On the construction of Restricted-Denominator Exponential W-methods

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Abstract

In this paper we consider the practical construction of exponential W-methods for the solution of large stiff nonlinear initial value problems, based on the Restricted-Denominator rational approach for the computation of the functions of matrices required. This approach is employed together with the Krylov subspace method based on the Arnoldi algorithm. Two integrators are constructed and tested on some classical stiff equations arising from the semidiscretization of parabolic problems.

1 Introduction

In recent years much interest has been devoted to the study of exponential integrators for initial value problems (IVPs). These integrators are based on the computation of the exponential function (or related functions) of the Jacobian or an approximation to it, inside the numerical method (see e.g. [12] for a wide survey). For large and stiff problems, such methods are commonly considered effective alternative to the classical implicit schemes and this is substantially due to the improvements in the efficient computation of the matrix exponential. Indeed, the most efficient iterative algorithms for the computation of $f(A)v$, where $A \in \mathbb{R}^{N\times N}$ and $v \in \mathbb{R}^N$, such as the Krylov expansion methods [18], converge superlinearly if f is an entire function, but only linearly in the contrary case. In this sense, the computation of $\exp(A)v$ is generally less expensive than the solution of a linear system. Actually, when solving IVPs, because of the large number of steps generally performed, it is not so clear if (and in which cases) an exponential integrator can outperform the most effective implicit solvers, that are able to exploit the sparsity pattern of the Jacobian (or an approximation to it) and consequently to use the sparse factorization techniques for the linear algebra problems inside the method. Up to now, the only exponential integrator implemented with stepsize selection is `exp4` [6], and hence few numerical comparisons between exponential integrators and classical implicit solvers are available.

The recent work on exponential integrators is mainly concerned with semi-linear problems of the type

$$y'(t) = Ly(t) + g(t, y(t)), \quad y(t_0) = y_0, \tag{1}$$

where $L \in \mathbb{R}^{N\times N}$ and g is a given function. Indeed, after spatial discretization, many parabolic problem can be well represented by (1), where the difficult part (stiff or oscillatory) is in the linear part. The main idea is to treat the linear part exactly, using the matrix exponential (or related matrix functions), whereas the remaining part of the integrator can be explicit (see e.g. [3], [7], [8], [11], [12]). Anyway, since many IVPs arising from spatial discretization of parabolic problems are well represented by (1) only locally, in this paper we want to consider the construction of exponential integrators for the general autonomous problem

$$y' = f(y), \quad y(t_0) = y_0. \tag{2}$$

We consider exponential integrators of the type

$$\begin{array}{c} k_i = \varphi(\gamma hW)\left(f\left(u_m^{(i)}\right) + hW\sum_{j=1}^{i-1}\gamma_{ij}k_j\right), \quad i = 1, ..., s, \\ u_m^{(i)} = y_m + h\sum_{j=1}^{i-1}\alpha_{ij}k_j, \\ y_{m+1} = y_m + h\sum_{i=1}^{s} b_i k_i, \end{array} \tag{3}$$

where W is an approximation of the Jacobian $f'(y_m)$ and the function φ is

$$\varphi(z) = \frac{e^z - 1}{z}. \tag{4}$$

In [6], the method (3) has been called *Exponential W-method*, since the only basic difference with respect to W- or ROW-methods (see [10] or [21] for a wide background) is the presence of $\varphi(\gamma hW)$ instead of $(I - \gamma hW)^{-1}$. The scheme (3) reduces to an explicit Runge-Kutta method for $\varphi(z) \equiv 1$ and $\gamma_{ij} \equiv 0$.

In [6] the authors use the Krylov expansion method for the computation of k_i, $i = 1, ..., s$, based on the Arnoldi or Lanczos algorithms. Krylov methods are commonly considered as a powerful tool for the computation of functions of large dimensional matrices times a vector, but they also present some disadvantages. Even in the case of entire functions such as (4), the theoretical superlinear convergence does not start immediately but depends on the spectral properties of the matrix involved in the computation. For instance, using the Arnoldi method for the computation of $\exp(A)v$ in which A is a sectorial matrix, the superlinear convergence starts after a phase whose length is proportional to $\|A\|$ (cf. [5]). However, it is worthwhile noting that a similar behavior (and hence a similar drawback), also regards all the existing iterative methods for functions of matrices, such as the methods based on the complex approximation of the function involved by series expansion or interpolation (see e.g. [1], [13]). In this sense, if we consider differential equations in which the Jacobian arises from the semidiscretization of unbounded operators the computation of $\varphi(\gamma hW)v$ can constitute a not negligible problem.

In order to partially overcome this kind of problems, that are particularly relevant in the context of the solution of (2) where a lot of function of matrices have to be computed, our idea is to use the Restricted-Denominator (RD) rational approach for the computation of k_i, $i = 1, ..., s$. This approach, firstly introduced in [17], is based on the approximation of $\varphi(z)$ by rational forms of the type

$$R_{n-1}(z;\delta) = \frac{p_{n-1}(z)}{(1-\delta z)^{n-1}}, \quad p_{n-1} \in \Pi_{n-1}, \quad n \geq 1, \tag{5}$$

where Π_n is the space of the algebraic polynomials of degree $\leq n$ and $\delta > 0$ is a suitable parameter. Setting

$$Z = (I - \delta W)^{-1},$$

the use of (5) means that $\varphi(\gamma hW)v$ is approximated by elements of the Krylov subspaces

$$K_n(Z, v) = span\left\{v, Zv, Z^2v, ..., Z^{n-1}v\right\}, \quad n \geq 1.$$

The aim of this paper is to construct an efficient integrator for (2) based on the scheme (3), in which the operations $\varphi(\gamma hW)v$ are performed using the RD approach together with the Krylov subspace approximation based on the Arnoldi method as described in [14], and already employed in [9] and [16] in the case of the exponential function. Indeed, even if this approach requires a matrix inversion, it is generally very fast, and moreover, as we explain in Section 5, such inversion can be reused many times during the integration. We construct two embedded method of order $p = 4$ and $s = 6$ internal stages: RDE43S that is A(α)-stable with $\alpha \approx 87.1^o$ with 6 function evaluations at each step, and RDE43L, an L-stable method with 4 function evaluation at each step.

The paper is structured as follows. In Section 2 we make some considerations about the linear stability of the exponential W-methods. In Section 3 we describe the construction of the methods RDE43s and RDE43L, whose complete sets of coefficients are given in the Appendix. In Section 4 we explain the Restricted-Denominator rational Arnoldi method for the computation of k_i, $i = 1, ..., s$. Section 5 is devoted to the numerical implementation of the two methods proposed. Finally in Section 6 we present some numerical experiments.

