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Numerical Treatment of Second Order Differential-Algebraic Systems

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We consider the numerical treatment of systems of second order differential-algebraic equations (DAEs). The classical approach of transforming a second order system to first order by introducing new variables can lead to difficulties such as an increase in the index or the loss of structure. We show how we can compute an equivalent strangeness-free second order system using the derivative array approach and we present Runge-Kutta methods for the direct numerical solution of second order DAEs.

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We discuss the numerical solution of the linear second order differential-algebraic initial value problem

$$M(t)\ddot{x}(t) + C(t)\dot{x}(t) + K(t)x(t) = f(t), \quad x(t_0) = x_0, \quad \dot{x}(t_0) = \dot{x}_0, \quad t_0 \in \mathbb{I}, \tag{1}$$

where $M, C, K \in \mathcal{C}(\mathbb{I}, \mathbb{C}^{m\times n})$ and $f(t) \in \mathcal{C}(\mathbb{I}, \mathbb{C}^m)$ are sufficiently smooth together with given initial values $x_0, \dot{x}_0 \in \mathbb{C}^n$. Usually, in the classical theory of ordinary differential equations, high order systems are turned into first order systems by introducing new variables for the derivatives. However, it has been discussed in several publications, see e.g. [1, 4], that for differential-algebraic equations (DAEs) this classical approach has to be performed with great care, since it may lead to a number of mathematical difficulties. In [3, 5] several examples show that the classical approach of introducing new variables may lead to higher smoothness requirements for the inhomogeneity, corresponding to an increase in the index of the DAE, or may result in a loss of structures in the system. Further, it is shown in [1, 2, 4, 6] that numerical methods can fail. Therefore, the direct discretization and numerical solution of the second order differential-algebraic system can yield better numerical results. The theoretical analysis of linear second order differential-algebraic equations is studied in [3, 5], where condensed forms for matrix triple and corresponding invariants under equivalence transformations are derived. One of the main results is the equivalence to a so-called *strangeness-free* system, that separates the given second order DAE into uncoupled subsystems of second order differential, first order differential and algebraic equations together with some consistency conditions for the right-hand side. The algebraic approach described in [3, 5] gives the theoretical analysis of second order DAEs including decisions about existence and uniqueness of solutions and consistency of initial values, but it cannot be used for the development of numerical methods as it is not feasible for numerical computations. Here, we introduce a numerical computable way for the determination of the characteristic invariants of a given DAE, i.e., the number of second order and the number of first order differential equations, the number of algebraic equations and the number of consistency conditions in the strangeness-free system, as well as for the extraction of an equivalent strangeness-free second order differential-algebraic system. The basic idea is to differentiate the DAE (1) a number of times and to put the original DAE together with the derivatives up to a sufficiently high order $\hat{\mu}$ into an enlarged system. In this way we obtain the so-called *derivative arrays* associated with (1)

$$\mathcal{M}_l(t)\ddot{z}_l + \mathcal{L}_l(t)\dot{z}_l + \mathcal{N}_l(t)z_l = g_l(t), \quad l = 0, \ldots, \hat{\mu}, \tag{2}$$

where $\mathcal{M}_l(t)$, $\mathcal{L}_l(t)$, $\mathcal{N}_l(t)$, $z_l(t)$ and $g_l(t)$ are defined by

$$\begin{aligned}
[\mathcal{M}_l]_{i,j} &:= \binom{i}{j} M^{(i-j)} + \binom{i}{j+1} C^{(i-j-1)} + \binom{i}{j+2} K^{(i-j-2)}, \quad i, j = 0, \ldots, l,\\
[\mathcal{L}_l]_{i,j} &:= \begin{cases} C^{(i)} + \binom{i}{j+1} K^{(i-j-1)} & \text{for } i = 0, \ldots, l,\ j = 0,\\ 0 & \text{otherwise,} \end{cases}\\
[\mathcal{N}_l]_{i,j} &:= \begin{cases} K^{(i)} & \text{for } i = 0, \ldots, l,\ j = 0,\\ 0 & \text{otherwise,} \end{cases}\\
[z_l]_i &:= x^{(i)}, \quad i = 0, \ldots, l,\\
[g_l]_i &:= f^{(i)}, \quad i = 0, \ldots, l.
\end{aligned} \tag{3}$$

The local characteristic values of the triple $(\mathcal{M}_l(\hat{t}), \mathcal{L}_l(\hat{t}), \mathcal{N}_l(\hat{t}))$ at a fixed $\hat{t} \in \mathbb{I}$ are invariant under global equivalence transformations of the original triple (M, C, K). Further, we are able to extract a strangeness-free triple $(\hat{M}, \hat{C}, \hat{K})$ using only

