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Jacobian-dependent vs Jacobian-free discretizations for nonlinear differential problems

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Abstract The paper provides a comparison between two relevant classes of numerical discretizations for stiff and nonstiff problems. Such a comparison regards linearly implicit Jacobian-dependent Runge-Kutta methods and fully implicit Runge-Kutta methods based on Gauss-Legendre nodes, both A-stable. We show that Jacobian-dependent discretizations are more efficient than Jacobian-free fully implicit methods, as visible in the numerical evidence.

Keywords Linearly-implicit methods, Jacobian-dependent methods, stiff problems.

Mathematics Subject Classification (2010) 65L04,65L05

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1 Introduction

The wide literature on the numerical solution for nonlinear differential problems

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where the vector field f is smooth enough to guarantee the well-posedness of the problem, is rich of general purpose methods, as well as on adapted methods, specially tuned to the problem under investigation. The numerical integration of (1.1) is important not only for itself but also for the time integration of spatially discretized time-dependent partial differential equations [8, 18, 21, 30, 31, 33, 38, 48–50] and, therefore, an adaptation of the numerical schemes to the problems may be particularly favourable for an efficient computation of the solutions. A relevant example of adaptation has been provided by the literature on the so-called exponentially fitted methods [9, 16, 19, 20, 22, 27, 28, 34, 45, 39, 43, 46, 47], whose coefficients are dependent on parameters which characterize the problem, such as the frequency oscillation for oscillatory solutions.

Clearly, this level of adaptation is feasible if a good approximation of the parameters is known in advance. If this is not the case, a competitive level of adaption is made possible by Jacobian-dependent discretizations, which are characterized by coefficients containing a correction term that depends on the Jacobian of the vector field f of (1.1). This correction contains the contribution to the error arising from the internal stages of the scheme and its presence creates a benefit in terms of stability and accuracy properties in comparison with the Jacobian-free case [26, 35, 40–42]. Focusing on the class of explicit Runge-Kutta methods, Ixaru found examples of A-stable Jacobian-dependent formulae in [40–42]. Actually, the computation of the coefficients requires the inversion of a matrix depending on the Jacobian at each step, making the resulting methods linearly implicit. Other examples of stabilized explicit methods are given in [1, 3, 44] and references therein.

It is the purpose of this paper to focus on Jacobian-dependent discretizations relying on Runge-Kutta schemes, by providing a fair comparison with the analogous Jacobian-free versions. We will show that such methods are more efficient than fully implicit methods, as for implicit methods Newton iterations may require more matrix inversions to achieve a prescribed tolerance. The comparison is performed between two A-stable classes of methods: the classical Gaussian Runge-Kutta methods versus the linearly implicit Jacobian-dependent Runge-Kutta methods developed in [42] and briefly reviewed in Section 2. Section 3 provides the numerical evidence originated on a selection of test problems, while some conclusions are given in Section 4.

2 Jacobian-dependent discretizations

Consider a two-stage explicit Runge-Kutta method for a scalar problem (1.1)

$$y_{n+1} = y_n + h\left(b_1 f(t_n, Y_1) + b_2 f(t_n + c_2 h, Y_2)\right),$$

with

$$\begin{aligned} Y_1 &= y_n \\ Y_2 &= y_n + h a_{21} f(t_n, Y_1), \end{aligned}$$

and $a_{21} = c_2$ for stage consistency. While for the Jacobian-free version of this method, b_1 and b_2 are constant coefficients, in the Jacobian-dependent version they assume the form

$$b_1 = 1 - \frac{1}{c_2\left(2 - c_2 M_2\right)}, \qquad b_2 = 1 - b_1, \tag{2.2}$$

with

$$M_2 = h f_y(t_n + c_2 h, Y_2). \tag{2.3}$$

The scheme has second order for any $c_2 \neq 2/3$, while for $c_2 = 2/3$ it achieves order $p = 3$. We observe that, for $c_2 = 1$, above linearly implicit method is A-stable. When $M_2 = 0$, the scheme is fully explicit, so it is never A-stable and (2.2) is the well-known condition of order 2 for a two-stage Runge-Kutta method [2].