2 Linear stability

Looking at the general formula (3) and working as with a ROW-method, we set

$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}, \quad \beta_{ij} = \alpha_{ij} + \gamma_{ij}, \quad \beta_i = \sum_{j=1}^{i-1} \beta_{ij}, \qquad i, j = 1, ..., s.$$

Defining $b = (b_1, ..., b_s)^T$, $\beta = (\beta_{ij})_{i,j=1,...,s}$, $e = (1, ..., 1)^T$, after some computation by (3) we get the relation

$$\begin{aligned} y_{m+1} &= \left(I + \sum_{k=0}^{s-1} b^T \beta^k e w^{k+1} \right) y_m + \\ & \quad h \sum_{k=0}^{s-1} \sum_{j=1}^{s} b^T \beta^k e_j w^k \left(I + \gamma w \right) \left(f\left(u_m^{(i)} \right) - W u_m^{(i)} \right), \end{aligned}$$

where $w = \varphi(\gamma h W) h W$ [22]. Applying the method to the scalar test equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C},$$

with $W = \lambda$ we get

$$y_{m+1} = R(z) y_m, \quad z = h\lambda,$$

where

$$R(z) = 1 + \sum_{k=0}^{s-1} b^T \beta^k e w^{k+1}, \tag{6}$$

is a sum of exponentials. Clearly, the A-stability is not ensured for an arbitrary choice of the coefficients of the method.

Theorem 1 *For an s-stage exponential W-method the conditions*

$$b^T \beta^k e = \frac{1}{(k+1)!} \gamma^{k+1} \prod_{j=0}^{k} \left(\frac{1}{\gamma} - j \right), \quad k = 0, ...p-1, \tag{7}$$

are necessary for having consistency order $p \leq s$.

Proof. By (6) we have

$$\begin{aligned} R(z) &= 1 + \sum_{k=0}^{s-1} \frac{b^T \beta^k e}{\gamma^{k+1}} \left(\exp(\gamma z) - 1 \right)^{k+1} \\ &= 1 + \sum_{k=0}^{s-1} \frac{b^T \beta^k e}{\gamma^{k+1}} (k+1)! \sum_{n=1}^{\infty} S(n, k+1) \gamma^n \frac{z^n}{n!} \\ &= 1 + \sum_{n=1}^{\infty} \left(\sum_{k=0}^{s-1} \frac{b^T \beta^k e}{\gamma^{k+1}} (k+1)! S(n, k+1) \gamma^n \right) \frac{z^n}{n!}, \end{aligned}$$

where

$$S(n, k+1) = \frac{1}{(k+1)!} \sum_{j=1}^{k+1} (-1)^{k+1-j} \binom{k+1}{j} j^n,$$

are the Stirling numbers of the second kind (see e.g. [2]). Hence, for having order $p \leq s$ it is necessary that

$$\gamma^n \sum_{k=0}^{n-1} \frac{b^T \beta^k e}{\gamma^{k+1}} (k+1)! S(n, k+1) = 1, \quad n = 1, ..., p,$$

since $S(n,k+1)=0$ for $k+1>n$. Defining $b^T\beta^k e$ as in (7) we get

$$\gamma^n \sum_{k=0}^{n-1} \frac{b^T\beta^k e}{\gamma^{k+1}}(k+1)!S(n,k+1) = \gamma^n \sum_{k=0}^{n-1}\prod_{j=0}^{k}\left(\frac{1}{\gamma}-j\right)S(n,k+1).$$

By [2] p.85 we know that

$$\sum_{k=0}^{n-1}\prod_{j=0}^{k}\left(\frac{1}{\gamma}-j\right)S(n,k+1) = \frac{1}{\gamma^n}, \quad n\geq 1,$$

and hence the Theorem is proved. ■

Theorem 2 *Assume that an s-stage exponential W-method satisfies (7) for* $k = 1,...,s-1$. *If* $\gamma = 1/k$ *for* $k \in \{1, 2..., s-1\}$ *then* $R(z) = \exp(z)$.

Proof. Let $1 \leq k \leq s-1$, and $\gamma = 1/k$. By (7) we clearly have $b^T\beta^n e = 0$ for $n = k,...,s-1$. Then

$$R(z) = 1 + \sum_{n=0}^{k-1} b^T\beta^n e k^{n+1}\left(\exp\left(\frac{z}{k}\right)-1\right)^{n+1}.$$

Since for $1 \leq n \leq k-1$

$$b^T\beta^n e = \frac{1}{n+1}\frac{1}{k^n}\binom{k-1}{n},$$

we get

$$\begin{aligned} R(z) &= 1 + \sum_{n=0}^{k-1}\frac{k}{n+1}\binom{k-1}{n}\left(\exp\left(\frac{z}{k}\right)-1\right)^{n+1} \\ &= 1 + \sum_{m=1}^{k}\binom{k}{m}\left(\exp\left(\frac{z}{k}\right)-1\right)^{m} \\ &= \exp(z). \end{aligned}$$

■

The above theorem explains how to choose γ and the entries of b and β in order to get an L-stable method. This result will be used in the next section.

3 The construction of two embedded methods of order 4

The construction of an embedded exponential W-method of order 4(3) requires 21 conditions for the basic method to get $p = 4$ and 8 conditions for the embedded one to achieve $p = 3$, if the Jacobian is approximated by an arbitrary

matrix [6]. However, since our idea is to start with the exact Jacobian, keep it constant for a certain number of steps and than recompute it, the approximations we consider are of the type $W = J + O(h)$. In this situation some of the order conditions can be shifted to higher order and some can be omitted since we assume to work with autonomous systems.

Hence, in our case there are 11 conditions for having order $p = 4$ (see [6] and [21]):

$$\begin{array}{lll} p=1 & \text{(R1)} & b^T e = 1 \\ p=2 & \text{(R2)} & b^T \beta e = 1/2\,(1-\gamma) \\ p=3 & \text{(R3a)} & b^T \alpha^2 = 1/3 \\ & \text{(R3b)} & b^T \beta^2 e = 1/3\,(1-\gamma)\,(1/2-\gamma) \\ & \text{(W3)} & b^T \alpha = 1/2 \\ p=4 & \text{(R4a)} & b^T \alpha^3 = 1/4 \\ & \text{(R4b)} & \varphi^T \overline{\alpha} \beta e = 1/8 - \gamma/6 \\ & \text{(R4c)} & b^T \beta \alpha^2 = 1/12 - \gamma/6 \\ & \text{(R4d)} & b^T \beta^3 e = 1/4\,(1-\gamma)\,(1/2-\gamma)(1/3-\gamma) \\ & \text{(W4a)} & b^T \overline{\alpha} \beta e = 1/6 - \gamma/4 \\ & \text{(W4b)} & b^T \beta \alpha = 1/6 - \gamma/4 \end{array} \tag{8}$$

where we define $\overline{\alpha} = (\alpha_{ij})_{i,j=1,...,s}$, and $\varphi = (b_1\alpha_1, ..., b_s\alpha_s)^T$. Of course, the embedded method, with weights $\overline{b}_i$, $i = 1, ..., s$, has to fulfil the first 5 conditions of (8). Moreover, for the basic method we set the additional condition

$$\text{(A3)} \quad b^T \overline{\alpha} \alpha = 1/6 \tag{9}$$

that completes the set of condition of order 3 for a general exponential W-method. In this way, whenever the condition $W = J+O(h)$ fails, the order of the basic method drops down to 3 instead of 2 whereas the order of the embedded one drops down to 2. In this section we present two methods, RDE43S and RDE43L. We choose to have $s = 6$ internal stages, since this is the minimum number for the construction of embedded pairs of order 4(3).

