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Applied Numerical Mathematics 53 (2005) 527–541
APPLIED NUMERICAL MATHEMATICS
www.elsevier.com/locate/apnum

Krylov-ROW methods for DAEs of index 1 with applications to viscoelasticity

Jörg Wensch

Martin-Luther-Universität Halle-Wittenberg, FB Mathematik und Informatik, 06099 Halle, Germany

Available online 21 December 2004

Abstract

The combination of Krylov techniques to Rosenbrock methods (Krylov-ROW methods) leads to an efficient class of methods for stiff problems. Here the extension to semi-explicit DAEs of index 1 is discussed. Several paths are possible to apply the direct and the indirect approach. The equivalence of different approaches is proved. Conclusions on the dimension of the Krylov spaces are drawn. The methods are applied to typical high-dimensional DAEs arising from viscoelastic materials. Numerical experiments confirm the theoretical predictions.

Keywords: Differential-algebraic equations; Rosenbrock methods; Krylov-ROW methods

1. Introduction

The solutions of stiff initial value problems

$$\begin{aligned} &y'(t) = f\big(y(t)\big), \quad y(t) \in \mathbb{R}^{n_y}, \quad t \in [t_0, t_e], \\ &y(t_0) = y_0, \end{aligned} \tag{1}$$

are characterised by the fact that both smooth components as well as strongly varying components occur. Explicit methods are not suitable for such systems. In a search for methods with as little implicitness as necessary one certainly reaches the point of linearly implicit methods where only a fixed number of linear systems has to be solved at each step. Even there we can improve efficiency by applying iterative solution techniques like Krylov methods to the linear systems—which results in Krylov-ROW methods.

E-mail address: wensch@informatik.uni-halle.de (J. Wensch).

0168-9274/$30.00
doi:10.1016/j.apnum.2004.08.012

An s-stage Rosenbrock method [13,21,6] for (1) is given by

$$Y_{mi} = y_m + h\sum_{j=1}^{i-1}\alpha_{ij}k_j, \quad i = 1,\dots,s, \tag{2a}$$

$$(I - h\gamma J)(k_i + \underline{k}_i) = f(Y_{mi}) + \underline{k}_i, \quad i = 1,\dots,s, \tag{2b}$$

$$y_{m+1} = y_m + h\sum_{i=1}^{s} b_i k_i, \tag{2c}$$

where α_{ij}, γ, γ_{ij}, b_i are the coefficients of the method and $\underline{k}_i = \sum_{j<i}(\gamma_{ij}/\gamma)k_j$. Rosenbrock methods are suitable for the solution of differential-algebraic equations, too. They have been successfully applied to systems of index 1 by several authors, we mention [12,11,1]. They can further be utilised for higher index systems like multibody systems in descriptor form, see [23].

We mention that a more general ansatz is offered by the adaptive Runge–Kutta methods developed by Strehmel and Weiner [17,18].

This paper is organised as follows: In Section 2 we give a brief overview of Krylov-ROW methods. The adaptation of Rosenbrock methods to DAEs is discussed in Section 3. Both approaches are combined in Section 4, where the application of Krylov-ROW methods to DAEs is investigated. Sections 5 and 6 deal with an application from viscoelasticity. We conclude with a summary.

2. Krylov-ROW methods

Many application problems consist of stiff and non-stiff components. For stability reasons the stiff components have to be treated implicitly, but the non-stiff components can be solved by explicit procedures. Krylov methods [20,14,19] constitute a way to accomplish this. The stiff components correspond to large eigenvalues of the Jacobian of the right-hand side. When the linear equation (2b) is solved by a Krylov method then the Krylov space will be dominated by the eigenmodes that correspond to large eigenvalues of the Jacobian. The application of a Krylov method constitutes automatic partitioning into stiff and non-stiff components—the more stiff a component the more it will be integrated implicitly.

We start with a Rosenbrock method. In the ith stage we have to solve a linear system $(I - h\gamma J)x_i = w_i$. When the system is solved by FOM (fully orthogonal method), the solution is given as the exact solution in a (lower-dimensional) Krylov space $\mathcal{K}_{\kappa_i}(J, w_i) \ni w_i$ via $(I - h\gamma Q_{\kappa_i} Q_{\kappa_i}^{\mathrm{T}} J)x_i = w_i$, where the matrix Q_{κ_i} is typically generated by an Arnoldi process [19]. A Krylov-ROW method is therefore given by

$$Y_{mi} = y_m + h\sum_{j=1}^{i-1}\alpha_{ij}k_j, \tag{3a}$$

$$\left(I - h\gamma Q_{\kappa_i} Q_{\kappa_i}^{\mathrm{T}} J\right)(k_i + \underline{k}_i) = f(Y_{mi}) + \underline{k}_i, \tag{3b}$$

$$y_{m+1} = y_m + h\sum_{i=1}^{s} b_i k_i, \tag{3c}$$

where the coefficients are taken from the underlying Rosenbrock method.

Schmitt and Weiner [16] showed that under fairly mild assumptions on the number of Krylov iterations the Krylov-ROW method will have the same non-stiff order as the underlying Rosenbrock method. The

basic idea in the proof is to estimate the difference between the Rosenbrock- and the Krylov-ROW solution by an expansion of $(I - h\gamma J)$ respectively $(I - h\gamma Q_{\kappa_i} Q_{\kappa_i}^{\mathrm{T}} J)$ in Neumann series.

