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A piecewise-linearized algorithm based on the Krylov subspace for solving stiff ODEs☆

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ABSTRACT

Numerical methods for solving Ordinary Differential Equations (ODEs) have received considerable attention in recent years. In this paper a piecewise-linearized algorithm based on Krylov subspaces for solving Initial Value Problems (IVPs) is proposed. MATLAB versions for autonomous and non-autonomous ODEs of this algorithm have been implemented. These implementations have been compared with other piecewise-linearized algorithms based on Padé approximants, recently developed by the authors of this paper, comparing both precisions and computational costs in equal conditions. Four case studies have been used in the tests that come from stiff biology and chemical kinetics problems. Experimental results show the advantages of the proposed algorithms, especially when the dimension is increased in stiff problems.

1. Introduction

Many scientific and engineering problems are described by ODEs where the analytic solution is unknown. In recent years many review articles and books have appeared on numerical methods for integrating stiff ODEs. Stiff problems are very common problems in many fields of the applied sciences: control theory, biology, chemical kinetics, electronic circuit theory, fluids, etc. There exist numerous one-step algorithms for solving stiff ODEs based on the implicit Runge–Kutta methods [1–3]. Another popular family of algorithms for solving these problems are the multistep algorithms based on the BDF method [4–7]. In this paper we have developed a one-step method based on a piecewise-linearized method [8]. These methods solve an IVP by approximating the right hand side of the corresponding ODE by a Taylor polynomial of degree 1. The resulting approximation can be integrated analytically to obtain the solution in each subinterval and yields the exact solution for linear problems. In [8,9] an exhaustive study of this method is introduced. The proposed method requires a non-singular Jacobian matrix on each subinterval.

In [10] the authors presented a piecewise-linearized method for solving ODEs. This method uses a theorem proved in that article, which enables the approximate solution to be computed at each time step by a block-oriented approach based on diagonal Padé approximations. In this work another approach based on the piecewise-linearized method is introduced. In this case, the matrix–vector product $e^A v$, which appears in these methods, is computed by a Krylov subspace approach. The computational costs and precisions of the algorithms are compared in equal conditions. The paper is structured as follows. The new approach for solving ODEs based on the Krylov subspace approach is presented in Section 2. The experimental results are shown in Section 3. Finally, conclusions and future expectations are given in Section 4.

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2. A piecewise-linearized algorithm for solving ODEs based on the Krylov subspace approach

In [10] the authors presented a piecewise-linearized method for solving ODEs, based on the following theorem which enables the approximate solution to be computed at each time step by a block-oriented approach based on diagonal Padé approximations.

Theorem 1 (*[10]*). *Let*

$$\dot{x}(t) = f(t, x(t)), \quad t \in [t_0, t_f], \tag{1}$$

be an ODE with initial value

$$x(t_0) = x_0 \in \mathbb{R}^n,$$

such that the first-order partial derivatives of $f(t, x)$ are continuous on $[t_0, t_f] \times \mathbb{R}^n$. Given a mesh $t_0 < t_1 < \cdots < t_{l-1} < t_l = t_f$, ODE (1) can be approximated by a set of LDEs obtained as a result of a linear approximation of $f(t, x(t))$ on each subinterval [9,11],

$$\begin{aligned} &\dot{y}(t) = f_i + J_i(y(t) - y_i) + g_i(t - t_i), \quad t \in [t_i, t_{i+1}], \\ &y(t_i) = y_i, \quad i = 0, 1, \ldots, l-1. \end{aligned} \tag{2}$$

The solution of (2) is

$$y(t) = y_i + E_{12}^{(i)}(t - t_i)f_i + E_{13}^{(i)}(t - t_i)g_i, \tag{3}$$

where $E_{12}^{(i)}(t - t_i)$ and $E_{13}^{(i)}(t - t_i)$ are blocks $(1, 2)$ and $(1, 3)$ of $E = \mathrm{e}^{C_i(t-t_i)}$, where

$$C_i = \begin{bmatrix} J_i & I_n & 0_n \\ 0_n & 0_n & I_n \\ 0_n & 0_n & 0_n \end{bmatrix}. \quad \square$$

If t is replaced by t_{i+1} in (3), the approximate solution of ODE (1) at t_{i+1}, $i = 0, 1, \ldots, l-1$, is given by

$$y_{i+1} = y_i + E_{12}^{(i)}(\Delta t_i)f_i + E_{13}^{(i)}(\Delta t_i)g_i, \quad \Delta t_i = t_{i+1} - t_i. \tag{4}$$

In this work, another approach based on the piecewise-linearized method is introduced as follows.