Let us now focus on the corresponding version for systems of differential equations (1.1). We observe that, in this case, M_2 in (2.3) is a matrix and, as a consequence, also the weights B_1 and B_2 of the corresponding Runge-Kutta method

$$y_{n+1} = y_n + h\left(B_1 f(t_n, Y_1) + B_2 f(t_n + c_2 h, Y_2)\right), \tag{2.4}$$

become matrices. In the above expression

$$\begin{aligned} Y_1 &= y_n \\ Y_2 &= y_n + h a_{21} f(t_n, Y_1), \end{aligned}$$

with $a_{21} = c_2$ for stage consistency. In the Jacobian-dependent version for systems (1.1) the matrices B_1 and B_2 assume the form

$$B_1 = I - \frac{1}{2c_2}\left(I - \frac{c_2}{2} M_2\right)^{-1}, \quad B_2 = I - B_1,$$

where I stands for the identity matrix of order d. The matrix M_2 is defined by

$$M_2 = hJ(t_n + c_2 h, Y_2),$$

where J is the Jacobian matrix of f. We observe that the Jacobian-free version of the method follows by setting M_2 equal to zero matrix and, therefore,

$$B_1 = b_1 I, \qquad B_2 = b_2 I,$$

where b_1 and b_2 are the scalar values given by (2.2).

We now consider a three-stage explicit Runge-Kutta method for systems of type (1.1)

$$y_{n+1} = y_n + h\left(B_1 f(t_n, Y_1) + B_2 f(t_n + c_2 h, Y_2) + B_3 f(t_n + c_3 h, Y_3)\right), \quad (2.5)$$

with

$$\begin{aligned} Y_1 &= y_n \\ Y_2 &= y_n + h a_{21} f(t_n, Y_1), \\ Y_3 &= y_n + h a_{31} f(t_n, Y_1) + h a_{32} f(t_n, Y_2), \end{aligned}$$

with $a_{21} = c_2$ and $a_{31} + a_{32} = c_3$ for stage consistency. While for the Jacobian-free version of this method, the weights are constant coefficients, in the Jacobian-dependent version they are matrices assuming the form

$$\begin{aligned} B_1 &= TQ^{-1}, \\ B_2 &= \frac{1}{c_2^2} B_3 \left((1 - c_2 - c_3(3c_3 - 2c_2))I + (-c_3^2 + c_2 c_3 + c_2^2)M_3\right), \\ B_3 &= I - B_1 - B_2, \end{aligned}$$

with

$$\begin{aligned} T &= (3c_2 - 2)I - c_2(c_2 - 1)M_2, \\ Q &= c_3\Big(6(c_2 - c_3)I + c_2(3c_3 - 2c_2)M_2 + c_3(2c_3 - 3c_2)M_3 \\ &\qquad + c_3 c_2(c_2 - c_3)M_3 M_2\Big), \end{aligned}$$

and

$$M_2 = hJ(t_n + c_2 h, Y_2), \quad M_3 = hJ(t_n + c_3 h, Y_3).$$

Such a linearly implicit method is A-stable for $c_2 = 1/2$ and $c_3 = 1$.

Remark 1 Jacobian-dependent methods allow to combine linear implicitness and A-stability but, on the other hand, they have the drawback of matrix inversions. However, as observed by Ixaru in [42], the required stepsize restrictions to guarantee the invertibility of the involved matrices is not severe. For instance, the A-stable two-stage method (2.4), with $c_1 = 0$ and $c_2 = 1$, requires $h|\lambda| < 10^{11}$, where λ is the spectral radius of the Jacobian. Moreover, for the A-stable three-stage method (2.5), with $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$, the restriction is $h|\lambda| < 10^6$. More details regarding the computation of these stepsize restrictions can be found in [42].