3.1 RDE43S

We require that the method fulfils the relations

$$b_i = \beta_{si}, \quad i = 1, ..., s-1, \quad b_s = \gamma \quad \text{and} \quad \alpha_s = 1, \tag{10}$$

$$\overline{b}_i = \beta_{s-1,i} = \alpha_{si} \quad i = 1, ..., s-1, \quad \alpha_{s-1} = 1. \tag{11}$$

The above relations, define a stiffly accurate embedded ROW-method (see e.g. the construction of RODAS in [10]) because they ensure $R(-\infty) = 0$. Anyway such definition can also be applied for an exponential ROW-method (that is, an exponential W-method in which $W = f'(y_m)$), as stated by the following.

Proposition 3 *For the exponential W-method (3)*

$$R(-\infty) = 1 - b^T(\gamma I + \beta)^{-1} e. \tag{12}$$

Proof. Since β is strictly lower triangular, by (6) we get

$$R(z) = 1 + z\varphi(\gamma z) b^T \left(I - z\varphi(\gamma z)\beta\right)^{-1} e.$$

Then, using

$$\lim_{z\to-\infty} z\varphi(\gamma z) = -\frac{1}{\gamma},$$

we easily get the thesis. ■

Formula (12) is exactly the same of ROW-methods (see [10]) so that the conditions (10)-(11) ensure that $R(-\infty) = 0$.

Using (10)-(11) and inserting them into (8)-(9) we can simplify the set of conditions. By direct computation it is not difficult to see that the conditions (10)-(11) together with the first 5 conditions of (8) that must be fulfilled by both methods imply $b_i = \bar{b}_i$, $i = 1, ..., 4$, and $b_5 = 0$. Therefore the conditions (8)-(9) become

$$\begin{array}{ll}
\text{(R1')} & b_1 + b_2 + b_3 + b_4 = 1 - \gamma \\
\text{(R2')} & b_2\beta_2 + b_3\beta_3 + b_4\beta_4 = 1/2 - 3\gamma/2 + \gamma^2 \\
\text{(R3a')} & b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2 = 1/3 - \gamma \\
\text{(R3b')} & b_3\beta_{32}\beta_2 + b_4(\beta_{42}\beta_2 + \beta_{43}\beta_3) = 1/6 - \gamma + 11\gamma^2/6 - \gamma^3 \\
\text{(W3')} & b_2\alpha_2 + b_3\alpha_3 + b_4\alpha_4 = 1/2 - \gamma \\
\text{(R4a')} & b_2\alpha_2^3 + b_3\alpha_3^3 + b_4\alpha_4^3 = 1/4 - \gamma \\
\text{(R4b')} & b_3\alpha_3\alpha_{32}\beta_2 + b_4\alpha_4(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = 1/8 - 2\gamma/3 + \gamma^2/2 \\
\text{(R4c')} & b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) = 1/12 - \gamma/2 + \gamma^2 \\
\text{(R4d')} & b_4\beta_{43}\beta_{32}\beta_2 = 1/24 - 5\gamma/12 + 35\gamma^2/24 - 25\gamma^3/12 + \gamma^4 \\
\text{(W4a')} & b_3\alpha_{32}\beta_2 + b_4(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = 1/6 - 3\gamma/4 + \gamma^2/2 \\
\text{(W4b')} & b_3\beta_{32}\alpha_2 + b_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) = 1/6 - 3\gamma/4 + \gamma^2 \\
\text{(A3')} & b_3\alpha_{32}\alpha_2 + b_4(\alpha_{42}\alpha_2 + \alpha_{43}\alpha_3) = 1/6 - \gamma/2
\end{array} \tag{13}$$

The above system can be solved in the following manner. Setting γ and $\alpha_2, \alpha_3, \alpha_4$, we find b_1, b_2, b_3, b_4 from (R1'), (R3a'), (W3'), (R4a')

Setting β_{32} we find β_{42} and β_{43} by (R3b') and (W4b'). Then from (R4d') we find β_2. By (R3b') we have β_3 and by (R2') we can compute β_4. Then, by (R4b'), (W4a') and (A3') we get α_{32}, α_{42} and α_{43}. Regarding γ, the choices $\gamma = 1, 1/2, 1/3, 1/4$ as suggested by Theorem 2 are unfeasible because they lead to a singular system. We set $\gamma = 0.23$, in order to get a compromise between a wide A-stability region and to stay far from singularities of (13). With our choice the method is not A-stable; it is A(α)-stable with $\alpha \approx 87.1^o$ but contains the whole half-plane $\{z \in C : \Re(z) < -0.65\}$. The remaining free parameters $\alpha_2, \alpha_3, \alpha_4, \beta_{32}, \alpha_{51}, \alpha_{52}, \alpha_{53}$ are fixed in order to maintain the error constant small. In Fig.1 the boundary of the A-stability region is plotted.

3.2 RDE43L

The second method we propose, RDE43L, is theoretically cheaper than RDE43S, because it requires only 4 function evaluations per step. Moreover for this method we require $R(z) = \exp(z)$. Therefore, setting $\alpha_{61} = \alpha_{51} = \alpha_{41}$, $\alpha_{62} =$

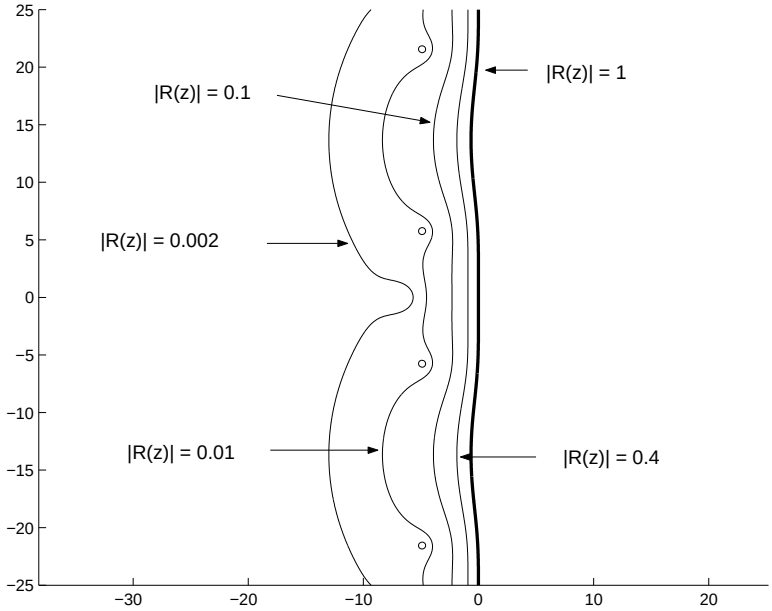

Figure 1: Boundary of the A-stability region of RDE43S and some contour lines.