From [10, p. 716], $\mathrm{e}^{C_i\Delta t_i}$ can be expressed as

$$\begin{bmatrix} \mathrm{e}^{J_i\Delta t_i} & E_{12}^{(i)}(\Delta t_i) & E_{13}^{(i)}(\Delta t_i) \\ 0_n & I_n & I_n\Delta t_i \\ 0_n & 0_n & I_n \end{bmatrix},$$

whereas the approximate solution y_{i+1} given in (4) can be obtained by adding to y_i the first n components of a vector

$$\mathrm{e}^{C_i\Delta t_i}v_i, \tag{5}$$

where

$$C_i = \begin{bmatrix} J_i & I_n & 0_n \\ 0_n & 0_n & I_n \\ 0_n & 0_n & 0_n \end{bmatrix}, \; v_i = \begin{bmatrix} 0_{n\times 1} \\ f_i \\ g_i \end{bmatrix}.$$

The matrix–vector product $\mathrm{e}^{C_i\Delta t_i}v_i$ can be obtained by a Krylov subspace method [12,13]. Given $A \in \mathbb{R}^{n\times n}$ and $v \in \mathbb{R}^n$, it is possible to compute an approximation to vector $\mathrm{e}^A v$ by using the Arnoldi method. This approximation is given by

$$\mathrm{e}^A v \cong v_{\mathrm{opt}} = \beta V_p \mathrm{e}^{H_p} e_1, \tag{6}$$

where $H_p = (h_{ij}) \in \mathbb{R}^{p\times p}$ is the Hessenberg matrix obtained from the Arnoldi method and $V_p = [v_1, v_2, \ldots, v_p] \in \mathbb{R}^{n\times p}$, with $\{v_i\}_{i=1,2,\ldots,p}$ an orthonormal basis of the Krylov subspace $K_p = \mathrm{span}\{v, Av, \ldots, A^{p-1}v\}$, $\beta = \|v\|_2$ and $e_1 = [1, 0, \ldots, 0]^T$.

In order to reduce computational and storage costs when we want to compute vector y_{i+1}, it is necessary to modify the classical Arnoldi algorithm without explicitly forming the matrix $C_i\Delta t_i$. Algorithm 1 solves IVPs for non-autonomous ODEs by the above piecewise-linearized method based on a Krylov subspace approach. This algorithm uses Algorithm 2, which computes the approximate solution at t_{i+1} of IVP (1) for non-autonomous ODEs, obtained after the piecewise-linearized process, by a block-oriented implementation of the Krylov subspace approach. Its computational cost is $2n^2p + 6np(p + 1) + 2(q + j_{H_p} + 1/3)p^3$ flops, where $j_{H_p} = \max(0, 1 + \mathrm{int}(\log_2(\|H_p\|)))$. It is possible to reduce the computational and storage costs of Algorithm 1 when IVP (1) is autonomous.

3. Experimental results

The main objective of this section is to compare the MATLAB implementations of algorithm developed in Section 2 with the implementations developed by the authors of this paper in [10].

Algorithm 1 Solves IVP (1) by a piecewise-linearized method based on a Krylov subspace approach.

Function $y = \texttt{inolkr}(t, \texttt{data}, x_0, p, tol, q)$
Inputs: Time vector $t \in \mathbb{R}^{l+1}$; function `data` computes $f(\tau, y) \in \mathbb{R}^n$, $J(\tau, y) \in \mathbb{R}^{n\times n}$ and $g(\tau, y) \in \mathbb{R}^n$ ($\tau \in \mathbb{R}, y \in \mathbb{R}^n$); vector $x_0 \in \mathbb{R}^n$; dimension $p \in \mathbb{N}$ of the Krylov subspace; tolerance $tol \in \mathbb{R}^+$; order $q \in \mathbb{N}$ of the diagonal Padé approximation of the exponential function
Output: Matrix $Y = [y_1, \ldots, y_l] \in \mathbb{R}^{n\times l}$, $y_i \in \mathbb{R}^n$, $i = 1, 2, \ldots, l$
Compute the vectors c_1 and c_2 that contain the coefficients of terms of degree greater than 0 in the diagonal Padé approximation of the exponential function
$y_0 = x_0$
for $i = 0 : l - 1$ **do**
    $[J_i, f_i, g_i] = \texttt{data}(t_i, y_i)$
    $\Delta t_i = t_{i+1} - t_i$
    $y_{i+1} = \texttt{inlbkr}(J_i, f_i, g_i, y_i, \Delta t_i, p, tol, c_1, c_2)$ (Algorithm 2)
end for