3 Numerical illustration

We now present the results of the comparison on selected problems among the following methods:

- RK2, two-stage fully implicit Runge-Kutta method based on Gaussian collocation points, of order 4 [37];

– Ix2(c_2), two-stage linearly implicit Jacobian-dependent method (2.4), with $c_1 = 0$. We consider Ix2(2/3) having order 3 and Ix2(1) of order 2 and A-stable;
– Ix3, three-stage linearly implicit Jacobian-dependent Runge-Kutta method (2.5), with nodes $c_1 = 0$, $c_2 = 1/2$ and $c_3 = 1$, of order 4 and A-stable.

Such a comparison aims to show the advantages of Jacobian-dependent discretizations with respect to the analog Jacobian-free version, with the same order or the same number of stages. The provided experiments, carried out in a fixed stepsize environment, are given for selected stiff and nonstiff problems [36,37]. In the remainder of the section, nval is the overall number of function evaluations, cd is the achieved number of correct digits at the endpoint T of the integration interval.

We first consider the following Euler problem

$$\begin{cases} y_1'(t) = -2y_2(t)y_3(t), \\ y_2'(t) = \dfrac{5}{4}y_1(t)y_3(t), \\ y_3'(t) = -\dfrac{1}{2}y_1(t)y_2(t), \end{cases} \tag{3.6}$$

with $t \in [0, 10]$ and initial value $y_0 = [1 \quad 0 \quad 0.9]^\intercal$. As visible from Tables 1 and 2, all the implemented methods converge with their expected orders, without exhibiting any order reduction, since Euler problem (3.6) is nonstiff. A detailed analysis of order reduction for one-step methods can be found in [37]. The estimated orders are computed by the usual formula

$$p(h) = \frac{cd(h) - cd(2h)}{\log_{10} 2}.$$

Figure 1 shows the corresponding work precision diagram and reveals that, for low accuracy, both Ix2 and Ix3 are competitive with the RK2 method. Clearly, for high accuracy demandings, the higher order methods perform better and, in particular, Ix3 is more efficient than the Jacobian-free RK2 method. Clearly, the implicit method results to be more expensive, since the involved Newton iterations may require more matrix inversions to achieve a prescribed tolerance. On the contrary, a linearly implicit scheme requires only one matrix inversion per step.

We next consider the Brusselator model

$$\begin{cases} y_1'(t) = 1 + y_1(t)^2 y_2(t) - 4y_1(t), \\ y_2'(t) = 3y_1(t) - y_1(t)^2 y_2(t), \end{cases} \tag{3.7}$$

with $t \in [0, 20]$ and initial value $y_0 = [1.5 \quad 3]^\intercal$. Tables 3 and 4 and Figure 2 reveal that, for any level of accuracy, Ix3 is more efficient than the RK2 method. Moreover, Ix2(2/3) remains competitive up to 6 correct digits. We observe that both Jacobian-dependent methods, with $h = 1/2$, are not applicable, since the stepsize does not fulfill the requirements of Remark 1.

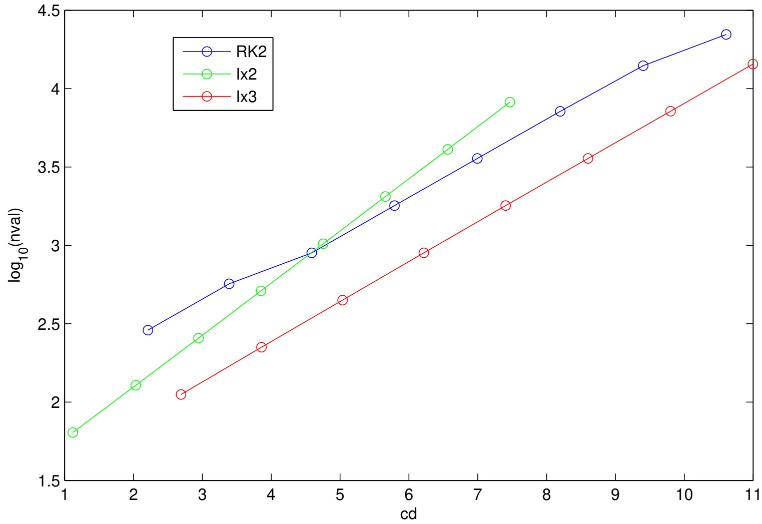

Fig. 1 Work precision diagram related to Euler problem (3.6). The method Ix2 is Ix2(2/3).