$\alpha_{52} = \alpha_{42}$, $\alpha_{63} = \alpha_{53} = \alpha_{43}$, $\alpha_{64} = \alpha_{54} = 0$, $\alpha_{65} = 0$, and $\alpha_6 = \alpha_5 = \alpha_4 = 1$, conditions (8)-(9) becomes

(R1)	$b_1 + b_2 + b_3 + b_4 + b_5 + b_6 = 1$
(R2)	$b_2\beta_2 + b_3\beta_3 + b_4\beta_4 + b_5\beta_5 + b_6\beta_6 = 1/2(1-\gamma)$
(R3a")	$b_2\alpha_2^2 + b_3\alpha_3^2 + (b_4 + b_5 + b_6) = 1/3$
(R3b)	$b_3\beta_{32}\beta_2 + b_4(\beta_{42}\beta_2 + \beta_{43}\beta_3) + b_5(\beta_{52}\beta_2 + \beta_{53}\beta_3 + \beta_{54}\beta_4)$ $+b_6(\beta_{62}\beta_2 + \beta_{63}\beta_3 + \beta_{64}\beta_4 + \beta_{65}\beta_5) = 1/3(1-\gamma)(1/2-\gamma)$
(W3")	$b_2\alpha_2 + b_3\alpha_3 + (b_4 + b_5 + b_6) = 1/2$
(R4a")	$b_2\alpha_2^3 + b_3\alpha_3^3 + (b_4 + b_5 + b_6) = 1/4$
(R4b")	$b_3\alpha_3\alpha_{32}\beta_2 + (b_4 + b_5 + b_6)\,(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = 1/8 - \gamma/6$
(R4c")	$b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) + b_5(\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54})$ $+b_6(\beta_{62}\alpha_2^2 + \beta_{63}\alpha_3^2 + \beta_{64} + \beta_{65}) = 1/12 - \gamma/6$
(R4d)	$b_4\beta_{43}\beta_{32}\beta_2 + b_5(\beta_{53}\beta_{32}\beta_2 + \beta_{54}\beta_{43}\beta_3 + \beta_{54}\beta_{42}\beta_2)$ $+b_6(\beta_{63}\beta_{32}\beta_2 + \beta_{64}\beta_{42}\beta_2 + \beta_{64}\beta_{43}\beta_3 + \beta_{65}\beta_{52}\beta_2 + \beta_{65}\beta_{53}\beta_3 + \beta_{65}\beta_{54}\beta_4)$ $= 1/4(1-\gamma)(1/2-\gamma)(1/3-\gamma)$
(W4a")	$b_3\alpha_{32}\beta_2 + (b_4 + b_5 + b_6)\,(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) = 1/6 - \gamma/4$
(W4b")	$b_3\beta_{32}\alpha_2 + b_4(\beta_{42}\alpha_2 + \beta_{43}\alpha_3) + b_5(\beta_{52}\alpha_2 + \beta_{53}\alpha_3 + \beta_{54})$ $+b_6(\beta_{62}\alpha_2 + \beta_{63}\alpha_3 + \beta_{64} + \beta_{65}) = 1/6 - \gamma/4$
(A3")	$b_3\alpha_{32}\alpha_2 + (b_4 + b_5 + b_6)\,(\alpha_{42}\alpha_2 + \alpha_{43}\alpha_3) = 1/6$

Hence, setting α_2, α_3 we find b_1, b_2, b_3 and $\eta = b_4 + b_5 + b_6$. Defining b_4, b_5 we get b_6. Setting α_{42} and α_{43} by (A3") we obtain α_{32}. Defining γ, from

(W4a") and (R4b") we get β_2 and $(\alpha_{42}\beta_2 + \alpha_{43}\beta_3)$, and then β_3. We set $\beta_{42} = \beta_{53} = \beta_{64} = \beta_{52} = \beta_{63} = \beta_{62} = 0$ and $\beta_{43} = \beta_{65} = 0$ in order that $b^T\beta^k e = 0$ for $k = 3, 4, 5$ (cf. Theorem 2). In this way, with $\gamma = 1/3$ and setting β_{32} such that $b_3\beta_{32} = 0.5$, we chose $\alpha_2 = 1/2 - \sqrt{5}/6$ between the two roots of the equation arising from (W4b") and (R4c"). Therefore, by (W4b") we find β_{54}. Then we get β_4 from (R3b). Defining β_5 we find β_6 by (R2). For the embedded method we set $\bar{b}_6 = 0$ so that the other weights are uniquely determined.

The following theorem summarizes the properties of the methods proposed, whose complete sets of coefficients are given in the Appendix.

Theorem 4 *RDE43S and RDE43L are method of order 4 for differential equations (2) when they are used with exact Jacobian or when $W = f'(y_m) + O(h)$, $m \geq 0$. When used with an arbitrary approximation of the Jacobian they are of order 3. Moreover RDE43L is L-stable and exact for linear problems of the type $y' = Ay + b$. RDE43S is $A(\alpha)$-stable with $\alpha = 87.1^o$ and fulfils $R(-\infty) = 0$.*

4 The Restricted-Denominator rational Arnoldi method

In this section we consider the practical computation of $\varphi(\gamma hW)v$ by means of the RD rational Arnoldi method (we refer to [14] for a complete background). We assume that the numerical range of W

$$F(W) = \left\{ \frac{x^H W x}{x^H x}, x \in \mathbb{C} \backslash \{0\} \right\},$$

is strictly contained in the left-half complex plane. In the sequel we denote by $\|\cdot\|$ the Euclidean norm.

As already explained in the introduction, the RD rational approach is based on the approximation of $\varphi(z)$ by rational forms of the type

$$R_{n-1}(z;\delta) = \frac{p_{n-1}(z)}{(1-\delta z)^{n-1}}, \quad p_{n-1} \in \Pi_{n-1}, \quad n \geq 1, \tag{14}$$

where $\delta > 0$ is a suitable parameter. Setting

$$Z = (I - \delta W)^{-1} \tag{15}$$

the use of (14) means that $\varphi(\gamma hW)v$ is approximated by elements of the Krylov subspaces $K_n(Z, v)$.Because of the spectral properties of W the matrix Z is well defined for each $\delta > 0$. Using the Arnoldi algorithm for the construction of the subspaces $K_n(Z, v)$ we get an orthonormal sequence $\{v_1, v_2, ..., v_j, ...\}$, with $v_1 = v/\|v\|$, such that $K_n(Z, v) = span\{v_1, v_2, ..., v_n\}$. Moreover, for each $n \geq 1$,

$$ZV_n = V_n H_n + h_{n+1,n} v_{n+1} e_n^T.$$

where $V_n = [v_1, v_2, ..., v_n]$, e_j is the j-th vector of the canonical basis of $\mathbb{R}^n$, H_n is an upper Hessenberg matrix whose entries are $h_{i,j}$, $i, j = 1, ..., n$.

