PAMM · Proc. Appl. Math. Mech. **3**, 573–574 (2003) / **DOI** 10.1002/pamm.200310554

J. Wensch, H. Podhaisky and S. Hartmann

Time integration of index 1 DAEs with Rosenbrock methods using Krylov subspace techniques

The derivation of Rosenbrock-Krylov methods for index 1 DAEs involves two well known techniques: a limit process which transforms a singular perturbed ODE to an index 1 DAE and the use of Krylov iterations instead of direct linear solvers for the stage equations. We show that our derived class of Rosenbrock-Krylov schemes is independent of the order in which we apply these techniques. We also conclude that for convergence a rather accurate solution of the algebraic part is always needed.

1. Problem

We deal with large structured systems of differential algebraic systems of index 1

$$\begin{aligned} y' &= f(y,z), \\ 0 &= g(y,z), \quad \text{where } g_z \text{ is regular.} \end{aligned} \tag{1}$$

The special application we have in mind is the simulation of viscoelastic media by a quasi-stationary approach that couples evolution equations for inelastic strains with linear elasticity [3]. A spatial discretization using a finite element ansatz leads to a large DAE-system, where the inelastic strains are given at the Gaussian points that are used by the finite elements. Index 1 is guaranteed by the fact that the linear elastic problem possesses a unique solution. The differential part of those systems is mildly stiff in typical applications.

2. Rosenbrock methods

For an ODE $y' = f(y)$ a timestep with a Rosenbrock method is given by the scheme $y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$ with s internal stages k_i defined by (cf. [2])

$$(I - h\gamma J)k_i = \underbrace{f\left(y_n + h\sum_{j=1}^{i-1} \alpha_{ij} k_j\right)}_{=:f_i} + hJ\sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, \ldots, s \tag{2}$$

or, equivalently, $(I - h\gamma J)(k_i + k_i^{(0)}) = f_i + k_i^{(0)}$ where $k_i^{(0)} := \sum_{j=1}^{i-1} \frac{\gamma_{ij}}{\gamma} k_j$. For large stiff ODE systems it might be favorable to use Krylov techniques for the solution of the linear stages. Due to a fast damping of stiff modes they have good stability properties with a fraction of the numerical effort that the direct solution of the linear systems requires. With fairly low Krylov dimensions (ca. $4 - 15$) the order of the underlying Rosenbrock method can be guaranteed [4]. The Jacobian J is replaced by a low rank approximation $QQ^T J$ where Q is an orthogonal basis of the Krylov-subspace $\mathcal{K} = \text{span}\{r_i, Jr_i, \ldots, J^\kappa r_i\}$ which can be computed sucessively using Arnoldi's algorithm.

3. Krylov-Rosenbrock methods for DAEs of index 1

A general recipe to apply ODE methods to DAEs is the direct approach. The DAE is interpreted as the limit of a singularly perturbed problem

$$\begin{array}{rl} y' = & f(y,z) \\ 0 = & g(y,z) \end{array} \quad \longleftarrow \quad \begin{array}{rl} y' = & f(y,z) \\ z' = & \frac{1}{\varepsilon} g(y,z). \end{array} \tag{3}$$

The method of choice is (formally) applied to the singularly perturbed problem. The limit case $\varepsilon \to 0$ results in a numerical method for the DAE. As illustrated by diagram (4) below we have two options: first (*right-down*), we apply a Rosenbrock method to (3), put $\varepsilon \to 0$ and employ Krylov techniques afterwards in the Rosenbrock scheme for the DAE, or second (*down-right*), we can apply a Krylov method to (3) and study $\varepsilon \to 0$. This gives raise to the question: does the diagram (4) commute?

$$\begin{array}{ccc} \text{ROW}(\varepsilon\text{-ODE}) & \xrightarrow{\varepsilon \to 0} & \text{ROW(DAE)} \\ \Big\downarrow \text{Krylov} & & \Big\downarrow \text{Krylov} \\ \text{Krylov}(\varepsilon\text{-ODE}) & \xrightarrow{\varepsilon \to 0} & \text{Krylov(DAE)} \end{array} \tag{4}$$