It seems natural to reuse the Krylov spaces from preceding stages. This leads to the so-called multiple Arnoldi process. For a detailed description see [22]. The multiple Arnoldi process for Krylov-ROW methods is implemented in the code ROWMAP by Weiner, Schmitt and Podhaisky.

Further applications of Krylov subspace techniques can be found in [9]. The usage of Krylov techniques for BDF methods is described in [3], the techniques are implemented in the code VODPK.

3. Rosenbrock methods for DAEs of index 1

We consider a semi-explicit DAE of index 1:

$$y' = f(y, z), \quad y \in \mathbb{R}^{n_y},\ z \in \mathbb{R}^{n_z}, \tag{4a}$$

$$0 = g(y, z), \tag{4b}$$

whenever the Jacobian g_z is regular the system is of index 1. In that case the constraint (4b) can be solved uniquely for the algebraic variable $z = G(y)$ in a neighbourhood of the solution via the implicit relation $0 = g(y, G(y))$. By inserting $z = G(y)$ in Eq. (4a) we obtain an ODE. We suppose that the resulting ODE $y' = f(y, G(y))$ is stiff. Such systems occur when parabolic differential equations are solved by semi-discretisation where the boundary conditions lead to constraints (4b). Typically, in that case the number of constraints will be fairly low compared with the number of differential equations. We are also interested in the opposite case where a large number of constraints occurs.

ODE methods have to be adapted to be applicable to DAEs. There are two principal ways to make an ODE method suitable for differential-algebraic systems of index 1. These two approaches are called the direct and the indirect approach, respectively.

3.1. The indirect approach

The indirect approach exploits the fact that the system can be transformed in an ODE by solving the constraint for z and replacing z by $G(y)$. The resulting ODE is then solved by the basic method. For an s-stage Rosenbrock method (2) the new Jacobian becomes

$$J = \frac{\partial}{\partial y} f\big(y, G(y)\big) = f_y - f_z g_z^{-1} g_y. \tag{5}$$

We obtain

$$y_{m+1} = y_m + h \sum_i b_i k_i, \qquad 0 = g(y_{m+1}, z_{m+1}), \tag{6a}$$

with

$$Y_{mi} = y_m + h \sum_{j=1}^{i-1} \alpha_{ij} k_j, \qquad 0 = g(Y_{mi}, Z_{mi}), \quad i = 1, \ldots, s, \tag{6b}$$

$$\big(I - h\gamma\big(f_y - f_z g_z^{-1} g_y\big)\big)(k_i + \underline{k}_i) = f(Y_{mi}, Z_{mi}) + \underline{k}_i, \quad i = 1, \ldots, s. \tag{6c}$$

The computation of the function $z = G(y)$ is realized by the implicit relation in Eqs. (6b), (6a).

3.2. The direct approach

The direct approach is also applicable to higher index systems. Note that it is only a recipe. The resulting method has to be analysed for each individual case with care.

The system is formally regularised by an ε-embedding

$$y' = f(y,z), \qquad \varepsilon z' = g(y,z). \tag{7}$$

On the ODE system (7) the basic method is formally applied, afterwards we let $\varepsilon \to 0$. The resulting method is our DAE method. Methods based on that approach have been investigated by several authors, we mention [11,12,1].

The direct approach results in:

$$y_{m+1} = y_m + h\sum_{i=1}^{s} b_i k_i, \qquad z_{m+1} = z_m + h\sum_{i=1}^{s} b_i l_i, \tag{8a}$$

$$Y_{mi} = y_m + h\sum_{j=1}^{i-1} \alpha_{ij} k_j, \qquad Z_{mi} = z_m + h\sum_{j=1}^{i-1} \alpha_{ij} l_j, \tag{8b}$$

$$\left[\begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} - h\gamma \begin{pmatrix} f_y & f_z \\ g_y & g_z \end{pmatrix}\right] \begin{pmatrix} k_i + \underline{k}_i \\ l_i + \underline{l}_i \end{pmatrix} = \begin{pmatrix} f(Y_{mi}, Z_{mi}) + \underline{k}_i \\ g(Y_{mi}, Z_{mi}) \end{pmatrix}, \tag{8c}$$

where $\underline{k}_i = \sum_{j=1}^{i-1} (\gamma_{ij}/\gamma) k_j$ and $\underline{l}_i$ are given analogously. An advantage of the direct approach is that the z-component needs not to be determined by the solution of the constraint. The price to be paid for that is that the constraint is satisfied only up to the accuracy order of the solution. To have stability for the z-component typically $|R(\infty)| < 1$ is necessary [6].

4. Krylov-ROW methods for DAEs

We can simply apply the direct and indirect approach to Krylov-ROW methods, or, go a step back, and apply the direct and indirect approach to Rosenbrock methods and solve the resulting equations by Krylov techniques. These 4 approaches are discussed in the following. A brief overview on these alternatives is also given in [24].