In this way, the n-th RD rational Arnoldi approximation to $q = \varphi(\gamma h W)v$ is defined as

$$q_n = \|v\| \, V_n \phi(H_n) e_1,$$

where

$$\phi(z) = \varphi\left(\frac{\gamma h}{\delta}\left(1 - \frac{1}{z}\right)\right), \tag{16}$$

or equivalently

$$q_n = \|v\| \, V_n \varphi(B_n) e_1,$$

where

$$B_n = \frac{\gamma h}{\delta}\left(I - H_n^{-1}\right).$$

Writing

$$q_n = p_{n-1}^*(Z)v,$$

it is known that $p_{n-1}^* \in \Pi_{n-1}$ interpolates, in the Hermite sense, the function $\phi(z)$ in the eigenvalues of H_n.

Besides the fast convergence, an important feature of such method, pointed out in [9] and [16], is that, contrary to the classical polynomial approach based on the construction of the Krylov subspaces $K_n(W, v)$, the convergence does not depend on the norm of W. In particular, if W is a sectorial matrix and $F(W) \subset \mathbb{C}^-$, the method attains the so called mesh independence property, because $F(Z)$ is contained in the disk centered in $1/2$ and with radius $1/2$ for each $\delta > 0$. In other words, as pointed out in [9], the method produces classical Krylov polynomial approximations just for a preconditioned problem.

Clearly the main drawback of these methods regards the computation of the matrix Z. Actually, as suggested in [9], this computation can be avoided using an iterative method for linear systems within the Arnoldi iterations. Anyhow, in the context of the solution of differential equations, the explicit computation of Z (by means of a factorization) is preferable, since this matrix can be reused many times during the integration (see Section 5 for more details).

Regarding the error $e_n = q - q_n$ of the method just explained, in [14] the author shows that it can be bounded as

$$\|e_n\| \leq C_n \prod_{i=1}^{n} h_{i+1,i} \, \|v\|, \tag{17}$$

where $h_{i+1,i}$ are the subdiagonal entries of H_n and C_n depends on δ and the spectral properties of W. For the symmetric case, in [14] a useful bound has been derived, by means of Laguerre polynomials. Such bound can be obtained defining

$$C_n = \frac{\exp\left(\frac{h\gamma}{\delta} - n\right) 2^{n+2} n^n}{\left(\frac{h\gamma}{\delta}\right)^{n+1}}. \tag{18}$$

The nonsymmetric case is a bit more complicate because the angle of the sector containing $F(W)$ must be taken into account [15]. In this case one typically makes use of the *generalized residual* [6], but, as explained in next section, we adopt a different approach.

5 Numerical implementation

In this section we want to provide some details concerning the practical implementation of the methods proposed in Section 3, RDE34S and RDE43L. We have created a Matlab code `RDE43` available at `http://univaq.it/~novati`. The code is written following the format used in THE MATLAB ODE SUITE [19], and allows to choose between the two methods.

5.1 Stepsize control

Regarding the local error estimate at the m-th step, denoted by τ_m, we consider the weighted norm

$$err_m = \left(\frac{1}{N} \sum_{i=1}^{N} \left(\frac{\tau_{m,i}}{atol_i + \max\left(|y_{m,i}|, |y_{m-1,i}|\right) rtol} \right)^2 \right)^{1/2},$$

where $atol \in \mathbb{R}^N$ and $rtol \in \mathbb{R}$ are the absolute and relative tolerances respectively. As usual, the stepsize is accepted if $err_m \leq 1$. In our numerical experiments, we adopt the stepsize selection due to Gustafsson (see [10])

$$h_{m+1} = h_m \min\left\{ fac_{\overline{M}}, \max\left\{ fac_{\underline{M}}, fac_s \frac{h_m}{h_{m-1}} \left(\frac{err_{m-1}}{err_m^2} \right)^{1/p} \right\} \right\}, \qquad (19)$$

where we chose $fac_{\overline{M}} = 5$, $fac_{\underline{M}} = 0.2$ and $fac_s = 0.8$.

5.2 Stopping criterion in the computation of $\varphi(h\gamma W)v$

As discussed in Section 4, for the computation of $\varphi(h\gamma W)v$ we employ the RD rational Arnoldi method. In order to monitor the error during the Arnoldi iteration one typically uses the so-called generalized residual. Anyway this approach requires the solution of all (or several) subproblems during the iteration, that is, the computation of $\phi(H_n)$, where ϕ is defined by (16), for $n \geq 1$. Since we want to avoid this computation we define (cf. (17)-(18))

$$d_n := \frac{\exp\left(\frac{h\gamma}{\delta} - n\right) 2^{n+2} n^n}{\left(\frac{h\gamma}{\delta}\right)^{n+1}} \prod_{i=1}^{n} h_{i+1,i} \left\| v \right\|, \qquad (20)$$

and then, since k_i $(i = 1, ..., s)$ is multiplied by h, the idea is to use the stopping criterion

$$h \frac{d_n}{rtol} K \leq 1, \qquad (21)$$

where $K \geq 1$ is a safety factor, whose introduction is motivated by the fact that formula (20) holds only in the symmetric case. Many numerical experiments with $1 \leq K \leq 2$ on stiff equations with unsymmetric Jacobian arising from parabolic problems confirmed the effectiveness of this heuristic approach. For the experiments of next section we set $K = 1$.

5.3 The choice of δ

As pointed out in [16] and [9] in the case of the exponential function, if one looks at the error of the n-th approximation a value like $\delta = h\gamma/n$ turns out to be the optimal one. This seems a reasonable choice even for our case. For instance if we take δ in order to minimize d_n in (20) we just obtain $\delta = h\gamma/(n+1)$. In this sense one can use a formula of the type

$$\delta = h\gamma/n^*, \tag{22}$$

with n^* chosen by means of some a-priori error estimates. For our method, given the initial step we define initially $\delta = h\gamma/5$, and then at each accepted step we observe the maximum number Krylov iterations $\overline{n}$ performed for the computation of the 6 stages. Then we use $\overline{n}$ as the a priori estimate for the required number of iterations to get (21).

5.4 Savings from previous steps

The method proposed may reuse the Jacobian of a previous step as an approximation of the current Jacobian. Similarly to the code `VODE` (see e.g. [4]), we adopt the following controls in order to decide wether to compute the Jacobian or not.

1. $$\left| \frac{h_{m+1} - h_m}{h_m} \right| \geq c;$$
2. the Jacobian has not been updated since $\overline{m}$ steps.

Typical values in this context are $c \in [0.2, 0.4]$, $\overline{m} \in [10, 40]$ depending on the accuracy requirements and the problem to be solved. In this sense, our methods are implemented computing the new Jacobian if one of the above conditions holds.