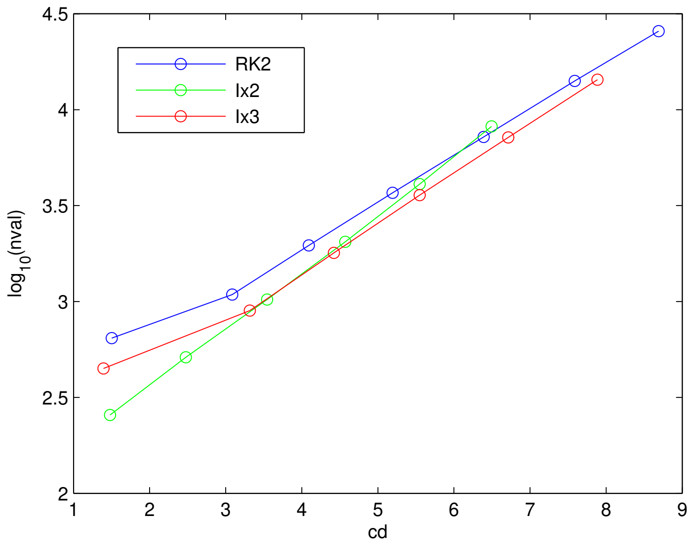

Fig. 2 Work precision diagram related to Brusselator problem (3.7). The method Ix2 is Ix2(2/3).

h	RK2	Ix2(2/3)	Ix3
1/2	2.5910e-03	3.8651e-02	9.0258e-04
1/4	1.6755e-04	4.7054e-03	5.7404e-05
1/8	1.0565e-05	5.7968e-04	3.8272e-06
1/16	6.6180e-07	7.1946e-05	2.5170e-07
1/32	4.1386e-08	8.9621e-06	1.6205e-08
1/64	2.5869e-09	1.1184e-06	1.0290e-09
1/128	1.6156e-10	1.3968e-07	6.4954e-11
1/256	9.9786e-12	1.7452e-08	4.2064e-12

Table 1 Absolute errors at the endpoint T on Euler problem (3.6), in correspondence of several values of the stepsize h.

h	RK2	Ix2(2/3)	Ix3
1/4	3.9509	3.0381	3.9748
1/8	3.9872	3.0210	3.9068
1/16	3.9968	3.0103	3.9265
1/32	3.9992	3.0050	3.9572
1/64	3.9999	3.0025	3.9771
1/128	4.0010	3.0012	3.9857
1/256	4.0171	3.0006	3.9488

Table 2 Estimated order $p(h)$ on Euler problem (3.6).

h	RK2	Ix2(2/3)	Ix3
1/2	2.3356e-02	-	-
1/4	7.7100e-04	1.5112e-02	2.4211e-03
1/8	3.9150e-05	1.5267e-03	2.1457e-04
1/16	2.6447e-06	1.3159e-04	1.6592e-05
1/32	1.6703e-07	1.2853e-05	1.1989e-06
1/64	1.0885e-08	1.3902e-06	8.0831e-08
1/128	1.1044e-09	1.6097e-07	5.6483e-09
1/256	4.9279e-10	1.9703e-08	7.8217e-10

Table 3 Absolute errors at the endpoint T on Brusselator problem (3.7), in correspondence of several values of the stepsize h.

h	RK2	Ix2(2/3)	Ix3
1/4	4.9209	-	-
1/8	4.2997	3.3073	3.4961
1/16	3.8878	3.5363	3.6929
1/32	3.9849	3.3558	3.7907
1/64	3.9397	3.2088	3.8906
1/128	3.3010	3.1104	3.8390
1/256	1.1642	3.0302	3.7341

Table 4 Estimated order $p(h)$ on Brusselator problem (3.7).