Algorithm 2 Computes the approximate solution at t_{i+1} of IVP (1) for non-autonomous ODEs, obtained after the piecewise-linearized process, by a block-oriented implementation of the Krylov subspace approach.

Function $y_{i+1} = \texttt{inlbkr}(J_i, f_i, g_i, y_i, \Delta t_i, p, tol, c_1, c_2)$
Inputs: Matrix $J_i \in \mathbb{R}^{n\times n}$; vector $f_i \in \mathbb{R}^n$; vector $g_i \in \mathbb{R}^n$; vector $y_i \in \mathbb{R}^n$; step size $\Delta t_i \in \mathbb{R}$; dimension $p \in \mathbb{N}$ of the Krylov subspace; tolerance $tol \in \mathbb{R}^+$; vectors $c_1, c_2 \in \mathbb{R}^q$ with the coefficients of terms of degree greater than 0 in the diagonal Padé approximation of the exponential function
Output: Vector $y_{i+1} \in \mathbb{R}^n$ given by expression (5)
$V(1 : n, 1) = 0_n$
$V(n + 1 : 2n, 1) = f_i$
$V(2n + 1 : 3n, 1) = g_i$
$\beta = \|V(n + 1 : 3n, 1)\|_2$
if $\beta == 0$ **then**
    $y_{i+1} = y_i$
    Return
end if
$V(n + 1 : 3n, 1) = V(n + 1 : 3n, 1)/\beta$
for $j = 1 : p$ **do**
    $w(1 : n) = J_i V(1 : n, j) + V(n + 1 : 2n, j)$
    $w(n + 1 : 2n) = V(2n + 1 : 3n, j)$
    $w(1 : 2n) = \Delta t_i w(1 : 2n)$
    $w(2n + 1 : 3n) = 0_n$
    for $i = 1 : j$ **do**
        $H(i, j) = w^T V(1 : 3n, i)$
        $w = w - H(i, j)V(1 : 3n, i)$
    end for
    $s = \|w\|_2$
    if $s < tol$ **then**
        $p = j$
        Leave for loop
    end if
    $H(j + 1, j) = s$
    $V(1 : 3n, j + 1) = w/s$
end for
computes $E = \mathrm{e}^{H_p}$
$y_{i+1} = y_i + \beta V(1 : n, 1 : p)E(1 : p, 1)$

As test battery, four case studies of stiff ODEs, which come from stiff biology and chemical kinetics problems, were considered. Numerous tests were made on them. For each case study and algorithm, the characteristic parameters were varied, although only the parameters which offered the same accuracy for the two implementations with the lower computational cost are presented.

What follows is a short description of the implemented algorithms and the characteristic parameters:

- `iaolwp` and `inolwp` solve IVPs for ODEs by a piecewise-linearized approach and a block-oriented version without scaling–squaring implementation of the diagonal Padé approximation method:
  – Order $q = 2$ of the diagonal Padé approximation of the exponential function.

Table 1
Relative error (E_r) with $t = 10$ and Δt variable (case study 1).

E_r	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.01$	$\Delta t = 0.005$	$\Delta t = 0.001$
`iaolwp`	2.809e−04	7.523e−05	2.390e−06	5.840e−07	2.366e−08
`iaolkr`	2.348e−04	6.928e−05	2.759e−06	6.423e−07	2.399e−08

Table 2
Execution time (T_e) in seconds with $t = 10$ and Δt variable (case study 1).

T_e	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.01$	$\Delta t = 0.005$	$\Delta t = 0.001$
`iaolwp`	0.014	0.021	0.114	0.257	6.231
`iaolkr`	0.025	0.048	0.201	0.428	6.802

Table 3
Relative error (E_r) $\Delta t = 0.01$ and t variable (case study 1).