4.1. The indirect approach

We have to solve the ODE $y' = f(y, G(y))$, where $G(y)$ is defined by $g(y, G(y)) = 0$. Obviously the application of Krylov techniques and the application of the indirect approach are independent of each other, i.e., the diagram

$$\begin{array}{ccc} \text{ROW(ODE)} & \xrightarrow{\text{indirect}} & \text{ROW(DAE)} \\ \big\downarrow \text{Krylov} & & \big\downarrow \text{Krylov} \\ \text{Krylov(ODE)} & \xrightarrow{\text{indirect}} & \text{Krylov(DAE)} \end{array} \tag{9}$$

commutes. The complete method is obtained from (6), where in (6c) the Jacobian $J = f_y - f_z g_z^{-1} g_y$ has to be replaced by $Q_i Q_i^{\mathrm{T}} J$.

4.2. The direct approach for Rosenbrock methods

Here we have to take care what we do first—direct approach or Krylov space approximation. The diagram

$$\begin{array}{ccc} \text{ROW}(\varepsilon\text{-ODE}) & \xrightarrow{\text{direct}} & \text{ROW(DAE)} \\ \Big\downarrow \text{Krylov} & & \Big\downarrow \text{Krylov} \\ \text{Krylov}(\varepsilon\text{-ODE}) & \xrightarrow{\text{direct}} & \text{Krylov(DAE)} \end{array} \tag{10}$$

illustrates the possible paths. First the DAE is transformed into an ODE by ε-embedding. On the path including the upper-right corner first ε is set to zero which gives a DAE method. Afterwards we apply Krylov iterations to the linear equations.

On the path including the lower-left corner we apply Krylov techniques on the singularly perturbed problem (containing the formal parameter ε). Then we set ε to zero. We will compare both strategies in the following.

4.2.1. The Krylov solution of ROW(DAE)

We set first $\varepsilon = 0$ and apply the Krylov method afterwards. The first step leads to system (8).

In the Krylov procedure the Jacobian J is replaced by a low rank approximation. In the ODE case we can prove consistency easily because the coefficient matrix of the linear system is in the form $I + \mathcal{O}(h)$—and we only approximate in the $\mathcal{O}(h)$-part. But here, in the DAE case, the situation is more difficult. For the algebraic variables the iteration matrix is g_z—in principle. Without further information on the matrix g_z a general iterative procedure cannot be advised.

We have several ways to deal with the situation:

KODE The algebraic equations are solved exactly at each Krylov step. We have already discussed that approach in the context of the indirect approach.

KDAE We apply Krylov techniques to the system (8c).

PREC We use a suitable preconditioner, especially with respect to the constraints.

The last proposal seems to be a natural choice, but preconditioning is beyond the scope of this paper. For systems with a large number of constraints one has to solve the—possibly nonlinear—constraint equations exactly at each step when using approach KODE. Therefore we concentrate on studying the approach KDAE. We have by an elimination of the algebraic variables from the upper equation in (8c) with $f_i = f(Y_{mi}, Z_{mi})$ and $g_i = g(Y_{mi}, Z_{mi})$ as in (3b)

$$\begin{pmatrix} I - h\gamma\, Q_i\, Q_i^{\mathrm{T}}(f_y - f_z g_z^{-1} g_y) & 0 \\ -h g_y & -h g_z \end{pmatrix} \begin{pmatrix} k_i + \underline{k}_i \\ l_i + \underline{l}_i \end{pmatrix} = \begin{pmatrix} f_i - f_z g_z^{-1} g_i + \underline{k}_i \\ g_i \end{pmatrix}.$$

The upper block of the system is iteratively solved by an Krylov method.

We will later reconsider the approach KDAE in a numerical experiment.

4.2.2. ε-embedding of the Krylov method

The Krylov method is originally formulated for an explicit differential equation. Using the direct approach, the DAE transforms into an explicit ODE

$$y' = f(y,z), \qquad z' = 1/\varepsilon g(y,z). \tag{11}$$

The stages of the Krylov method are given by

$$\left(\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - h\gamma \begin{pmatrix} f_y & f_z \\ \frac{1}{\varepsilon} g_y & \frac{1}{\varepsilon} g_z \end{pmatrix}\right) \begin{pmatrix} k_i + \underline{k}_i \\ l_i + \underline{l}_i \end{pmatrix} = \begin{pmatrix} f(Y_{mi}, Z_{mi}) \\ \frac{1}{\varepsilon} g(Y_{mi}, Z_{mi}) \end{pmatrix} + \begin{pmatrix} \underline{k}_i \\ \underline{l}_i \end{pmatrix}. \tag{12}$$

The linear system (12) denoted by $A(\varepsilon)x = b(\varepsilon)$ is solved iteratively whereby Krylov spaces $\mathcal{K}(A(\varepsilon), b(\varepsilon))$ are generated. We are interested in the limit of the Krylov spaces in case of $\varepsilon \to 0$.

