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Constraint partitioning in dynamic iteration methods

*Dynamic iteration (*waveform relaxation*) is a well approved approach to the numerical solution of coupled instationary differential equations that is based on a splitting into several subsystems. If the subsystems are coupled by constraints then there is no generic way to assign these constraints to the subsystems. In the present paper we consider three partitioning strategies for constraints that couple two differential-algebraic systems. An error analysis shows that the stability of the dynamic iteration method depends strongly on the partitioning of the constraints.*

1. Introduction

In a modular approach to the modelling of coupled physical phenomena and coupled technical systems the overall problem is splitted into several subsystems that are in a first step modelled separately. In the second (and final) step these models for the subsystems are coupled to obtain a full model for the overall coupled problem. Typical coupling conditions are, e. g., balance equations, continuity conditions, and contact conditions [3].

The modular approach results in coupled systems of model equations. The special structure of such coupled systems may be exploited in the numerical solution [6]. As in the previous paper [1] we focus again on dynamic iteration methods for coupled differential-algebraic systems. Dynamic iteration (or waveform relaxation) methods have originally been introduced for the simulation of large scale electrical circuits [5]. Similar to the classical Picard iteration the dynamic iteration works in a function space, the iterates are continuous functions that approximate the solution of an initial or boundary value problem.

Dynamic iteration is a promising approach to the numerical solution of coupled differential equations since within each step of iteration the system is decoupled and the subsystems may be solved separately (*modular* time integration [4]). If the subsystems are coupled by constraints then each constraint has to be assigned to (at least) one of the subsystems. The partitioning of the overall coupled system into subsystems includes a partitioning of the constraints.

In the present paper we consider dynamic iteration methods with three different partitioning strategies for the constraints. Stability and convergence of these methods may be studied on the basis of the corresponding analysis for a special Gauss–Seidel type method that has been developed in detail in [1]. The error bounds indicate that the stability of the dynamic iteration depends strongly on the partitioning of the constraints.

The paper is organized as follows: In Section 2 we start with a more precise description of the coupled system. The class of dynamic iteration methods is defined in Section 3. In Section 4 stability and convergence of these methods are analysed. In the present paper we restrict ourselves to these theoretical investigations. A discussion of practical applications in mechanical engineering and results of numerical tests may be found in [1].

2. The problem class

As a typical but nevertheless simple problem class we consider the coupling of two differential-algebraic systems

$$\left.\begin{array}{rclcrcl} \dot y_1(t) &=& f_1(y_1,y_2,z_1)\,, & \qquad & \dot y_2(t) &=& f_2(y_1,y_2,z_2)\,, \\ 0 &=& h_1(y_1,y_2,z_1,u)\,, & & 0 &=& h_2(y_1,y_2,z_2,u) \end{array}\right\} \tag{1a}$$

by n_u algebraic equations

$$0 = g(y_1,y_2,z_1,z_2)\ . \tag{1b}$$

The i-th subsystem of (1a) consists of n_{y_i} differential equations $\dot y_i = f_i$ and n_{z_i} algebraic equations $0 = h_i$, $(i = 1, 2)$. The subsystems are coupled by the arguments y_1, y_2 in the right hand sides of (1a) and by the constraints (1b). We assume that the initial value problem

$$y(0) = y_0\ ,\quad z(0) = z_0\ ,\quad u(0) = u_0 \tag{2}$$

for (1) has a unique solution $y = (y_1,y_2)^\top\colon [0,T_e] \to \mathbb{R}^{n_y}$, $z = (z_1,z_2)^\top\colon [0,T_e] \to \mathbb{R}^{n_z}$, $u : [0,T_e] \to \mathbb{R}^{n_u}$ on the finite time interval $[0,T_e]$, $n_y = \sum n_{y_i}$, $n_z = \sum n_{z_i}$. In a neighbourhood of this solution the functions $f=(f_1,f_2)^\top$, $h=(h_1,h_2)^\top$, and g are supposed to be sufficiently often differentiable. Furthermore, it is supposed that the Jacobians