E_r	$t = 20$	$t = 30$	$t = 40$	$t = 50$	$t = 60$
`iaolwp`	2.015e−06	1.744e−06	1.537e−06	1.374e−06	1.240e−06
`iaolkr`	2.327e−06	2.013e−06	1.775e−06	1.585e−06	1.431e−06

Table 4
Relative error (E_r) with $\Delta t = 0.1$ and t variable (case study 2).

E_r	$t = 15\,400$	$t = 16\,400$	$t = 17\,400$	$t = 18\,400$	$t = 19\,400$
`inolwp`	4.410e−14	8.833e−14	1.431e−13	1.980e−13	2.528e−13
`inolkr`	4.410e−14	8.833e−14	1.431e−13	1.980e−13	2.528e−13

- `iaolkr` and `inolkr` solve IVPs for ODEs by a piecewise-linearized method based on Krylov subspaces:
  - Dimension $p = 4$ of the Krylov subspace. In Ref. [12] there is an exhaustive study of the computation of the product of the exponential of a matrix and a vector by using Krylov subspaces. We have proved experimentally that when considering low or medium dimension matrices, it is only necessary to consider a very much reduced subspace dimension. In this work $p = 4$.
  - Tolerance $tol = 10^{-6} \in \mathbb{R}^+$.
  - Order $q = 2$ of the diagonal Padé approximation of the exponential function.

For each test, the following results are shown:

- Tables which contain the relative error

$$E_r = \frac{\|x - x^*\|_\infty}{\|x\|_\infty},$$

where x^* is the computed solution and x is the analytic solution (case study 2) or the solution computed by the MATLAB function ode15s with a vector of relative error tolerances $rtol = 10^{-13}$ and a vector of absolute error tolerances $atol = 10^{-13}$ [14].
- Tables/figures with the execution time.

The algorithms were implemented in MATLAB 7.9 and tested on an Intel Core 2 Duo processor at 2.66 GHz with 2 GB main memory. Several tests have been developed in order to determine the accuracy and efficiency of the algorithms. The implemented algorithms are available online at http://www.grycap.upv.es/odelin.

3.1. Case study 1 (the pollution problem [15])

This case study corresponds to a stiff IVP of dimension 20. The problem describes a chemical process consisting of 25 reactions and 20 species. The following tests were done:

- First test (Tables 1 and 2): $t = 10$ and Δt variable.
- Second test (Table 3 and Fig. 1): $\Delta t = 0.01$ and t variable.

3.2. Case study 2 (the EMEP problem [15])

In this case study a stiff IVP for ODEs of dimension 66 is solved. The problem describes a problem which consists of 66 chemical species and about 140 reactions. The following tests were done:

- In the first test $t = 14\,450$ was considered. With $\Delta t = 0.1$ the relative errors of the three implementations were equal to $2.219 \cdot 10^{-15}$, with executions times equal to 1.290 (`inolwp`) and 0.266 (`inolkr`) seconds.
- Second test (Tables 4 and 5, and Fig. 2): $\Delta t = 0.1$ and t variable.

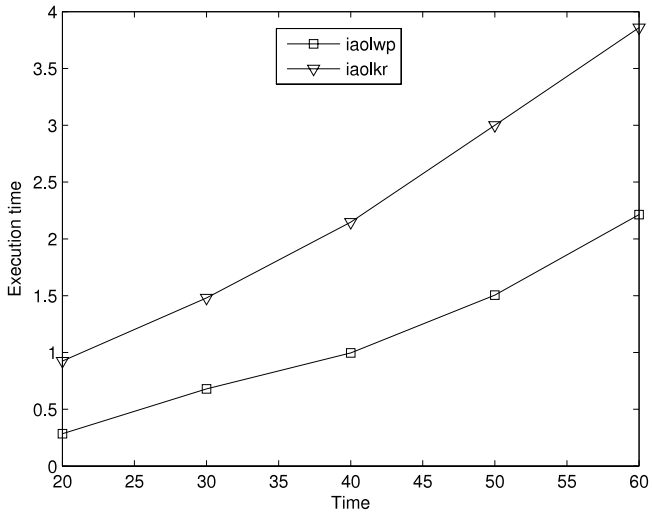

Fig. 1. Execution time in seconds of the MATLAB implementations considering $\Delta t = 0.01$ and varying t (case study 1).

