	58	5083	847	1.10	1.0×10^{-8}
bruss	ode45	Crude	46	12	349	0	1	7.7×10^{-2}
		Mild	148	13	967	0	1	8.7×10^{-6}
		Refined	558	4	3373	0	1	1.5×10^{-8}
	LLDP45	$4.6 \times$ Crude	28	7	211	35	1.16	7.5×10^{-2}
		$1.2 \times$ Mild	101	13	685	114	1.27	8.1×10^{-6}
		$3.5 \times$ Refined	309	8	1903	330	1.05	1.3×10^{-8}
vdp1	ode45	Crude	59	10	415	0	1	2.0
		Mild	204	32	1417	0	1	2.8×10^{-4}
		Refined	785	19	4825	0	1	5.6×10^{-7}
	LLDP45	$3.2 \times$ Crude	42	10	313	52	1.21	1.47
		$3.2 \times$ Mild	128	26	925	154	1.12	2.4×10^{-4}
		$4.0 \times$ Refined	461	10	2827	471	0.95	4.1×10^{-7}
vdp100	ode45	Crude	16916	1074	107941	0	1	1.9×10^4
		Mild	17516	1540	114337	0	1	0.42
		Refined	31253	9	187573	0	1	1.2×10^{-3}
	LLDP45	$10 \times$ Crude	3780	24	22825	3804	0.34	1.9×10^4
		$39 \times$ Mild	5026	731	34543	5757	0.50	0.26
		$98.5 \times$ Refined	10719	37	64537	10756	0.53	1.1×10^{-3}

Table 8: Code performance in the integration of the nonlinear examples with similar accuracy.

5. Discussion

The results of the previous section show the following: 1) on the same time partition (Tables 3 and 4), the embedded LLRK formulas are significantly much accurate than the classical embedded RK formulas of Dormand & Prince. 2) with identical tolerances and adaptive strategy (Tables 5 and 6), the LLDP45 code is

more accurate than the ode45 code and requires much less time steps for integrating the whole intervals. For highly oscillatory, stiff linear, stiff semilinear and mildly stiff nonlinear problems the overall time of the adaptive LLDP45 code is lower than that of the ode45 code, whereas it is similar or bigger for equations with smooth solution; 3) for reaching similar - but always lower - accuracy (Tables 7 and 8), the LLDP45 code also requires much less time steps than the ode45 code for integrating the whole intervals. In this situation, the overall time of the adaptive LLDP45 code is again much lower than that of the ode45 code for highly oscillatory, stiff linear, stiff semilinear and mildly stiff nonlinear problems, whereas it is slightly bigger only for two equations with smooth solution (bruss and vdp1 examples); and 4) the accuracy of the dense output of the LLDP45 code is, in general, higher than the accuracy of the ode45 code (Tables 9 and 10).

Example	Code	Tol	Time steps	Dense OutPut	Relative Error
PerLin	ode45	Crude	147	589	10.2
		Mild	598	2393	2.6×10^{-2}
		Refined	2394	9577	1.6×10^{-3}
	LLDP45	Crude	14	57	2.0×10^{-9}
		Mild	14	57	3.0×10^{-9}
		Refined	15	61	4.1×10^{-9}
PerNoLin	ode45	Crude	105	313	4.8×10^{-3}
		Mild	411	1169	3.0×10^{-6}
		Refined	1634	4625	2.7×10^{-9}
	LLDP45	Crude	42	101	1.5×10^{-3}
		Mild	137	293	8.7×10^{-7}
		Refined	534	1073	9.2×10^{-10}
StiffLin	ode45	Crude	60	241	1.1×10^{-3}
		Mild	78	313	1.1×10^{-6}
		Refined	172	689	8.1×10^{-10}
	LLDP45	Crude	14	53	2.7×10^{-12}
		Mild	14	57	2.7×10^{-12}
		Refined	15	61	2.7×10^{-12}
StiffNoLin	ode45	Crude	104	417	1.4×10^{-2}
		Mild	133	533	3.0×10^{-5}
		Refined	294	1177	2.6×10^{-8}
	LLDP45	Crude	21	85	6.4×10^{-3}
		Mild	43	173	2.9×10^{-5}
		Refined	132	525	7.3×10^{-8}

Table 9: Relative error of the continuous formulas of the codes over their dense output after integrating the semilinear examples.