$$\begin{pmatrix} \frac{\partial h}{\partial z} & \frac{\partial h}{\partial u} \\ \frac{\partial g}{\partial z} & 0 \end{pmatrix}, \quad \begin{pmatrix} \frac{\partial h_i}{\partial z_i} & \frac{\partial h_i}{\partial u} \\ \frac{\partial g}{\partial z_i} & 0 \end{pmatrix}, \quad \frac{\partial h_i}{\partial z_i}, \quad (i=1,2) \tag{3}$$

are non-singular such that the coupled system (1) has index one [2]. Condition (3) guarantees that for $i=1$ and $i=2$ the equations $h_i(y_1,y_2,z_i,u)=0$ are (locally) uniquely solvable w. r. t. z_i and the systems of equation

$$0 = h_i(y_1,y_2,z_i,u)\,, \qquad 0 = g(y_1,y_2,z_1,z_2)$$

are (locally) uniquely solvable w. r. t. z_i and u.

3. The class of dynamic iteration methods

In a dynamic iteration method the numerical solution of the initial value problem (2) for the coupled system (1) is composed of analytical solutions for initial value problems for the individual subsystems. Instead of considering the time integration for the subsystems in detail the convergence analysis for dynamic iteration focusses on the *coupling* between the subsystems.

Example 1. The iterates $(y_1^{(k)},y_2^{(k)})$ of the classical Gauss–Seidel method for a system of two coupled ordinary differential equations (ODEs)

$$\dot y_1(t) = f_1(y_1,y_2)\,, \qquad \dot y_2(t) = f_2(y_1,y_2) \tag{4}$$

with initial values $y_i(0)=y_{i,0}$, $(i=1,2)$ are defined as solutions of the initial value problems

$$\dot y_1^{(k)}(t) = f_1(y_1^{(k)},y_2^{(k-1)})\,, \qquad y_1^{(k)}(0)=y_{1,0}\,, \tag{5a}$$

$$\dot y_2^{(k)}(t) = f_2(y_1^{(k)},y_2^{(k)})\,, \qquad y_2^{(k)}(0)=y_{2,0}\,. \tag{5b}$$

The initial guesses $y_i^{(0)}$ may be set, e. g., to $y_i^{(0)}(t) := y_{i,0}$, $(t\in[0,T_e],\ i=1,2)$. If the right hand sides f_i satisfy a Lipschitz condition and the time interval of interest is bounded then (5) is convergent [7].

Dynamic iteration may suffer from very slow convergence on large time intervals. Therefore a practical implementation is based on a splitting of $[0,T_e]$ into *windows* $[T_n,T_{n+1}]$ with a discrete time grid $0=T_0<T_1<\ldots<T_N=T_e$. In each window an initial guess $y_{n,i}^{(0)} \in C(\,(T_n,T_{n+1}],\mathbb{R}^{n_{y_i}})$ is obtained extrapolating the numerical solution $\tilde y_i$ from $[0,T_n]$ to $(T_n,T_{n+1}]$. Then a finite number k_n of dynamic iteration steps is performed such that the numerical solution $\tilde y_i$ is continued from $[0,T_n]$ to $(T_n,T_{n+1}]$ by

$$\tilde y_i\,\big|_{(T_n,T_{n+1}]} := y_{n,i}^{(k_n)}\,. \tag{6}$$

The coupled system (1) goes beyond the classical framework of Example 1 since the subsystems are coupled not only by the right hand sides in (1a) but additionally by constraints (1b). There is no generic way to consider these constraints in the dynamical iteration.