We finally consider the Van der Pol oscillator

$$\begin{cases} y_1'(t) = y_2(t), \\ \varepsilon y_2'(t) = (1 - y_1(t)^2)y_2(t) - y_1(t), \end{cases} \tag{3.8}$$

with $t \in [0, 2/3]$ and initial value $y_0 = [2 \quad -2/3]^\intercal$. We consider the values $\varepsilon = 10^{-3}, 10^{-5}, 10^{-6}$, corresponding to nonstiff, mildly stiff and stiff prolems,

h	RK2	Ix2(1)	Ix3
$(T-t_0)/2^4$	1.2527e-03	3.8670e-03	-
$(T-t_0)/2^5$	1.6858e-04	7.0246e-04	8.3320e-05
$(T-t_0)/2^6$	1.4886e-05	1.7230e-04	6.7424e-06
$(T-t_0)/2^7$	1.0415e-06	4.3261e-05	4.0699e-07
$(T-t_0)/2^8$	6.7128e-08	1.0827e-05	2.3142e-08
$(T-t_0)/2^9$	4.2308e-09	2.7075e-06	1.2956e-09
$(T-t_0)/2^{10}$	2.6707e-10	6.7693e-07	7.5512e-11
$(T-t_0)/2^{11}$	1.8817e-11	1.6923e-07	6.5652e-12

Table 5 Absolute errors at the endpoint T on the van der Pol problem (3.8) with $\varepsilon = 10^{-3}$, in correspondence of several values of the stepsize h.

h	RK2	Ix2(1)	Ix3
$(T-t_0)/2^5$	2.8935	2.4607	-
$(T-t_0)/2^6$	3.5014	2.0275	3.6273
$(T-t_0)/2^7$	3.8372	1.9938	4.0502
$(T-t_0)/2^8$	3.9556	1.9984	4.1364
$(T-t_0)/2^9$	3.9879	1.9996	4.1588
$(T-t_0)/2^{10}$	3.9856	1.9999	4.1008
$(T-t_0)/2^{11}$	3.8271	2.0000	3.5238

Table 6 Estimated order $p(h)$ on the van der Pol problem (3.8) with $\varepsilon = 10^{-3}$.

respectively. The dashes appearing in the following tables are related to the cases of non applicability of the Jacobian-dependent methods, according to Remark 1.

Tables 5 and 6 show that all the implemented methods converge with their expected orders, without exhibiting any order reduction, since the problem is nonstiff. Similarly to the case of the Euler problem, Figure 3 shows the corresponding work precision diagram and reveals that, for low accuracy, both Ix2 and Ix3 are competitive with the RK2 method. Clearly, for high accuracy demandings, the higher order methods perform better and, in particular, Ix3 is more efficient than the Jacobian-free RK2 method. Tables 7–10, referring to the mildly stiff and stiff cases, show that only Ix2(1) converges with its expected order, while the other two methods suffer from order reduction. The corresponding work precision diagrams, reported in Figures 4 and 5, show that Ix3 is always more efficient than the RK2 method, while Ix2(1) is more competitive up to 7 correct digits for the mildly stiff case and up to 8 for the stiff case.