Since we intend to solve exactly the linear systems within the Arnoldi iteration using the LU (or Cholesky) decomposition of $I - \delta W$, the reuse of a previous Jacobian clearly can reduce the number of such decompositions. In fact, when a new stepsize h_{m+1} is predicted without Jacobian update, the previous LU factorization of

$$I - \frac{h_m \gamma}{n_m} W,$$

(cf. (22)) where n_m is the a-priori estimate explained above, the current LU factorization is the same if we define $n_{m+1} = n_m\,(h_{m+1}/h_m)$.

The numerical experiments reveal that the RD rational Arnoldi method and also formula (20) preserve their effectiveness for a window of value of δ (cf. [14]). In this sense in our code we allow the reuse of a previous LU decomposition whenever

$$\max(1, \lambda n_m) \leq n_{m+1} \leq \mu n_m,$$

where $\lambda < 1$, $\mu > 1$. This is done even when a failed attempt occurs (note that the value of n_m comes from an accepted step). Although this may seem a bit complicate the reuse of previous LU decompositions is fundamental for the construction of an efficient integrator based on the RD Arnoldi method because the LU decompositions can have a great influence on the global cost of the method.

5.5 Computational costs

Many numerical experiments revealed that formula (21) is even too much conservative even in the nonsymmetric cases. The reason lies in the use of the bound (20) when the value δ is far from the optimal one. However there is also the advantage of avoiding the computation of $\phi(H_n)$ at each Krylov step, that would be necessary using the generalized residual as estimator.

Therefore, because of the mesh-independence property of the RD-based approach, at each step of the method we have $s\upsilon$ Krylov iterations, typically with $\upsilon \leq 10$ for sectorial matrices, independently of the dimension of the problem. This is the major advantage of this approach with respect to the classical Arnoldi method, where for large dimensional problems the superlinear convergence could require a large number of iterations.

6 Numerical Experiments

In this section we compare the methods RDE43S and RDE43L implemented in `RDE43` with the Matlab stiff solver `ode15s` (a BDF method), `exp4` [6], the only existing variable stepsize exponential integrator for (2), and `RODASP` (by Steinebach [20]), a powerful fourth order ROW-method used with the incomplete LU preconditioning together with the BI-CGSTAB for the linear algebra required. Regarding `RDE43` we set $c = 0.3$, $\overline{m} = 30$, $\lambda = 1/3$, $\mu = 3$ (cf. 5.3, 5.4).

The test problems we consider are well-known nonlinear equations arising from parabolic PDEs.

1. The Fischer's equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u^2(1-u),$$

with initial condition $u(x,0) = \sin(\pi x)$ and Dirichlet boundary conditions, for $0 \leq x \leq 1$ and $0 \leq t \leq 2$. We discretize with central differences and the method of lines with meshsize $\Delta = 1/1001$, getting a system of 1000 equations.

2. The equation

$$\frac{\partial u}{\partial t} = \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - u \frac{\partial u}{\partial x} - u \frac{\partial u}{\partial y}, \tag{23}$$

on $[0, 1/2] \times [0, 1/2]$ and $0 \leq t \leq 0.1$, with $\nu = 0.1$. Initial and time-dependent boundary conditions are taken from the exact solution

$$u(x, y, t) = \frac{1}{1 + \exp\left(\frac{x+y-t}{2\nu}\right)}.$$

Discretizing as before with $\Delta = 1/62$ we get a system of 900 equations. We solve this system after writing it in the corresponding autonomous form.

3. The NILIDI problem [23], i.e., the two-dimensional nonlinear diffusion equation

$$\frac{\partial u}{\partial t} = e^u \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + u \left(18 e^u - 1 \right),$$

on $[0, \pi/3] \times [0, \pi/3]$ and $0 \leq t \leq 1$. We consider the initial condition $u(x, y, 0) = \sin(3x) \sin(3y)$ and Dirichlet boundary conditions. We discretize as before with uniform meshsize $\Delta = \pi/105$, getting a system of 1225 equations.

4. The Burgers' equation

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} - u \frac{\partial u}{\partial x},$$

with initial condition $u(x, 0) = x \left(1 - x\right)^2$ and Dirichlet boundary conditions, for $0 \leq x \leq 1$ and $0 \leq t \leq 1$. We discretize with meshsize $\Delta = 1/1001$ getting a systems of 1000 equations. We set $\nu = 1$.

For each example, we compare the obtained numerical results for each methods with a reference solution for the given ODE. The computing time ($NSEC$) is displayed as a function of the Euclidean norm of the error at the endpoint (ERR). For each problem we set $atol_i = rtol = TOL$, $i = 1, ..., N$, and the methods have been applied with

$$TOL = 10^{-2}, 10^{-3}, ...$$

In Figures 2-5 the diagrams relative to the test problems considered are shown. The results prove that the code `RDE43` represents an efficient solver for such problems. The RD rational approach for the computation of the functions of matrices inside the method appears as a powerful tool in the context of the solution of differential equations arising from parabolic problems, where the Jacobian is generally sparse and structured. In particular, with the exception of the ODE arising from (23), RDE43L seems to be the best of the methods considered, especially for high accuracy requirements. Moreover, for all the examples

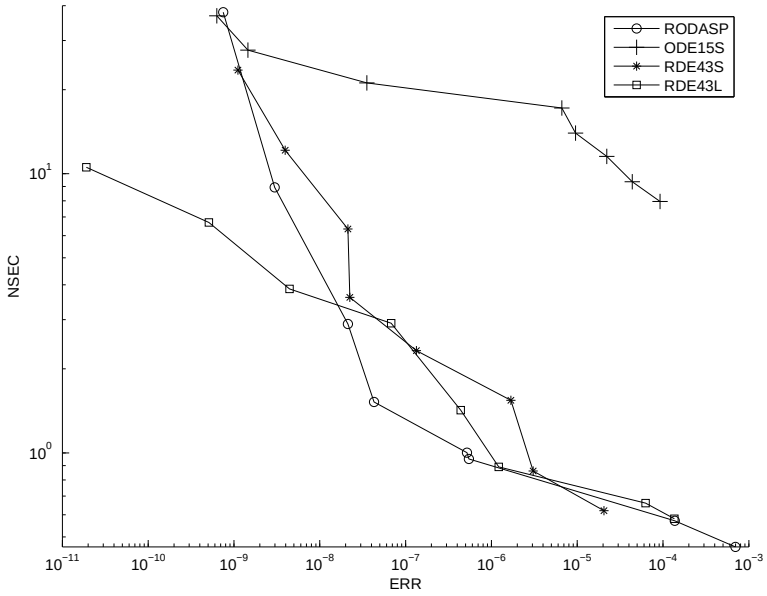

Figure 2: Work-precision diagram for the Fischer problem.