In [1] we generalized the Gauss–Seidel iteration (5) assigning all constraints (1b) to the second subsystem. In the first stage of the k-th Gauss–Seidel step the functions $y_{n,2}^{(k-1)}$ and $u_n^{(k-1)}$ are given and the initial value problem

$$\begin{aligned} \dot y_{n,1}^{(k)}(t) &= f_1(y_{n,1}^{(k)},y_{n,2}^{(k-1)},z_{n,1}^{(k)})\,, \qquad y_{n,1}^{(k)}(T_n)=\tilde y_1(T_n)\,,\\ 0 &= h_1(y_{n,1}^{(k)},y_{n,2}^{(k-1)},z_{n,1}^{(k)},u_n^{(k-1)}) \end{aligned} \tag{7a}$$

is solved w. r. t. $y_{n,1}^{(k)}$ and $z_{n,1}^{(k)}$. In the second stage these functions are inserted in the initial value problem

$$\begin{aligned} \dot y_{n,2}^{(k)}(t) &= f_2(y_{n,1}^{(k)},y_{n,2}^{(k)},z_{n,2}^{(k)})\,, \qquad y_{n,2}^{(k)}(T_n)=\tilde y_2(T_n)\,,\\ 0 &= h_2(y_{n,1}^{(k)},y_{n,2}^{(k)},z_{n,2}^{(k)},u_n^{(k)})\,,\\ 0 &= g(y_{n,1}^{(k)},y_{n,2}^{(k)},z_{n,1}^{(k)},z_{n,2}^{(k)}) \end{aligned} \tag{7b}$$

that defines the remaining solution components $y_{n,2}^{(k)}$, $z_{n,2}^{(k)}$, and $u_n^{(k)}$.

On the other hand a Gauss–Seidel method for (1) may consider the constraints (1b) as well in the first subsystem:

$$\begin{aligned} \dot y_{n,1}^{(k)}(t) &= f_1(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}) \,, \qquad y_{n,1}^{(k)}(T_n) = \tilde y_1(T_n) \,, \\ 0 &= h_1(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}, u_n^{(k)}) \,, \\ 0 &= g(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}, z_{n,2}^{(k-1)}) \,, \end{aligned} \tag{8a}$$

$$\begin{aligned} \dot y_{n,2}^{(k)}(t) &= f_2(y_{n,1}^{(k)}, y_{n,2}^{(k)}, z_{n,2}^{(k)}) \,, \qquad y_{n,2}^{(k)}(T_n) = \tilde y_2(T_n) \,, \\ 0 &= h_2(y_{n,1}^{(k)}, y_{n,2}^{(k)}, z_{n,2}^{(k)}, u_n^{(k)}) \,. \end{aligned} \tag{8b}$$

Obviously, the approaches (7) and (8) may also be combined such that coupling conditions (1b) are considered in both subsystems. A typical method of this type is

$$\begin{aligned} \dot y_{n,1}^{(k)}(t) &= f_1(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}) \,, \qquad y_{n,1}^{(k)}(T_n) = \tilde y_1(T_n) \,, \\ 0 &= h_1(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}, U_1) \,, \\ 0 &= g(y_{n,1}^{(k)}, y_{n,2}^{(k-1)}, z_{n,1}^{(k)}, z_{n,2}^{(k-1)}) \,, \end{aligned} \tag{9a}$$

$$\begin{aligned} \dot y_{n,2}^{(k)}(t) &= f_2(y_{n,1}^{(k)}, y_{n,2}^{(k)}, Z_2) \,, \qquad y_{n,2}^{(k)}(T_n) = \tilde y_2(T_n) \,, \\ 0 &= h_2(y_{n,1}^{(k)}, y_{n,2}^{(k)}, Z_2, U_2) \,, \\ 0 &= g(y_{n,1}^{(k)}, y_{n,2}^{(k)}, z_{n,1}^{(k)}, Z_2) \,. \end{aligned} \tag{9b}$$

The functions $U_1(t)$, $U_2(t)$, $Z_2(t)$ are auxiliary functions that define the new iterates

$$z_{n,2}^{(k)}(t) := Z_2(t) + A(t)\big(U_2(t) - U_1(t)\big) \,, \quad u_n^{(k)}(t) := U_2(t) + B(t)\big(U_2(t) - U_1(t)\big) \,. \tag{9c}$$

The matrix valued functions $A : [0, T_e] \to \mathbb{R}^{n_{z_2} \times n_u}$, $B : [0, T_e] \to \mathbb{R}^{n_u \times n_u}$ are free parameters of method (9).