4 Conclusions

We have focused our attention on advantages and drawbacks of Jacobian-dependent discretizations introduced by Ixaru [42] versus Jacobian-free ones, both based on Runge-Kutta methods. When the problem is stiff, the methods by Ixaru do not suffer from order reduction, while Runge-Kutta methods exhibit lower effective order. The three-stage method by Ixaru outperforms the Runge-Kutta method in terms of efficiency. In future developments of this

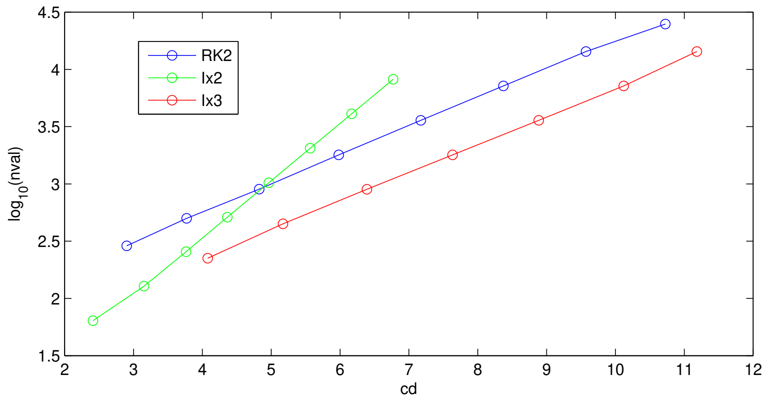

Fig. 3 Work precision diagram related to the van der Pol problem (3.8) with $\varepsilon = 10^{-3}$. The method Ix2 is Ix2(1).

h	RK2	Ix2(1)	Ix3
$(T - t_0)/2^7$	2.4021e-05	1.1597e-04	-
$(T - t_0)/2^8$	3.6979e-06	1.1969e-05	-
$(T - t_0)/2^9$	3.6951e-07	2.7125e-06	1.4935e-07
$(T - t_0)/2^{10}$	2.7393e-08	6.7792e-07	1.2417e-08
$(T - t_0)/2^{11}$	1.8002e-09	1.6948e-07	7.7927e-10
$(T - t_0)/2^{12}$	1.1635e-10	4.2368e-08	4.9905e-11
$(T - t_0)/2^{13}$	9.7311e-12	1.0590e-08	5.3797e-12
$(T - t_0)/2^{14}$	3.0422e-12	2.6455e-09	2.7631e-12

Table 7 Absolute errors at the endpoint T on the van der Pol problem (3.8) with $\varepsilon = 10^{-5}$, in correspondence of several values of the stepsize h.

h	RK2	Ix2(1)	Ix3
$(T - t_0)/2^8$	2.6995	3.2764	-
$(T - t_0)/2^9$	3.3230	2.1416	-
$(T - t_0)/2^{10}$	3.7537	2.0004	3.5883
$(T - t_0)/2^{11}$	3.9276	2.0000	3.9940
$(T - t_0)/2^{12}$	3.9516	2.0001	3.9649
$(T - t_0)/2^{13}$	3.5798	2.0003	3.2136
$(T - t_0)/2^{14}$	1.6775	2.0011	0.9612

Table 8 Estimated order $p(h)$ on the van der Pol problem (3.8) with $\varepsilon = 10^{-5}$.

h	RK2	Ix2(1)	Ix3
$(T - t_0)/2^7$	3.0194e-05	4.2640e-02	-
$(T - t_0)/2^8$	6.9312e-06	1.7456e-03	-
$(T - t_0)/2^9$	1.3337e-06	4.2164e-06	-
$(T - t_0)/2^{10}$	1.7743e-07	7.0058e-07	-
$(T - t_0)/2^{11}$	1.5668e-08	1.6948e-07	5.8589e-09
$(T - t_0)/2^{12}$	1.1000e-09	4.2367e-08	4.9426e-10
$(T - t_0)/2^{13}$	7.3710e-11	1.0590e-08	3.3979e-11
$(T - t_0)/2^{14}$	7.4523e-12	2.6451e-09	4.9178e-12

Table 9 Absolute errors at the endpoint T on the van der Pol problem (3.8) with $\varepsilon = 10^{-6}$, in correspondence of several values of the stepsize h.