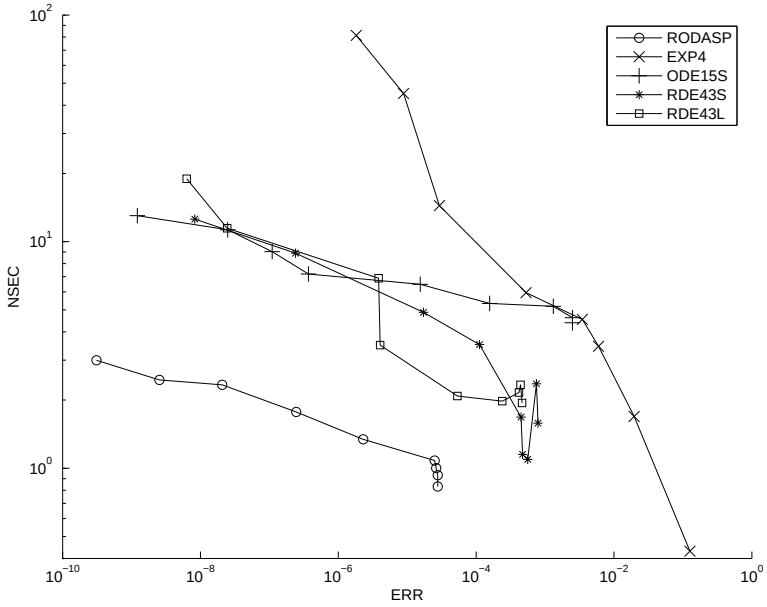

Figure 3: Work-precision diagram for the problem (23).

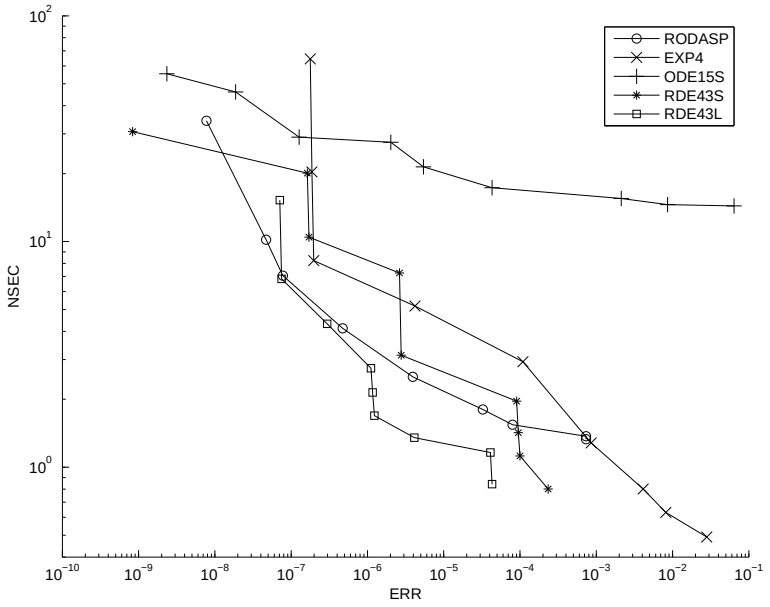

Figure 4: Work-precision diagram for the NILIDI problem.

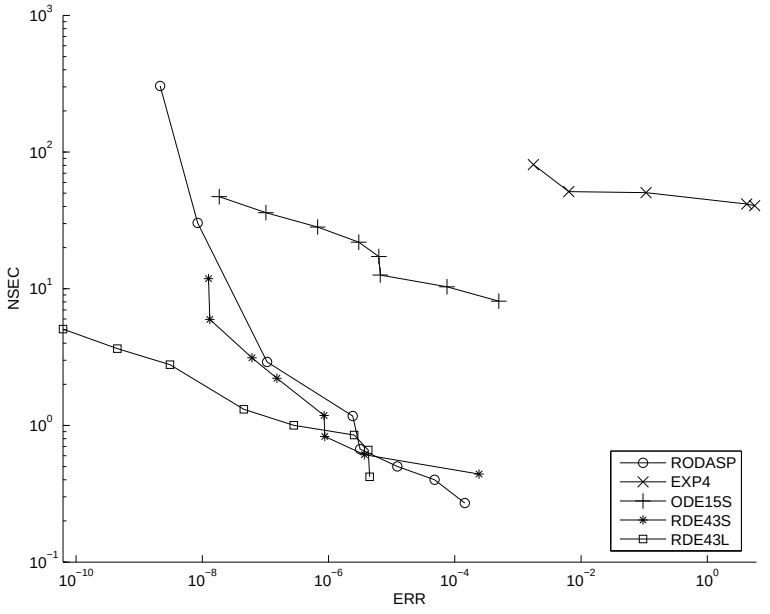

Figure 5: Work-precision diagram for the Burgers problem.

we can also appreciate the error curves of `RODASP` that uses the incomplete LU preconditioning together with the BI-CGSTAB method for the linear systems inside the integrator. Maybe this approach could represent an improvement also for the methods presented in the paper. We must point out that for the Fischer problem (Figure 2) the behavior of `exp4` is very bad and hence it is not represented.

For the Burgers problem, in Table 1 we also report the statistics for RDE43S and RDE43L respectively. In the table, $NSTP$ is the number of steps, PD is the number of Jacobian evaluations, LU is the number of LU decompositions, $KSTP$ is the total number of Krylov steps and MKS is the mean value of Krylov steps. It is interesting to observe that MKS is considerably small with respect to the dimension of the problem.

TOL	$NSTP$	PD	LU	$KSTP$	MKS	ERR	$NSEC$
10^{-2}	8	8	9	165	3.43	$2.42\ 10^{-4}$	2.80
	8	8	9	149	3.10	$4.47\ 10^{-5}$	2.64
10^{-3}	11	11	12	250	3.78	$3.68\ 10^{-6}$	2.88
	10	10	11	228	3.80	$5.08\ 10^{-5}$	2.76
10^{-4}	15	12	13	369	4.10	$8.69\ 10^{-7}$	3.07
	12	12	13	317	4.40	$2.54\ 10^{-6}$	2.92
10^{-5}	21	16	17	545	4.32	$8.52\ 10^{-7}$	3.42
	13	13	14	410	5.25	$2.81\ 10^{-7}$	3.09
10^{-6}	38	18	19	1096	4.80	$1.51\ 10^{-7}$	4.46
	17	17	18	570	5.58	$4.54\ 10^{-8}$	3.38
10^{-7}	52	43	44	1439	4.61	$6.12\ 10^{-8}$	5.25
	36	15	16	1392	6.44	$3.07\ 10^{-9}$	4.92
10^{-8}	85	80	81	2813	5.51	$1.31\ 10^{-8}$	8.02
	52	19	20	1823	5.84	$4.49\ 10^{-10}$	5.70
10^{-9}	164	19	22	6672	6.78	$1.45\ 10^{-9}$	9.60
	76	10	12	2694	5.91	$5.60\ 10^{-11}$	4.53

Table 1. Statistics for RDE43S / RDE43L for Burgers' problem.

