

A Combined Structural-Algebraic Approach for the Regularization of Coupled Systems of DAEs

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A Combined Structural-Algebraic Approach for the Regularization of Coupled Systems of DAEs^{*}

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Abstract

The automated modeling of multi-physical dynamical systems is usually realized by coupling different subsystems together via certain interface or coupling conditions. This approach results in large-scale high-index differential-algebraic equations (DAEs). Since the direct numerical simulation of these kind of systems leads to instabilities and possibly non-convergence of the numerical methods a regularization or remodeling of the system is required. In many simulation environments a kind of structural analysis based on the sparsity pattern of the system is used to determine the index and a reduced system model. However, this approach is not reliable for certain problem classes, in particular we show that it is not suited for coupled systems of DAEs. We will present a new approach for the regularization of coupled dynamical systems that combines the structural analysis, in particular the Signature Method [11], with classical algebraic regularization techniques and thus allows to handle so-called structurally singular systems and also enables a proper treatment of redundancies or inconsistencies in the system.

Keywords: Differential-algebraic equation, coupled system, regularization, structural analysis, signature method, structural singularity.

AMS(MOS) subject classification: 65L80, 34A09

1 Introduction

Modeling and simulation of multi-physics dynamical systems is an important issue in many industrial applications. In modern simulation packages like DYMOLA, MATLAB/SIMULINK, MAPLESIM, SIMULATIONX, etc. the modeling process is automated using various sophisticated libraries for the different system components (from different physical domains). Then, these subcomponent can be interconnected in a network structure in a hierarchical way. During the compilation process these subsystems are coupled together via certain interface or coupling conditions. This way of modeling dynamical systems via a network of subcomponents leads to large (but usually sparse) systems of differential-algebraic equations (DAEs).

In this paper, we will consider coupled systems consisting of a set of subsystems S_i , where the dynamical behavior of each subsystem is described by a system of nonlinear DAEs

$$F^i(t, z^i, \dot{z}^i, u^i) = 0,$$

with states $z^i : \mathbb{I} \to \mathbb{R}^{n_i}$, inputs $u^i : \mathbb{I} \to \mathbb{R}^{p_i}$, and compact interval $\mathbb{I} \subset \mathbb{R}$. The coupling of a subsystem S_i with other subsystems S_{j_1}, \ldots, S_{j_k} is realized via coupling conditions of the form

$$u^i = G_{ij_1\dots j_k}(t, z^{j_1}, \dots, z^{j_k})$$

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Altogether, this yields a large nonlinear DAE system.

If this resulting system of DAEs is of high index, then the direct numerical simulation of these kinds of systems leads to instabilities and possibly non-convergence of the numerical methods, see [1, 3, 6]. Thus, a regularization or remodeling of the DAE is required to guarantee stable and robust numerical computations [6].

In most modeling and simulation tools the current state of the art to deal with high index DAEs is to use some kind of structural analysis based on the sparsity pattern of the system, e.g., the Signature Method [11] or Pantelides Algorithm [10]. Here, generic structural information together with certain computer-algebra packages or symbolic differentiation is used to identify the constraints and interface conditions, to determine the index of the system and to compute an index reduced system model. Furthermore, symbolically sorting the equations by using graph-theoretical algorithms enables the efficient solution of sparse equation systems. However, this approach is not reliable for certain problem classes, e.g., for so-called *structurally singular* problems, and, in particular, we will show that this is the case for certain coupled systems of DAEs.

In this paper, we will present a new approach for the remodeling of coupled dynamical systems that combines the structural analysis with classical algebraic regularization techniques and allows to handle structurally singular systems and also a proper treatment of redundancies or inconsistencies in the system.

The paper is organized as follows. In Section 2 we introducing some notation and present the main results concerning general DAE theory and regularization techniques, including the structural analysis for DAEs based on the Signature Method. In Section 3 we describe a regularization technique for structurally well-posed problems. Furthermore, in Section 4, we show that the structural analysis fails for coupled systems if the coupling leads to higher index DAEs. Thus, we show how a combined structural-algebraic approach can be used in case of structurally singular problems. Finally, in Section 5 we present some numerical examples.