Assumption (3) guarantees that all three methods (7), (8), (9) are well defined since the subsystems (7a), (7b), ..., (9b) form differential-algebraic systems of index 1, see [2]. The initial values for the algebraic components $z_{n,i}^{(k)}$, $u_n^{(k)}$, Z_2, and U_i are defined by the algebraic equations $h_i = 0$, $g = 0$.

4. Error estimates

Dynamic iteration methods for coupled ODEs define a contractive mapping in a scaled L^∞–norm on $[0, T_e]$ such that convergence follows from the Fixed point Theorem [7]. If dynamic iteration is applied to coupled differential-algebraic systems then a *contractivity condition* has to be satisfied to guarantee also contractivity w. r. t. the algebraic solution components [5]. An additional contractivity condition is necessary for a stable error propagation from window to window [1].

The error is essentially influenced by the choice of the initial guesses $(y_n^{(0)}, z_n^{(0)}, u_n^{(0)})$ and by the number k_n of iteration steps in each window $[T_n, T_{n+1}]$. For simplicity of presentation we restrict ourselves to fixed window sizes $H := T_{n+1} - T_n$. It is supposed that the initial guesses for the **d**ifferential components y and the **a**lgebraic components z and u are obtained extrapolating continuously from $(T_{n-1}, T_n]$ to $(T_n, T_{n+1}]$:

$$y_n^{(0)} := \Phi_n^{(\mathrm{d})}\big(\tilde y|_{(T_{n-1},T_n]}\big) \,, \qquad (z_n^{(0)}, u_n^{(0)}) := \Phi_n^{(\mathrm{a})}\big((\tilde z, \tilde u)|_{(T_{n-1},T_n]}\big) \,.$$

Here $(\tilde y, \tilde z, \tilde u)$ is the result of the dynamic iteration method with a finite number of iteration steps, see (6). We assume that the extrapolation operators $\Phi_n^{(\mathrm{d})}$, $\Phi_n^{(\mathrm{a})}$ satisfy a Lipschitz condition

$$\|\Phi_n^{(\mathrm{d})}(\hat Y) - \Phi_n^{(\mathrm{d})}(Y)\| \le L \|\hat Y - Y\| \,, \qquad \|\Phi_n^{(\mathrm{a})}(\hat Z, \hat U) - \Phi_n^{(\mathrm{a})}(Z, U)\| \le L(\|\hat Z - Z\| + \|\hat U - U\|)$$

with a Lipschitz constant L being independent of H ($\|.\|$ denotes the L^∞–norm).

The *extrapolation errors* are defined applying $\Phi_n^{(\mathrm{d})}$, $\Phi_n^{(\mathrm{a})}$ to the analytical solution of (1):

$$\delta_n^{(\mathrm{d})} := \Phi_n^{(\mathrm{d})}\big(y|_{(T_{n-1},T_n]}\big) - y|_{(T_n,T_{n+1}]} \,, \qquad \delta_n^{(\mathrm{a})} := \Phi_n^{(\mathrm{a})}\big((z,u)|_{(T_{n-1},T_n]}\big) - \begin{pmatrix} z \\ u \end{pmatrix}\Big|_{(T_n,T_{n+1}]} \,.$$

With these assumptions the convergence result of Theorem 2.2 in [1] may be generalized to (7), (8), and (9):