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local information from $(\mathcal{M}_{\hat{\mu}}(t), \mathcal{L}_{\hat{\mu}}(t), \mathcal{N}_{\hat{\mu}}(t))$. By determining matrix functions Z_3, Z_2 and Z_1 of appropriate dimensions, that span certain coranges of the triple $(\mathcal{M}_{\hat{\mu}}(\hat{t}), \mathcal{L}_{\hat{\mu}}(\hat{t}), \mathcal{N}_{\hat{\mu}}(\hat{t}))$, we can construct a triple of matrix functions

$$(\hat{M}, \hat{C}, \hat{K}) = \left(\begin{bmatrix} \hat{M}_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \hat{C}_1 \\ \hat{C}_2 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \hat{K}_1 \\ \hat{K}_2 \\ \hat{K}_3 \\ 0 \end{bmatrix} \right) = \left(\begin{bmatrix} Z_1^H M \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} Z_1^H C \\ Z_2^H \mathcal{L}_{\hat{\mu}} \mathcal{I}_n \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} Z_1^H K \\ Z_2^H \mathcal{N}_{\hat{\mu}} \mathcal{I}_n \\ Z_3^H \mathcal{N}_{\hat{\mu}} \mathcal{I}_n \\ 0 \end{bmatrix} \right) \tag{4}$$

with $\mathcal{I}_n = \begin{bmatrix} I_n & 0 & \dots & 0 \end{bmatrix}^H$. This triple has the same size as the original triple and we can show that it is strangeness-free with the same characteristic values as the strangeness-free system obtained via the algebraic approach described in [5]. Setting $\hat{f}_1 = Z_1^H f$, $\hat{f}_2 = Z_2^H g_{\hat{\mu}}$, $\hat{f}_3 = Z_3^H g_{\hat{\mu}}$ and $\hat{f}_4 = 0$ (assuming that the system is solvable) we obtain from the inflated DAE (2) a system

$$\hat{M}(t)\ddot{x}(t) + \hat{C}(t)\dot{x}(t) + \hat{K}(t)x(t) = \hat{f}(t),$$

which has the same solution set as the original system (1) and can easily be solved numerically as it is strangeness-free.

Such second order strangeness-free differential-algebraic systems then have to be solved numerically. For the direct discretization of second order DAEs we can use BDF methods, Runge-Kutta methods and General Linear Methods. In the following we will only present a Runge-Kutta discretization for some general nonlinear second order DAE of the form

$$F(t, y(t), \dot{y}(t), \ddot{y}(t)) = 0, \quad y(t_0) = y_0 \in \mathbb{C}^n, \quad \dot{y}(t_0) = \dot{y}_0 \in \mathbb{C}^n, \quad t_0 \in \mathbb{I},$$

with $F \in \mathcal{C}(\mathbb{I} \times \mathbb{C}^m \times \mathbb{C}^m \times \mathbb{C}^m, \mathbb{C}^m)$ sufficiently smooth. Similar approaches can be made to construct BDF methods and General Linear Methods for second order systems. Such an s-stage Runge-Kutta method is given by

$$y_{n+1} = y_n + h\dot{y}_n + h^2 \sum_{i=1}^{s} \tilde{b}_i \ddot{Y}_{ni},$$

$$\dot{y}_{n+1} = \dot{y}_n + h \sum_{i=1}^{s} b_i \ddot{Y}_{ni},$$

with internal stages

$$Y_{ni} = y_n + hc_i\dot{y}_n + h^2 \sum_{j=1}^{s} \tilde{a}_{ij} \ddot{Y}_{nj},$$

$$\dot{Y}_{ni} = \dot{y}_n + h \sum_{j=1}^{s} a_{ij} \ddot{Y}_{nj},$$

which have to satisfy for $i = 1, \dots, s$ the nonlinear system

$$F(t_n + c_i h, Y_{ni}, \dot{Y}_{ni}, \ddot{Y}_{ni}) = 0.$$

This means that from given approximations y_n, $\dot{y}_n$ at time t_n new approximations y_{n+1} and $\dot{y}_{n+1}$ to the exact solutions $y(t_{n+1})$ and $\dot{y}(t_{n+1})$ at time $t_{n+1} = t_n + h = t_0 + (n+1)h$ are computed with a given stepsize h and coefficient a_{ij}, $\tilde{a}_{ij}$, b_i, $\tilde{b}_i$, c_i of a specific Runge-Kutta method. A detailed description of the discretization of semi-explicit second order DAEs with BDF methods, Runge-Kutta methods and General Linear Methods can be found in [6], where certain numerical examples illustrate that we can obtain better numerical results solving second order systems directly, particularly with regard to changes in the stepsize or order of BDF methods.

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