Theorem 4.1. *Suppose the Krylov space $\mathcal{K}_{n_z}(g_z, g)$ is of full dimension n_z (the dimension of the algebraic variables). Then Krylov iterations for* (12) *give in the limit case $\varepsilon \to 0$ a series of spaces*

$$\lim_{\varepsilon \to 0} \mathcal{K}_n\big(A(\varepsilon), b(\varepsilon)\big) = \operatorname{span}\{u_1, \ldots, u_n\}, \quad \text{for } n = 1, \ldots, \tag{13}$$

that is spanned by a series of vectors u_n with

$$u_n = \begin{pmatrix} 0 \\ g_z^{n-1} g \end{pmatrix}, \qquad \text{for } n \leqslant n_z, \tag{14}$$

$$u_n = \begin{pmatrix} f + \underline{k} - f_z g_z^{-1} g \\ 0 \end{pmatrix}, \qquad \text{for } n = n_z + 1, \tag{15}$$

$$u_n = \begin{pmatrix} I - h\gamma(f_y - f_z g_z^{-1} g_y) & 0 \\ 0 & 0 \end{pmatrix} u_{n-1}, \quad \text{for } n > n_z + 1. \tag{16}$$

Proof. For notational convenience we scale the (complete!) linear equation by ε. This operation leaves the Krylov spaces unchanged. We consider the Krylov space $\mathcal{K}(A, b)$ with $A = A_0 + \varepsilon A_1$ and $b = b_0 + \varepsilon b_1$, where

$$A_0 = -h\gamma \begin{pmatrix} 0 & 0 \\ g_y & g_z \end{pmatrix}, \qquad A_1 = I - h\gamma \begin{pmatrix} f_y & f_z \\ 0 & 0 \end{pmatrix}, \tag{17}$$

$$b_0 = \begin{pmatrix} 0 \\ g \end{pmatrix}, \qquad b_1 = \begin{pmatrix} f + \underline{k} \\ \underline{l} \end{pmatrix}. \tag{18}$$

A straightforward calculation gives that the generating vectors $u_n = A^{n-1}b$, $n = 1, \ldots$ of the Krylov space possess for $n \geqslant 2$ the asymptotic ε-expansion

$$u_n = \begin{pmatrix} \varepsilon(-h\gamma)^{n-1} f_z g_z^{n-2} g \\ (-h\gamma)^{n-1} g_z^{n-1} g \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}. \tag{19}$$

To include the case $n = 1$, too, we write

$$u_n = \begin{pmatrix} \varepsilon(-h\gamma)^{n-1} f_z g_z^{n-2} g \\ (-h\gamma)^{n-1} g_z^{n-1} g \end{pmatrix} + \delta_{n1}\varepsilon \begin{pmatrix} f + \underline{k} - f_z g_z^{-1} g \\ 0 \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}. \tag{20}$$

Considering the matrix U_n consisting of columns $u_1, \ldots, u_n$, we have

$$U_n = \begin{pmatrix} \varepsilon V_n \\ W_n \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}, \tag{21}$$

where it follows from (20) that

$$V_n = f_z g_z^{-1} W_n + \begin{pmatrix} f + \underline{k} - f_z g_z^{-1} g \\ 0 \end{pmatrix} e_1^{\mathrm{T}} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}. \tag{22}$$

When the Krylov space is built by the Arnoldi process then in each step the vectors are normalised and orthogonalised. Because we are interested in the spaces that are spanned by the vectors u_n but not in the vectors u_n itself, we neglect the orthonormalisation for the vectors u_k for $k \leqslant n_z$ completely and put them together as columns of the matrix U_{n_z}. Because of our assumption on g_z, the matrix U_{n_z} has full rank. In the limit case $\varepsilon \to 0$ the columns of U_{n_z} span the space of algebraic variables, which establishes Eq. (14).

To prove Eq. (15), we have to compute the result of an orthogonalisation of u_{n_z+1} against the preceding u_k when we orthogonalise and normalise *before* $\varepsilon \to 0$. Note, that in the limit case $\varepsilon \to 0$ the vector u_{n_z+1} depends linearly on the preceding vectors u_k, $k = 1, \ldots, n_z$. In the following we compute how a vector is orthogonalised against the columns of U_{n_z}. This formula is then used to establish relations (15) and (16).

We ignore $\mathcal{O}(\varepsilon)$ terms in the orthogonalisation of vectors u_n for $n > n_z$ against the columns of U_{n_z}, i.e., we have

$$u_n^{\mathrm{T}} u_k = \mathcal{O}\big(\varepsilon \|u_n\| \|u_k\|\big), \quad k \leqslant n_z. \tag{23}$$

Afterwards we normalise to have $\|u_n\| = \mathcal{O}(1)$, which results in $u_n^{\mathrm{T}} u_k = \mathcal{O}(\varepsilon)$ for $k \leqslant n_z$ respectively $u_n^{\mathrm{T}} u_k \to 0$ when $\varepsilon \to 0$.

Let an arbitrary vector u be given in the form of Eq. (20)

$$u = \begin{pmatrix} \varepsilon v \\ w \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}. \tag{24}$$

The partial orthogonalisation of u is realized in two steps. First eliminate the $\mathcal{O}(1)$-terms in the second component and then replace V_{n_z} by (22):

$$u \mapsto u - \begin{pmatrix} \varepsilon V_{n_z} + \mathcal{O}(\varepsilon^2) \\ W_{n_z} + \mathcal{O}(\varepsilon) \end{pmatrix} W_{n_z}^{-1} w \tag{25}$$

$$= \begin{pmatrix} \varepsilon(v - V_{n_z} W_{n_z}^{-1} w) + \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix} \tag{26}$$

$$= \begin{pmatrix} \varepsilon(v - f_z g_z^{-1} w + (f + \underline{k} - f_z g_z^{-1} g) e_1^{\mathrm{T}} W_{n_z}^{-1} w) + \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix}. \tag{27}$$