2 Preliminaries

2.1 DAE Theory

In this section, we review the basic facts of DAE theory following the presentation in [6]. We consider a general nonlinear DAE given by

$$F(t, z, \dot{z}) = 0, \tag{1}$$

with a sufficiently smooth function $F : \mathbb{I} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^m$, $z : \mathbb{I} \to \mathbb{R}^n$ and compact interval $\mathbb{I} \subset \mathbb{R}$. In the following, for a differentiable time depending function x the *i*th (total) derivative of x(t) with respect to t is denoted by $x^{(i)}(t) = d^i x(t)/dt^i$ for $i \in \mathbb{N}_0$, using the convention $x^{(0)}(t) = x(t)$, $x^{(1)}(t) = \dot{x}(t)$, and $x^{(2)}(t) = \ddot{x}(t)$. For a differentiable function f depending on x the (partial) derivative of f(x) with respect to x is denoted by $f_{,x}(x) = \frac{\partial}{\partial x}f(x)$. The same notation is used for differentiable vector and matrix functions.

A regularization of the DAE (1) is an equivalent formulation of the system

$$\hat{F}(t,\hat{z},\dot{\hat{z}}) = 0, \tag{2}$$

in such a way that the index of the regularized system (2) is reduced and both systems have the same solution sets, whereupon there is a unique mapping from the state \hat{z} of the regularized system (2) to the state z of the original system (1).

In order to obtain a regularization, we introduce the *derivative array* \mathcal{D}_i of level *i* of the form

$$\mathcal{D}_i(t, z, \dot{z}, \dots, z^{(i+1)}) := \begin{bmatrix} F(t, z, \dot{z}) \\ \frac{d}{dt} F(t, z, \dot{z}) \\ \vdots \\ \frac{d^i}{dt^i} F(t, z, \dot{z}) \end{bmatrix} = 0,$$
(3)

which stacks the original equations of the DAE and all its derivatives up to level i into one large system. To obtain existence and uniqueness results for general DAEs, a hypothesis was introduced in [4].

Hypothesis 1. [4] Consider a nonlinear DAE (1). There exist integers μ, r, a, d and v such that the solution set of the derivative array \mathcal{D}_{μ}

$$\mathbb{L}_{\mu} = \{ (t, z, \dot{z}, \dots, z^{(\mu+1)}) \in \mathbb{I} \times \mathbb{R}^{(\mu+2)n} | \mathcal{D}_{\mu}(t, z, \dot{z}, \dots, z^{(\mu+1)}) = 0 \}$$

is not empty, and the following properties hold:

- 1. The set $\mathbb{L}_{\mu} \subset \mathbb{R}^{(\mu+2)n+1}$ forms a manifold of dimension $(\mu+2)n+1-r$.
- 2. We have rank $\mathcal{D}_{\mu,[z,\dot{z},...,z^{(\mu+1)}]} = r \text{ on } \mathbb{L}_{\mu}$.
- 3. We have corank $\mathcal{D}_{\mu,[z,\dot{z},...,z^{(\mu+1)}]}$ corank $\mathcal{D}_{\mu-1,[z,\dot{z},...,z^{(\mu)}]} = v$ on \mathbb{L}_{μ} . (The corank is the codimension of the range and we use the convention that corank $\mathcal{D}_{-1,z} = 0$.)
- 4. We have rank $\mathcal{D}_{\mu,[\dot{z},...,z^{(\mu+1)}]} = r a$ on \mathbb{L}_{μ} such that there are smooth full rank matrix functions Z_2 and T_2 defined on \mathbb{L}_{μ} of size $((\mu+1)m,a)$ and (n,n-a), respectively, satisfying

$$Z_2^T \mathcal{D}_{\mu,[\dot{z},...,z^{(\mu+1)}]} = 0, \quad \operatorname{rank} Z_2^T \mathcal{D}_{\mu,z} = a, \quad Z_2^T \mathcal{D}_{\mu,z} T_2 = 0$$

on \mathbb{L}_{μ} .

5. We have rank $F_{,z}T_2 = d = m - a - v$ on \mathbb{L}_{μ} such that there exists a smooth matrix function Z_1 defined on \mathbb{L}_{μ} of size (m, d) with $Z_1^T F_{,z} T_2$ having full rank.

The smallest possible μ in Hypothesis 1 is called the *strangeness index* (s-index) of the DAE (1) and a system with vanishing strangeness index is called *strangeness-free*. Further, a DAE (1) with m = n that satisfies Hypothesis 1 with v = 0 is called *regular*, otherwise it is called *singular*. The quantities d and a are the numbers of differential and algebraic equations of the DAE.