Example	Code	Tol	Time steps	Dense OutPut	Relative Error
fpu	ode45	Crude	964	3857	9.5×10^2
		Mild	4474	17897	19.0
		Refined	19190	76761	0.86
	LLDP45	Crude	377	1497	33.8
		Mild	1496	5985	2.8×10^{-2}
		Refined	6021	24085	0.15
rigid	ode45	Crude	19	77	0.31
		Mild	66	265	3.4×10^{-4}
		Refined	256	1025	1.1×10^{-6}
	LLDP45	Crude	16	65	0.19
		Mild	53	213	1.7×10^{-4}
		Refined	201	805	2.3×10^{-7}
chm	ode45	Crude	679	2717	1.1×10^{-3}
		Mild	723	2893	1.1×10^{-6}
		Refined	1521	6085	5.7×10^{-8}
	LLDP45	Crude	152	609	9.4×10^{-4}
		Mild	357	1429	9.2×10^{-7}
		Refined	859	3409	5.8×10^{-8}
bruss	ode45	Crude	46	185	8.8×10^{-2}
		Mild	148	593	1.0×10^{-5}
		Refined	558	2233	1.7×10^{-8}
	LLDP45	Crude	36	145	6.2×10^{-3}
		Mild	105	421	2.4×10^{-5}
		Refined	396	1585	1.1×10^{-8}
vdp1	ode45	Crude	59	237	2.9×10^2
		Mild	204	817	6.9×10^{-4}
		Refined	785	3141	4.3×10^{-6}
	LLDP45	Crude	44	177	2.25
		Mild	162	649	2.3×10^{-4}
		Refined	609	2437	1.9×10^{-7}
vdp100	ode45	Crude	16916	67665	2.0×10^4
		Mild	17516	70065	0.47
		Refined	31253	125013	4.4×10^{-3}
	LLDP45	Crude	3866	15457	2.0×10^4
		Mild	7893	31573	4.1×10^{-2}
		Refined	19887	79509	2.1×10^{-3}

Table 10: Relative error of the continuous formulas of the codes over their dense output after integrating the nonlinear examples.

These simulations results clearly shown that, in the ten examples, the local linearization of the embedded Runge-Kutta formulas of Dormand and Prince produces a significant improvement of the accuracy of the classical formulas. However, this is clearly not a result that could be expected according to the local truncation errors given in Theorem 1. This indicates that, most likely, sharper error estimates could be obtained for the locally linearized formulas, which is certainly an important open problem to solve.

Note that the significantly better accuracy of the locally linearized formulas implies a substantial reduction of the number of time steps and, consequently, a

sensitive reduction of the overall computation cost in eight of the ten test equations (see Tables 7 and 8). This indicates that, for various classes of equations, the additional computational cost of computing the exponential of a Jacobian matrix at each time step is compensated for the gain of accuracy. This result certainly agrees with previous reports in the same direction as that given in [19]: "supplying a function for evaluating the Jacobian can be quite advantageous, both with respect to reliability and cost".

Further, note that three of the eight test equations for which the application of locally linearized formulas yields a sensitive reduction of the overall computation cost are systems of twelve equations. This illustrates the usefulness of these integrators for low dimensional problems in general. However, because the locally linearized formulas (9) are expressed in terms of the Padé algorithm for computing exponential matrices, it is expected that they are unable to integrate moderately large system of ODE with a rational computational cost. In this case, because of the flexibility in the numerical implementation of the LLRK methods mentioned in the introduction, the local linearization of the embedded Runge Kutta formulas of Dormand and Prince can be easily formulated in terms of the Krylov-type methods for exponential matrices. In effect, this can be done just by replacing the Padé formula in (10) and (12) by the Krylov-Padé formula as performed in [5, 16, 17] for the local linearizations schemes for ordinary, random and stochastic differential equations. In this way, the Locally Linearized formulas of Dormand and Prince could be applied to high dimensional ODEs with a reasonable computational cost [23].

On the other hand, we recall that, in order to study the effect of the local linearization on the conventional RK scheme of Dormand and Prince, the LLDP45 code considered in this work is an exact copy of the code ode45 with the exception of the program lines corresponding to the embedded and continuous formulas. In this way, the LLDP45 code does not include a number of convenient modifications that might improve its performance. Some of they are the following:

- the initial h at t_0 , which can be estimated by means the exact second derivative of the solution \mathbf{x} with no extra cost (as in [22]);
- online smoothness and stiffness control for estimating the new h at each step (as, e.g., in [9]);
- the automatic detection of constant Jacobian matrix (as in [6, 24, 26]);
- option for using exact, numerical or automatic Jacobian matrices (as in [19, 20, 1]);

- faster algorithms to compute the Padé approximation to exponential matrix (as, e.g., in [11])
- a parallel implementation of matrix multiplications involved in the exponential matrix evaluations for taking advantage of the multi core technology available in the current microprocessors;
- increase the number of times of the dense outputs: a) up to twelve per each pair of consecutive times of the partition $(t)_h$ with no extra computation of exponential matrices; or b) up to ninety with some few extra matrix multiplications;
- a new continuous formula that replace the current one based on the continuous RK formula by other based on a polynomial interpolation of the LLRK formula itself (i.e, derived from the standard way of constructing continuous RK formulas as in [8]); and
- change of h_{max} , which seems to be too short for semilinear equations.

6. Conclusions

In this paper, embedded Locally Linearized Runge-Kutta formulas for initial value problems were introduced and their performance analyzed by means of exhaustive numerical simulations. In this way, the effect that produces the local linearization of the classical embedded Runge-Kutta formulas of Dormand and Prince were studied. It was shown that, for a variety of well-known physical equations usually taken in simulations studies as test equations, the local linearization of the embedded Runge-Kutta formulas of Dormand & Prince produces a significant improvement of the accuracy of classical formulas, which implies a substantial reduction of the number of time steps and, consequently, a sensitive reduction of the overall computation cost of their adaptive implementation.

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