In a second step we eliminate the $\mathcal{O}(\varepsilon)$-terms in the second component:

$$u \mapsto u - \begin{pmatrix} \varepsilon V_{n_z} + \mathcal{O}(\varepsilon^2) \\ W_{n_z} + \mathcal{O}(\varepsilon) \end{pmatrix} W_{n_z}^{-1} \mathcal{O}(\varepsilon) \tag{28}$$

$$= \begin{pmatrix} \varepsilon(v - f_z g_z^{-1} w + (f + \underline{k} - f_z g_z^{-1} g) e_1^{\mathrm{T}} W_{n_z}^{-1} w) + \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon^2) \end{pmatrix}. \tag{29}$$

By that we have established condition (23). Scaling to a norm of $\mathcal{O}(1)$ results finally in the partially orthogonalised vector q

$$\begin{pmatrix} \varepsilon v \\ w \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix} \mapsto q = \begin{pmatrix} v - f_z g_z^{-1} w + (f + \underline{k} - f_z g_z^{-1} g) e_1^{\mathrm{T}} W_{n_z}^{-1} w \\ 0 \end{pmatrix} + \mathcal{O}(\varepsilon). \tag{30}$$

Consider now the partial orthogonalisation by (30) of u_{n_z+1} given by (20). The term $v - f_z g_z^{-1} w$ vanishes so that afterwards we have

$$u_{n_z+1} \mapsto q_{n_z+1} = \begin{pmatrix} f + \underline{k} - f_z g_z^{-1} g \\ 0 \end{pmatrix} + \mathcal{O}(\varepsilon). \tag{31}$$

A necessary assumption for that is $e_1^{\mathrm{T}} W_{n_z}^{-1} w_{n_z+1} \neq 0$. This is indeed the case because of the regularity of g_z we have the constant term in the characteristic polynomial of g_z non-vanishing.

By induction we see that by partial orthogonalisation (30) and normalisation subsequent vectors in the Krylov sequence can be brought to the form

$$u = \begin{pmatrix} v \\ 0 \end{pmatrix} + \mathcal{O}(\varepsilon). \tag{32}$$

In a Krylov step u given by (32) is multiplied by A and via (30) projected:

$$Au = \begin{pmatrix} \varepsilon(I - f_y)v \\ g_y v \end{pmatrix} + \begin{pmatrix} \mathcal{O}(\varepsilon^2) \\ \mathcal{O}(\varepsilon) \end{pmatrix} \to q, \tag{33}$$

$$q = \begin{pmatrix} (I - (f_y - f_z g_z^{-1} g_y))v \\ 0 \end{pmatrix} + e_1^{\mathrm{T}} W_{n_z}^{-1} g_y v \begin{pmatrix} (f + \underline{k} - f_z g_z^{-1} g) \\ 0 \end{pmatrix} + \mathcal{O}(\varepsilon). \tag{34}$$

The second term in the sum vanishes after an orthogonalisation with u_{n_z+1}, which completes our proof. □

This approach takes us to version KODE of the preceding section where the iterative solution of Eq. (8c) is discussed. When we execute $n_z + \kappa$ iterations then the equations for the constraints are solved exactly whereas for the differential components κ iterations are executed.

The two ways in diagram (10) are closely connected. We conclude that by an application of Krylov techniques to Eq. (8c), as in version KDAE, a limitation of the number of Krylov iterations to approximately 10 to 30—as it is successfully practised in the case of ODEs—cannot be recommended. When the number of algebraic conditions is relatively small then the conclusions from Theorem 4.1 are not too restrictive. But in cases where there are many algebraic components, a larger number of Krylov iterations might be necessary.

We will check the relevance of Theorem 4.1 in the last sections. An application that leads to a system with a large number of algebraic equations is solved numerically by Krylov techniques.

5. An application from viscoelasticity

5.1. The linear elastic case

The deformation of elastic bodies under the actions of volume and surface forces is described by a displacement function u defined on the domain $\Omega \in \mathbb{R}^d$ that is occupied by the undeformed body.

The strong formulation [2] describing u, the strain tensor $\boldsymbol{\varepsilon}$ and the stress tensor $\boldsymbol{\sigma}$

$$0 = \nabla \cdot \boldsymbol{\sigma} + f, \tag{35a}$$

$$\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon} + \lambda(\operatorname{tr}\boldsymbol{\varepsilon})I =: C\boldsymbol{\varepsilon}, \tag{35b}$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla u + \nabla u^{\mathrm{T}}\right) =: Du, \tag{35c}$$

consists of the balance law (35a), the material law or stress–strain relation (35b) and the definition of the linear strain tensor. It is completed by Dirichlet (fixed boundaries) and Neumann conditions (surface forces or free boundaries).

If a solution u of the strong formulation (strong solution) exists, it is also a solution of the weak formulation. It has the advantage that the existence of a solution can be proved under very weak smoothness assumptions on the boundary and the boundary values (Korns inequality, see [2]). The weak formulation for u is given by the equation

$$\int_{\Omega} (Du : C\,Dv - fv)\,\mathrm{d}x - \int_{\gamma_N} gv\,\mathrm{d}A = 0, \quad \forall v \in H^1_{\Gamma_D}(0), \tag{36}$$

where $\boldsymbol{\varepsilon} : \boldsymbol{\sigma} := \sum_{i,j} \varepsilon_{ij}\sigma_{ij}$. Note, that the Neumann boundary conditions are included in Eq. (36). The Dirichlet boundary conditions are built into the solution space

$$H^1_{\Gamma_D}(u_D) := \left\{u \in H^1(\Omega):\ u(x) = u_D(x) \text{ for } x \in \Gamma_D\right\}. \tag{37}$$

5.2. Viscoelasticity

In pure elasticity there is a pointwise relation between stress and strain. In viscoelastic processes the rate of change and the deformation history are also included in this relation. For very slow deformations viscoelastic materials exhibit a nearly elastic behaviour. The case where even this condition is violated is denoted by plasticity.