Table 5
Execution time (T_e) in seconds with $\Delta t = 0.1$ and t variable (case study 2).

T_e	$t = 15\,400$	$t = 16\,400$	$t = 17\,400$	$t = 18\,400$	$t = 19\,400$
`inolwp`	52.830	157.465	316.257	529.469	790.217
`inolkr`	26.547	102.401	227.630	400.672	623.248

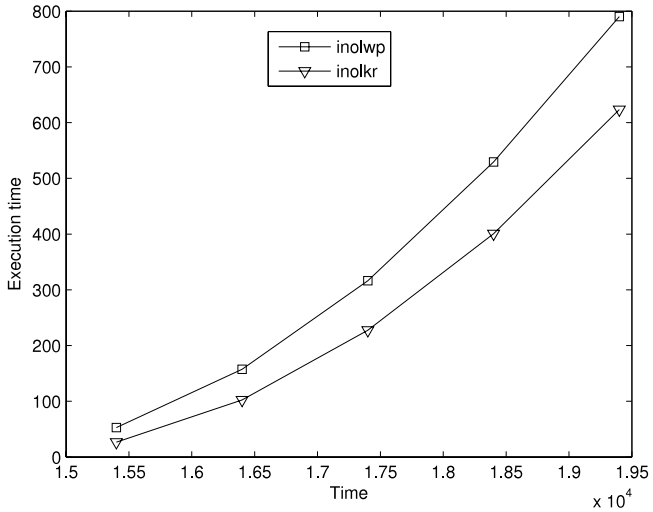

Fig. 2. Execution time in seconds of the MATLAB implementations considering $\Delta t = 0.1$ and varying t between 15 400 and 19 400 (case study 2).

3.3. Case study 3 (the Medical Akzo Nobel problem [15])

This case study corresponds to a stiff non-autonomous ODE [15] of variable dimension $2N$. This problem studies the penetration of radio-labeled antibodies into tissue infected by a tumor.

The following tests were made:

- First test (Tables 6 and 7): $n = 100$ ($N = 50$), $t = 1$ and Δt variable.
- Second test (Tables 8 and 9): $\Delta t = 0.001$, $t = 1$ and varying n from 50 to 250 ($N = 25$ to 125).

3.4. Case study 4 (the Brusselator problem) [1, pp. 6]

This case study corresponds to a stiff non-autonomous ODE of variable dimension N. This problem comes from chemical kinetics where the model of Lefever and Nicolis [16] is used and the method of lines is applied on a grid of N points:

- First test (Tables 10 and 11): $n = 100$ ($N = 50$), $t = 1$ and Δt variable.
- Second test (Tables 12 and 13, and Fig. 3): $t = 1$, $\Delta t = 0.001$ and n variable.

Table 6
Relative error (E_r) considering $n = 100$, $t = 1$ and Δt variable (case study 3).

E_r	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$	$\Delta t = 0.00001$
inolwp	1.572e−02	1.726e−03	1.741e−04	1.742e−05
inolkr	1.663e−02	1.728e−03	1.741e−04	1.742e−05

Table 7
Execution time (T_e) in seconds considering $n = 100$, $t = 1$ and Δt variable (case study 3).

T_e	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$	$\Delta t = 0.00001$
inolwp	0.301	4.926	144.484	6362.490
inolkr	0.036	0.538	50.044	5263.304

Table 8
Relative error (E_r) considering $\Delta t = 0.001$, $t = 1$ and n variable (case study 3).

E_r	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$
inolwp	1.636e−03	1.726e−03	1.746e−03	1.743e−03	1.736e−03
inolkr	1.637e−03	1.728e−03	1.752e−03	1.763e−03	1.781e−03

Table 9
Execution time (T_e) in seconds considering $\Delta t = 0.001$, $t = 1$ and n variable (case study 3).

T_e	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$
inolwp	0.720	3.531	20.863	63.944	143.920
inolkr	0.288	0.482	0.740	1.159	1.367

Table 10
Relative error (E_r) considering $n = 100$, $t = 1$ and Δt variable (case study 4).