Finally, working once again with the Burgers' problem, in Table 2 we show the statistics for RDE43S and RDE43L changing the dimension of the problem N. For each case, we apply the methods with $TOL = 10^{-6}$.

N	$NSTP$	PD	LU	$KSTP$	MKS	ERR	$NSEC$
200	36	20	21	879	4.06	$6.95\ 10^{-8}$	0.75
	17	17	18	462	4.52	$1.01\ 10^{-7}$	0.39
400	37	19	20	968	4.36	$2.54\ 10^{-7}$	1.35
	17	17	18	509	4.99	$4.01\ 10^{-8}$	0.73
600	37	19	20	1007	4.53	$3.12\ 10^{-7}$	1.95
	17	17	18	518	5.07	$5.29\ 10^{-8}$	1.24
800	38	18	19	1098	4.81	$1.34\ 10^{-7}$	3.05
	17	17	18	545	5.34	$6.73\ 10^{-8}$	2.16
1000	38	18	19	1096	4.80	$1.51\ 10^{-7}$	4.46
	17	17	18	570	5.58	$4.54\ 10^{-8}$	3.38

Table 2. Statistics for RDE43S / RDE43L for Burgers' problem with different meshsizes.

The statistics reported in the above table show that the methods do not suffer from the dimension of the problem. This is due to the mesh independence property [16]. As already said, by (15) the underlying unbounded operator is transformed into a compact operator whose spectrum lies in the disk centered in 1/2 and with radius 1/2. In this way the error of the RD rational method does not depend on $\|W\|$. This is the fundamental reason that makes the RD approach attractive for large dimensional problems.

A concluding important remark regards the computation of $\phi(H_n)$ at each final Arnoldi iteration. Since the mean number of Arnoldi iterations is typically small and independent of the dimension of the problem, $\phi(H_n)$ can be computed with an "exact" method (for instance by means of the Schur decomposition). This is a clear advantage with respect to the polynomial approach, in which one is generally forced to use some Padé approximation, that can make the integrator unsuited for highly stiff equations.

7 Appendix

γ	=	$2.300000000000000e-01$			
α_{21}	=	$5.000000000000000e-01$	γ_{21}	=	$-5.896681739130403e-01$
α_{31}	=	$1.807491994894457e+01$	γ_{31}	=	$-2.184086875983300e+01$
α_{32}	=	$-1.727491994894457e+01$	γ_{32}	=	$1.777491994894457e+01$
α_{41}	=	$1.447619738931194e+01$	γ_{41}	=	$-1.824368347564758e+01$
α_{42}	=	$-1.363059573356356e+01$	γ_{42}	=	$1.338336415461619e+01$
α_{43}	=	$5.439834425162180e-02$	γ_{43}	=	$7.533995890474793e-05$
α_{51}	=	$2.000000000000000e-01$	γ_{51}	=	$-3.157407407407428e-02$
α_{52}	=	$5.000000000000000e-01$	γ_{52}	=	$1.455555555555555e-01$
α_{53}	=	$6.000000000000000e-01$	γ_{53}	=	$-4.680555555555555e-01$
α_{54}	=	$-3.000000000000000e-01$	γ_{54}	=	$1.240740740740740e-01$
α_{61}	=	$1.684259259259259e-01$	γ_{61}	=	$0.000000000000000e-00$
α_{62}	=	$6.455555555555555e-01$	γ_{62}	=	$0.000000000000000e-00$
α_{63}	=	$1.319444444444444e-01$	γ_{63}	=	$0.000000000000000e-00$
α_{64}	=	$-1.759259259259259e-01$	γ_{64}	=	$0.000000000000000e-00$
α_{65}	=	$2.300000000000000e-01$	γ_{65}	=	$-2.300000000000000e-01$
b_1	=	$1.684259259259259e-01$	$\overline{b}_1$	=	$1.684259259259259e-01$
b_2	=	$6.455555555555555e-01$	$\overline{b}_2$	=	$6.455555555555555e-01$
b_3	=	$1.319444444444444e-01$	$\overline{b}_3$	=	$1.319444444444444e-01$
b_4	=	$-1.759259259259259e-01$	$\overline{b}_4$	=	$-1.759259259259259e-01$
b_5	=	$0.000000000000000e-00$	$\overline{b}_5$	=	$2.300000000000000e-01$
b_6	=	$2.300000000000000e-01$	$\overline{b}_6$	=	$0.000000000000000e-00$

Table 3 - Set of coefficients of RDE34S

γ	=	$3.333333333333333e-01$			
α_{21}	=	$1.273220037500351e-01$	γ_{21}	=	$-9.803381697176562e-02$
α_{31}	=	$-9.226441186718157e-01$	γ_{31}	=	$8.275955106271749e-01$
α_{32}	=	$1.422644118671816e+00$	γ_{32}	=	$-6.726441186718158e-01$
α_{41}	=	$3.000000000000000e-01$	γ_{41}	=	$8.382963781060364e-01$
α_{42}	=	$2.000000000000000e-01$	γ_{42}	=	$-2.000000000000000e-01$
α_{43}	=	$5.000000000000000e-01$	γ_{43}	=	$-5.000000000000000e-01$
α_{51}	=	$3.000000000000000e-01$	γ_{51}	=	$1.606553370833683e-01$
α_{52}	=	$2.000000000000000e-01$	γ_{52}	=	$-2.000000000000000e-01$
α_{53}	=	$5.000000000000000e-01$	γ_{53}	=	$-5.000000000000000e-01$
α_{54}	=	$0.000000000000000e-00$	γ_{54}	=	$3.934466291663161e-02$
α_{61}	=	$3.000000000000000e-01$	γ_{61}	=	$7.893003817339626e-01$
α_{62}	=	$2.000000000000000e-01$	γ_{62}	=	$-2.000000000000000e-01$
α_{63}	=	$5.000000000000000e-01$	γ_{63}	=	$-5.000000000000000e-01$
α_{64}	=	$0.000000000000000e-00$	γ_{64}	=	$0.000000000000000e-00$
α_{65}	=	$0.000000000000000e-00$	γ_{65}	=	$0.000000000000000e-00$
b_1	=	$1.666666666666671e-01$	$\overline{b}_1$	=	$2.246940103828099e-01$
b_2	=	$0.000000000000000e-00$	$\overline{b}_2$	=	$-8.921028305556744e-02$
b_3	=	$6.666666666666667e-01$	$\overline{b}_3$	=	$7.063156813580298e-01$
b_4	=	$2.000000000000000e-01$	$\overline{b}_4$	=	$-3.223527511893778e-01$
b_5	=	$5.000000000000000e-01$	$\overline{b}_5$	=	$4.805533425041055e-01$
b_6	=	$-5.333333333333333e-01$	$\overline{b}_6$	=	$0.000000000000000e-00$

Table 4 - Set of coefficients of RDE34L

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