5.2.1. Atoms of viscoelasticity in 1D

There exists a variety of models to describe viscoelastic materials, see, for example, [8]. Whereas linear elasticity uses springs as a one-dimensional model, in viscoelasticity we use springs and dampers (Newtonian viscosity). From the various ways to connect these atoms serially or in parallel, different models result. The Maxwell model is a series connection of a spring and a damper, whereas the Kelvin–Voigt model is a parallel connection of a spring and a damper. The latter one is also known as Kelvin body. Properties of both models are united in 3-element models that can principally exhibit creep and relaxation behaviour (see Fig. 1). The constitutive equations are derived as follows: For a series connection the strains add, but the stresses are equal. For a parallel connection the stresses add, but strains are equal. The stress–strain relation for the spring is given by the classical law (Hookes law in 3D)

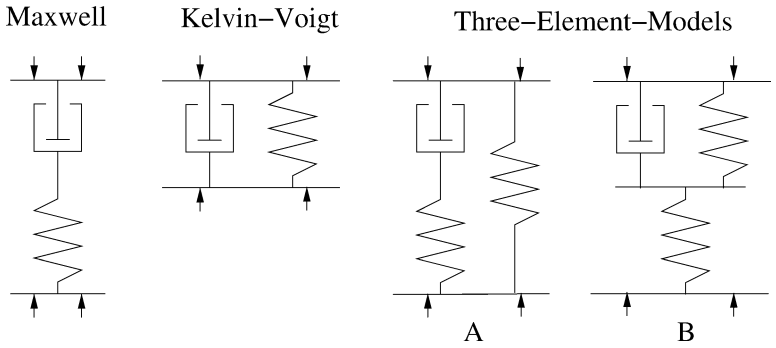

Fig. 1. Classical models of viscoelasticity.

$$\sigma = E\varepsilon, \quad E \ldots \text{modulus of elasticity}, \tag{38}$$

whereas the dampers react like a Newtonian fluid with viscosity η

$$\sigma = \eta\varepsilon', \quad \eta \ldots \text{viscosity}. \tag{39}$$

We concentrate in the following on the left 3-element model (A: parallel connection of a spring and a Maxwell element).

We have a single spring (parameters: $\varepsilon_0, \sigma_0, E_0$), a spring in the Maxwell element ($\varepsilon_M, \sigma_M, E_M$) and a Damper ($\varepsilon_D, \sigma_D, \eta$). We substitute total stress $\sigma = \sigma_0 + \sigma_M$ and total strain $\varepsilon = \varepsilon_0$ to obtain the constitutive equations consisting of an algebraic equation for ε, σ and an evolution equation for ε_D:

$$\sigma = E_0\varepsilon + E_M(\varepsilon - \varepsilon_D) = E\varepsilon - E_M\varepsilon_D, \tag{40}$$

$$\varepsilon_D' = \frac{E_M}{\eta}(\varepsilon - \varepsilon_D). \tag{41}$$

Note that E_0 is the elasticity modulus for the limit case of very slow deformations ($\varepsilon_D' = 0$), whereas in the case of very fast deformations we have elastic behaviour with a elasticity modulus given by $E = E_0 + E_M$ ($\varepsilon_D = 0$). In the 1D-case σ results from the outer forces. In that case we have a DAE of index 1 where ε_D are the differential variables and ε are the algebraic variables.

5.2.2. The extension of the model to three dimensions

We use the material law with compression modulus K and shear modulus G. By that we respect the fact that viscoelastic behaviour is restricted to the deviatoric part (no volume change) of the deformation. The deviatoric part A^D of a tensor A is given by

$$A^D := A - \frac{1}{3}(\operatorname{tr} A)I, \tag{42}$$

where the pure compression is given by $\frac{1}{3}(\operatorname{tr} A)I$. Obviously we have $\operatorname{tr} A^D = 0$. For the 3D-tensors $\boldsymbol{\varepsilon}^D$, $\boldsymbol{\sigma}^D$ we assume linear-elastic behaviour for the pure compression (given by the trace of the tensors), but that Eq. (40) holds for the deviatoric part. We end up with

$$\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon}^D - 2G_M\boldsymbol{\varepsilon}_D^D + K(\operatorname{tr}\boldsymbol{\varepsilon})I, \tag{43}$$

$$\eta\boldsymbol{\varepsilon}_D'^D = 2G_M\left(\boldsymbol{\varepsilon}^D - \boldsymbol{\varepsilon}_D^D\right). \tag{44}$$

When $\boldsymbol{\varepsilon}_D$ is given, we can determine $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$ from Eqs. (35a), (35c) and (43). Note, that by Eq. (44) $\boldsymbol{\varepsilon}_D$ evolves like a deviator whenever the prescribed initial values are a deviator.