E_r	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$	$\Delta t = 0.00001$
inolwp	2.162e−02	3.673e−04	3.715e−05	3.719e−06
inolkr	2.263e−02	3.672e−04	3.715e−05	3.719e−06

Table 11
Execution time (T_e) in seconds considering $n = 100$, $t = 1$ and Δt variable (case study 4).

T_e	$\Delta t = 0.01$	$\Delta t = 0.001$	$\Delta t = 0.0001$	$\Delta t = 0.00001$
inolwp	0.140	1.688	55.297	4106.738
inolkr	0.031	0.465	38.122	3710.951

Table 12
Relative error (E_r) considering $\Delta t = 0.001$, $t = 1$ and n variable (case study 4).

E_r	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$
inolwp	5.033e−04	3.673e−04	3.308e−04	3.170e−04	3.108e−04
inolkr	5.033e−04	3.672e−04	3.307e−04	3.169e−04	3.107e−04

Table 13
Execution time (T_e) in seconds considering $\Delta t = 0.001$, $t = 1$ and n variable (case study 4).

T_e	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$
inolwp	0.521	1.894	2.988	7.616	16.391
inolkr	0.279	0.506	0.701	0.963	1.256

4. Conclusions and future work

In this work a new piecewise-linearized approach for solving ODEs based on Krylov subspaces has been presented. Two algorithms based on this approach (`inolkr` and `iaolbk`) have also been proposed and compared to the piecewise-linearized algorithms `iaolwp` and `inolwp` based on Padé approximants developed by the authors of this paper in [10].

Numerous test have been made on four case studies that come from stiff biology and chemical kinetics problems. Experimental results show the advantages of the proposed algorithms, especially when they are integrating stiff problems. According to the experimental results, the new algorithms offer in general similar precision and smaller computational

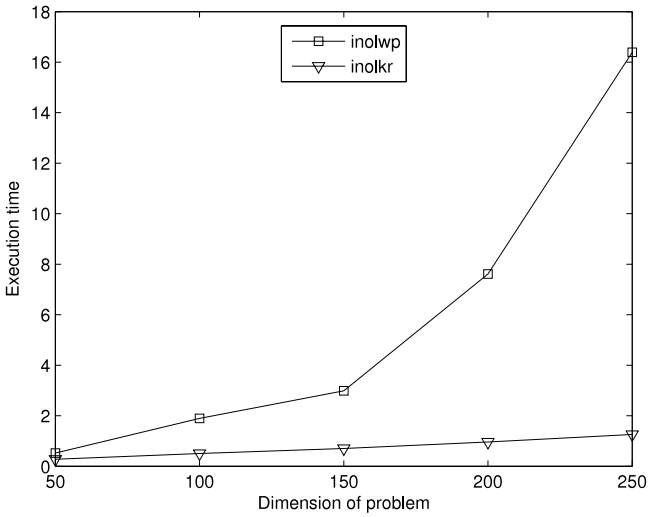

Fig. 3. Execution time in seconds of the MATLAB implementations considering $\Delta t = 0.001$ and varying t between 50 and 250 (case study 3).

cost when the problem size is increased. For example, Algorithm 1 (`inolkr`) was up to 111 times faster than `inolwp` for $n = 250$ and $t = 1$ in case study 3. This is because in the new approach the vector $e^A v$, $A \in \mathbb{R}^{n\times n}$, $v \in \mathbb{R}^n$, is approximated by the expression $\beta V_p e^{H_p} e_1$, where $p \ll n$. Nevertheless, when the problems are of small dimension, the computational costs of piecewise-linearized algorithms based on diagonal Padé approximants are smaller than the computational costs of piecewise-linearized algorithms based on Padé approximants. In general, all algorithms offer accuracy and good behaviour with stiff problems.

As future work new improvements will be developed such as:

1. Implementing algorithms based on the piecewise-linearized approach with error control in order to vary the step size dynamically. The tests reported here considered constant step size. It is possible to improve the algorithms developed, using a variable step size which can be used to estimate the error committed in each iteration [9].
2. Carrying out parallel implementation of the algorithms presented in this work in a distributed memory platform, using the message passing paradigm MPI [17] and BLACS [18] for communications, and PBLAS [19] and ScaLAPACK [20] for computations.

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