Theorem 1. *If the contractivity conditions $\alpha \le \bar{\alpha}$ and $L\alpha^{k_n} \le \bar{\alpha}$ are satisfied for all $n \ge 0$ with $nH \le T_N = T_e$ and a constant $\bar{\alpha} < 1$ then the dynamic iteration methods (7), (8) and (9) are convergent and there are constants $C_0, C^*, H_0 > 0$ such that for all $H \le H_0$*

$$\|\tilde{y} - y\|_{[0,T_e]} + \|\tilde{z} - z\|_{[0,T_e]} + \|\tilde{u} - u\|_{[0,T_e]} \le C^* \cdot \max_{0 \le n < N} \big(\mu^{\max(0,k_n-2)} \|\delta_n^{(\mathrm{d})}\| + \mu^{k_n - 1} \|\delta_n^{(\mathrm{a})}\| \big)$$

with a constant $\mu = \alpha + C_0 H \,/\, (\alpha + \sqrt{H})$. The constants C_0, C^*, and H_0 are independent of the contractivity constant α *that is given*

- *by* $\alpha := \max_{t \in [0,T_e]} \Big\| \Big[\Big(\frac{\partial g}{\partial z_2} \Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big)^{-1} \Big(\frac{\partial g}{\partial z_1} \Big(\frac{\partial h_1}{\partial z_1} \Big)^{-1} \frac{\partial h_1}{\partial u} \Big) \Big] (y(t), z(t), u(t)) \Big\|$ *for Method (7),*
- *by* $\alpha := \max_{t \in [0,T_e]} \Big\| \Big[\Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big(\frac{\partial g}{\partial z_1} \Big(\frac{\partial h_1}{\partial z_1} \Big)^{-1} \frac{\partial h_1}{\partial u} \Big)^{-1} \frac{\partial g}{\partial z_2} \Big] (y(t), z(t), u(t)) \Big\|$ *for Method (8), and*
- *by* $\alpha := \max_{t \in [0,T_e]} \Big\| \Big[\Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big(\frac{\partial g}{\partial z_2} \Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big)^{-1} \frac{\partial g}{\partial z_2} - A(t) R(t) \frac{\partial g}{\partial z_2} \Big] (y(t), z(t), u(t)) \Big\|$ *for Method (9),*

  $$R(t) := \Big(\frac{\partial g}{\partial z_1} \Big(\frac{\partial h_1}{\partial z_1} \Big)^{-1} \frac{\partial h_1}{\partial u} \Big)^{-1} + \Big(\frac{\partial g}{\partial z_2} \Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big)^{-1} .$$

Remark 1. a) If the contractivity conditions are violated and $\alpha > 1$ then the stability of the method may not be guaranteed. An exponential instability may be observed already in very simple model problems like (1) with scalar linear functions h_i and g.

b) The most important difference between (7), (8), and (9) is the way in that the constraints (1b) are assigned to the subsystems. Theorem 1 shows that this partitioning of the constraints has an essential influence on the stability of the dynamic iteration method.

c) In (9) constant α is independent of $B(t)$. For the most obvious choice $A(t) = 0$ constant α is given by the norm of a projector in $\mathbb{R}^{n_{z_2}}$ such that $\alpha \ge 1$ and the contractivity condition is always violated. However, stability and convergence may be achieved by an appropriate definition of $A(t)$. The optimal value $\alpha = 0$ is obtained for

$$A(t) := \Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big(\Big(\frac{\partial g}{\partial z_1} \Big(\frac{\partial h_1}{\partial z_1} \Big)^{-1} \frac{\partial h_1}{\partial u} \Big) + \Big(\frac{\partial g}{\partial z_2} \Big(\frac{\partial h_2}{\partial z_2} \Big)^{-1} \frac{\partial h_2}{\partial u} \Big) \Big)^{-1} \Big(\frac{\partial g}{\partial z_1} \Big(\frac{\partial h_1}{\partial z_1} \Big)^{-1} \frac{\partial h_1}{\partial u} \Big) .$$

5. Summary

In a dynamic iteration method for coupled differential-algebraic systems the coupling conditions have to be assigned to one or more of the subsystems. Three different strategies for the partitioning of the constraints in a Gauss–Seidel type method have been analysed. The convergence analysis indicates that the constraints should be partitioned such that a problem and method dependent contractivity constant α is minimized.

6. References

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