5.2.3. 2D-formulation as plane strain

Under the assumption of symmetries in the z-direction we obtain the thin plate model. In case of linear elasticity there is no strain in z-direction assumed. In case of viscoelasticity we have several strains in our model. We assume that the z-component of the displacement u vanishes. Further, the x-, y-components shall be independent of the z-value.

The strain tensor therefore has the form $\boldsymbol{\varepsilon}_{i3} = \boldsymbol{\varepsilon}_{3i} = 0$ for $i = 1, 2, 3$ and $\boldsymbol{\varepsilon}_{ij}(x, y, z) = \boldsymbol{\varepsilon}_{ij}(x, y)$. From the material equations we see that there is caused stress in z-direction. This is a typical phenomenon for the plane strain model. Physically the model corresponds to material that is fixed in z-direction—and this fixing causes stress.

In the elastic case we use the Lamé form of the material law $\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon} + (K - 2/3G)\operatorname{tr}\boldsymbol{\varepsilon} I$, which is simply restricted to the upper 2×2 block. The tr-expression causes stress is z-direction ($\boldsymbol{\sigma}_{33} \neq 0$) that is of no interest for us. From now on we consider $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}_D$ as the upper 2×2 blocks of the original $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}_D$.

In the viscoelastic case we have the equations in the formulation with shear and compression modulus. Further, the deviator (which is the 3D-deviator applied to 2D-matrices!) and the trace do not split the tensor in two independent parts. For $A, I \in \mathbb{R}^{2\times 2}$ it follows from $A^D = A - 1/3(\operatorname{tr} A)I$ that $\operatorname{tr} A^D = \operatorname{tr} A - 2/3 \operatorname{tr} A = 1/3 \operatorname{tr} A$ and therefore $A = A^D + (\operatorname{tr} A^D)I$. Because the 3D-deviator is an invertible map on $\mathbb{R}^{2\times 2}$ the internal variables are given by $q = \boldsymbol{\varepsilon}_D$ where only the symmetry restriction applies to q.

We further eliminate the deviator in the material law (43) and obtain with $\lambda = K - 2/3G$ again a Lamé formulation

$$\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon} - 2G_M q + \lambda(\operatorname{tr}\boldsymbol{\varepsilon})I, \tag{45}$$

$$\eta q' = 2G_M\big(\boldsymbol{\varepsilon}^D - q\big). \tag{46}$$

5.2.4. Weak formulation

We keep the evolution equations for the internal variables q, but the balance law is replaced by a variational principle. We use the so-called pure displacement ansatz [2] where the stress $\boldsymbol{\sigma}$ and the strain $\boldsymbol{\varepsilon}$ are expressed by the displacement u

$$q' = \frac{2G_M}{\eta}\big((Du)^D - q\big), \tag{47}$$

$$0 = \int_\Omega \big(2G\,Dv : Du + \lambda(\nabla\cdot u)(\nabla\cdot v)\big)\,\mathrm{d}x - \int_\Omega (2G_M\,Dv : q + v\cdot f)\,\mathrm{d}x - \int_{\Gamma_N} g\cdot v\,\mathrm{d}s. \tag{48}$$

The variational equation (48) and its discretisation have (for suitable solution spaces) a uniquely determined solution. Therefore we have a differential-algebraic system of index 1 in a function space—a so-called partial differential algebraic equation (PDAE). Such PDAEs arising from models for viscoelastic/viscoplastic behaviour have been investigated by several authors, see [5,7,8]. We mention that plasticity may lead to DAEs (PDAEs) of index 2, see [15,4].

6. Numerical tests on a shear experiment

6.1. Configuration and material parameters

We consider a thin rectangular plate under plane strain. The dimensions are given by $l_x = 1$ and $l_y = 0.1$. On the left side the plate is fixed, whereas on the right side there is a vertical shear force. We have chosen values typical for steel like $G = 200\,000$ and $\nu = 0.3$. For the Maxwell element we prescribe $G_M = G/2$ and $\eta = 1000$. We solve the problem for a constant shear force in the time interval $[0, 100]$.

6.2. Spatial discretisation

The weak formulation (48) makes finite elements the method of choice. For the computation of the stiffness matrix and the right-hand side often Gaussian quadrature of sufficiently high order is used

although the integrals can be evaluated analytically. This allows for an easy implementation. Therefore a natural choice is to consider the internal variables q in the Gaussian points, only. We will use the midpoint of the elements as Gaussian point for the internal variables. The integrals in (48) are computed analytically, where q is assumed as a piecewise (on each grid square) constant function for that purpose. The discussion of suitable pairs of function spaces for the variables u, q is beyond the scope of this paper.

For sufficiently smooth outer forces the space $H^1(\Omega)^2$ is a suitable solution space for the pure displacement method. We choose 4-node bilinear rectangular elements [10]. We have chosen 10×4 elements for the spatial discretisation.

6.3. Time integration

When Rosenbrock methods are applied to index 1 DAEs additional order conditions have to be fulfilled. We have chosen the method RODAS from Hairer and Wanner [6]. It fulfils the additional order conditions for index 1 systems. With $s = 6$ stages we have a solution of order 4 and an embedded solution of order 3.