4. The *right-down* way

After $\varepsilon \to 0$ the stages (augmented by additional entries l_i corresponding zo the z-component) of the Rosenbrock method have the form

$$\left(\begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} - h\gamma \begin{pmatrix} f_y & f_z \\ g_y & g_z \end{pmatrix}\right) \begin{pmatrix} k_i + k_i^{(0)} \\ l_i + l_i^{(0)} \end{pmatrix} = \begin{pmatrix} f_i \\ g_i \end{pmatrix} + \begin{pmatrix} k_i^{(0)} \\ 0 \end{pmatrix}, \quad i = 1, \ldots, s. \tag{5}$$

In contrast to ODEs the iteration matrix is not in the form $I + \mathcal{O}(h)$. This implies that additional preconditioning is required. Our ansatz is to eliminate l_i, to apply the Krylov solver to the ODE-part of the equation, only.

$$\Rightarrow (I - h\gamma(f_y - f_z g_z^{-1} g_y))(k_i + k_i^{(0)}) = f_i + k_i^{(0)} - f_z g_z^{-1} g_i \tag{6}$$

5. The *down-right* way

Applying the Rosenbrock method (2) to (3), leads for each stage to a linear system (scaled by ε, index i omitted)

$$\left(\begin{pmatrix} \varepsilon I & 0 \\ 0 & I \end{pmatrix} - h\gamma \begin{pmatrix} \varepsilon f_y & \varepsilon f_z \\ g_y & g_z \end{pmatrix}\right) \begin{pmatrix} k \\ l \end{pmatrix} = \begin{pmatrix} \varepsilon(f + k^{(0)}) \\ g + \varepsilon l \end{pmatrix}. \tag{7}$$

The solution is approximated by a Krylov method. We are interested in the limit of the Krylov subspaces for $\varepsilon \to 0$, i.e., we apply the direct approach to the Krylov method. We expand the Krylov iterates in powers of ε

$$\begin{aligned} k^{(\nu)} &= \varepsilon(-h\gamma)^\nu f_z g_z^{\nu-1} g + \mathcal{O}\left(\varepsilon^2\right) \\ l^{(\nu)} &= (-h\gamma g_z)^\nu g + \mathcal{O}(\varepsilon) \end{aligned} \tag{8}$$

to end up (after some tedious calculations) with

Theorem: Let the n_z eigenvalues of g_z be pairwise distinct. Let $\mathcal{K}_\nu$ be the ν-th Krylov space where $\mathcal{K}_{\nu+1} = \mathcal{K}_\nu \oplus \text{span}\{v_{\nu+1}\}$. For $\varepsilon \to 0$ it holds:
1.) The Krylov-space $\mathcal{K}_{n_z}$ is spaned by the algebraic variables.
2.) The vektors v_ν are given by

$$\begin{aligned} v_{n_z+1} &= \begin{pmatrix} f + k^{(0)} - f_z g_z^{-1} g \\ 0 \end{pmatrix} \\ v_{\nu+1} &= \begin{pmatrix} (I - h\gamma(f_y - f_z g_z^{-1} g_y) & 0 \\ 0 & 0 \end{pmatrix} v_\nu, \quad \nu \geq n_z + 1 \end{aligned} \tag{9}$$

□
We conclude that the *down-right* approach for the Krylov method leads to the exakt solution of the linear systems for the algebraic variables (if the Krylov dimension is at least n_z) whereas the differential variables are approximated by Krylov subspaces generated from equation (6). In this sense the diagram (4) commutes. This is accordance with the findings in [1] that an accurate solution for the algebraic part is always needed.

6. References

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J. Wensch, H. Podhaisky, Universität Halle, FB Mathematik&Informatik, 06099 Halle, Germany
{wensch, podhaisky}@mathematik.uni-halle.de
S. Hartmann, Universität Kassel, Mechanical Engineering, 34109 Kassel, Germany
hart@ifm.maschinenbau.uni-kassel.de