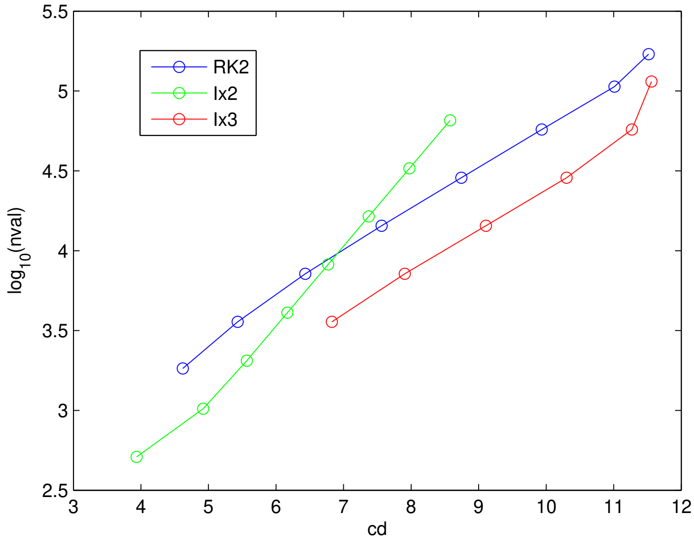

Fig. 4 Work precision diagram related to the van der Pol problem (3.8) with $\varepsilon = 10^{-5}$. The method Ix2 is Ix2(1).

h	RK2	Ix2(1)	Ix3
$(T-t_0)/2^8$	2.1231	4.6104	-
$(T-t_0)/2^9$	2.3777	8.6935	-
$(T-t_0)/2^{10}$	2.9101	2.5894	-
$(T-t_0)/2^{11}$	3.5014	2.0475	-
$(T-t_0)/2^{12}$	3.8322	2.0001	3.5673
$(T-t_0)/2^{13}$	3.8995	2.0003	3.8625
$(T-t_0)/2^{14}$	3.3061	2.0012	2.7886

Table 10 Estimated order $p(h)$ on the van der Pol problem (3.8) with $\varepsilon = 10^{-6}$.

research we aim to provide alternative formulation of the Jacobian-dependent discretizations that avoid the matrix inversion along the integration process, but take advantage from the structure of the involved matrices, especially when the ODE belongs to the discretization of PDEs in space. Moreover, it is worth assessing the effectiveness of the approach also to other kind of operators, such as problems with memory [4–6, 13, 14] and stochastic problems [7, 10–12, 17, 29], and other families of methods, such as multivalue methods [15, 23–25, 32]. In addition, we will consider the effectiveness of this approach on the parallel solution of high dimensional problems [18], for which a CPU time comparison is a further measure of efficiency.

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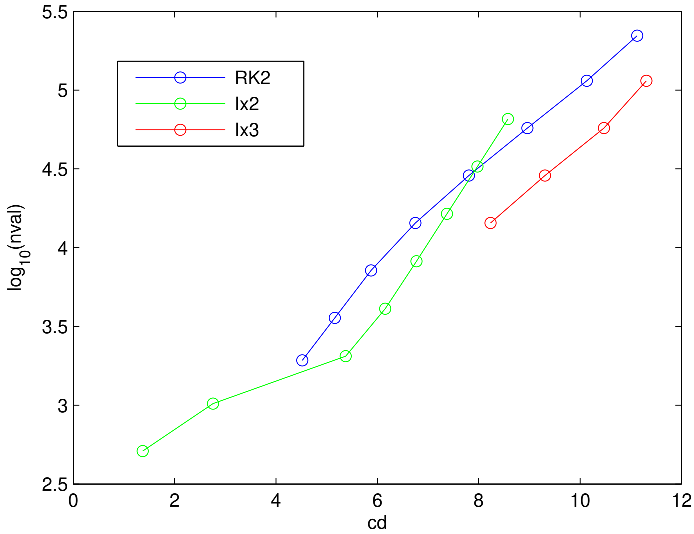

Fig. 5 Work precision diagram related to the van der Pol problem (3.8) with $\varepsilon = 10^{-6}$. The method Ix2 is Ix2(1).

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