We compare the method RODAS with direct solution of the linear systems with the Krylov method (based on RODAS) after version KDAE (4.2.1). For the iterative solution of the linear equations we have chosen GMRES. The tolerance for the solution of the linear system is coupled to the tolerance for the step size control of the time integrator. We have considered 3 variants:

$$TOL = 0.1 * RTOL, \qquad TOL = h * RTOL, \qquad TOL = 0.01 * RTOL/h. \tag{49}$$

The iterative solver has no influence on the accuracy in the solution. The errors, average number of Krylov steps and the number of steps are given in Tables 1–3.

Table 1
Maximum global error in the integration interval

RTOL	*TOL*(*GMRES*)			
	0	$0.1 * RTOL$	$h * RTOL$	$0.01 * RTOL/h$
3.59E−03	1.613E−02	1.613E−02	1.613E−02	1.620E−02
4.64E−04	1.458E−03	1.458E−03	1.458E−03	1.475E−03
5.99E−05	1.178E−04	1.178E−04	1.178E−04	1.178E−04
7.74E−06	7.169E−06	7.171E−06	7.170E−06	6.537E−06
1.00E−06	9.677E−07	9.679E−07	9.677E−07	9.400E−07

Table 2
Average number of Krylov iterations

RTOL	*TOL*(*GMRES*)			
	0	$0.1 * RTOL$	$h * RTOL$	$0.01 * RTOL/h$
3.59E−03	0.00	106.00	105.71	106.86
4.64E−04	0.00	106.62	106.25	107.31
5.99E−05	0.00	107.11	107.00	107.50
7.74E−06	0.00	107.44	107.52	116.31
1.00E−06	0.00	107.46	107.81	118.69

Table 3
Number of steps for different Krylov implementations and RODAS itself

RTOL	*TOL*(*GMRES*)			
	0	$0.1 * RTOL$	$h * RTOL$	$0.01 * RTOL/h$
3.59E−03	11	11	11	11
4.64E−04	14	14	14	14
5.99E−05	18	18	18	18
7.74E−06	26	26	26	27
1.00E−06	38	38	38	40

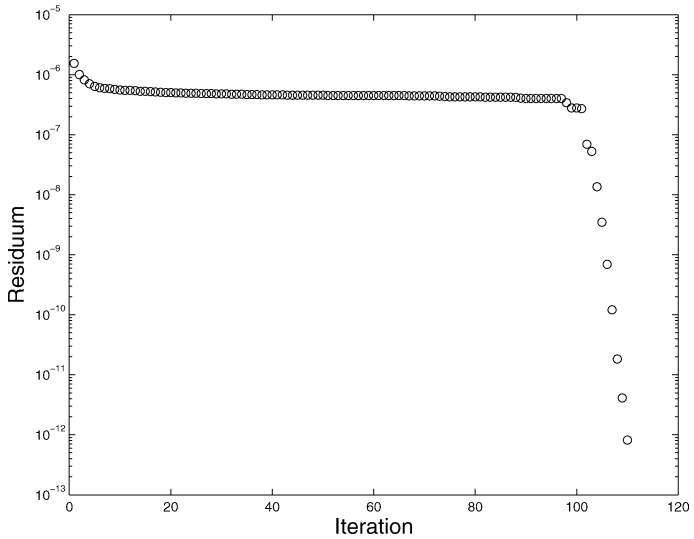

Fig. 2. Typical residual for a GMRES iteration.

Tables 1 and 3 illustrate that the stopping criterion in the iterative solver does not influence the accuracy in the solution significantly. The number of steps and global errors are almost identical for RODAS and the different Krylov implementations.

There has a price to be paid—the average number of Krylov iterations is approximately 100. This is in accordance with the analysis of Section 4. There is a close relation between the various ways to apply Krylov techniques to a DAE. Therefore it is not astonishing that we have to make almost as much iterations as the number of algebraic variables (110 in our case).

The typical residual for a Krylov iteration is shown in Fig. 2. After approximately 100 iterations the residual decreases remarkably.

Fig. 2 explains, too, why the attempt to restrict the number of iterations fails. We have set the maximum number of iterations at 30 and got completely useless results. One way to overcome this is to develop a suitable preconditioner for such systems. For medium-sized applications (up to several ten thousand equations) even the direct solution of the algebraic part or of the complete system (Rosenbrock method) can be a suitable choice if the sparse structure of the linear system is exploited.

7. Summary and conclusions

Krylov methods are suitable for the solution of stiff systems while offering the lowest possible degree of implicitness in a method. We have considered several ways to apply them to DAEs of index 1. In detail we have dealt with the direct approach. We have established an "almost" equivalence between the direct approach for the Krylov method and the Krylov solution of the direct approach. The most important conclusion is that the usual limitation of the dimension of the Krylov space as for ODEs, is not suitable in the DAE case.

In case of stiff systems where the number of algebraic constraints is low compared with the number of differential equations Krylov methods remain an attractive choice. To this class belong semi-discretised parabolic problems where the boundary conditions are added in the form of algebraic constraints.

We have illustrated the conclusion using an application with a large number of constraints—a shear experiment on a thin plate with viscoelastic behaviour. The theoretical results from Theorem 4.1 are confirmed by the numerical experiment. For systems with a relatively large number of constraints the Krylov dimensions become rather high. In this case either preconditioners have to be developed or an efficient direct solver exploiting the sparse structure of the system (Rosenbrock method) has to be used. The extension of these ideas to higher-dimensional applications and the comparison with established solution techniques is the subject of current research.

Acknowledgement

The author thanks the referees for their helpful comments.

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