It has been shown in [4] that Hypothesis 1 implies (locally) the existence of a reduced system (in the original variables) of the form

$$\hat{F}_1(t,z,\dot{z}) = 0, \tag{4a}$$

$$\hat{F}_2(t,z) = 0,\tag{4b}$$

with $\hat{F}_1 = Z_1^T F$, $\hat{F}_2 = Z_2^T \mathcal{D}_{\mu}$. An initial condition $z(t_0) = z_0$ with $t_0 \in \mathbb{I}$, $z_0 \in \mathbb{R}^n$ is said to be consistent with the DAE (1), if it satisfies the algebraic equation $\hat{F}_2(t_0, z_0) = 0$. Furthermore, it has been shown in [6] that the system (4) is locally equivalent to a semi-explicit DAE of the form

$$\dot{z}_1 = \mathcal{L}(t, z_1, z_2, \dot{z}_2),$$
 (5a)

$$z_3 = \mathcal{R}(t, z_1, z_2),\tag{5b}$$

with differential components $z_1 \in C^1(\mathbb{I}, \mathbb{R}^d)$, algebraic components $z_3 \in C^0(\mathbb{I}, \mathbb{R}^a)$, and undetermined components $z_2 \in C^1(\mathbb{I}, \mathbb{R}^u)$, with u = n - d - a. When the undetermined components z_2 are fixed, then the resulting system has (locally) a unique solution for z_1 and z_3 , provided that a consistent initial condition is given.

Theorem 1. [4] Let F in (1) be sufficiently smooth and satisfy Hypothesis 1 with μ , r, a, d, v and u = n - d - a. Then every solution of (1) also solves the reduced problems (4) and (5) consisting of d differential and a algebraic equations.

Note that in the reduced systems (4) and (5) we have not used the quantity v. This quantity measures the number of equations in the original system that give rise to trivial equations 0 = 0, i.e., it counts the number of redundancies in the system. Together with a and d it gives a complete classification of the m equations into d differential equations, a algebraic equations and v trivial

equations. Of course, trivial equations can be simply removed without altering the solution set. Thus, the reduced systems (4) and (5) are regularizations of the original system (1).

Note that it can be sufficient to differentiate only a subset of equations in order to be able to obtain a regularization. Then, the inflated system that is formed by adding only this subset of derivatives to the original system is called a *reduced derivative array*.

In the following, the previously described approach of obtaining a regularized system via Hypothesis 1 will be called the *derivative array approach* or *algebraic approach*.

Besides the strangeness index, another frequently used index concept is the concept of the differentiation index (d-index). Roughly speaking, the d-index is defined as the minimal number of times that all or part of the equations in the system must be differentiated in order to obtain an explicit ordinary differential system for the unknown function z, for details see e.g. [1, 2]. This approach, however, is only feasible for uniquely solvable square systems, since a DAE with free solution components cannot lead to an ordinary differential equation. For a regular DAE, i.e., m = n = d + a, with well-defined strangeness index μ the differentiation index ν_d is also well-defined and

$$\nu_d = \begin{cases} 0 & \text{for } a = 0, \\ \mu + 1 & \text{for } a \neq 0. \end{cases}$$

In the following, we will consider a class of specially structured DAE systems, namely *semi-explicit* DAEs of the form

$$\dot{x} = f(t, x, y), \tag{6a}$$

$$0 = g(t, x, y), \tag{6b}$$

with $f: \mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \to \mathbb{R}^{n_x}$ and $g: \mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \to \mathbb{R}^{n_y}, x: \mathbb{I} \to \mathbb{R}^{n_x}, y: \mathbb{I} \to \mathbb{R}^{n_y}$. We assume that $\mathbb{L}_0 \neq \emptyset$, where

$$\mathbb{L}_0 = \{ (t, x, y, \dot{x}) \, | \, \dot{x} = f(t, x, y), 0 = g(t, x, y) \},\$$

i.e., in particular, the constraints g(t, x, y) = 0 can be satisfied. Then, if the Jacobian

$$g_{,y}$$
 is nonsingular for all points in \mathbb{L}_0 , (7)

the system (6) satisfies Hypothesis 1 with $n = m = n_x + n_y$ and characteristic values $\mu = 0$, $a = n_y$, and $d = n_x$, see [6]. In particular, semi-explicit systems (6) that satisfy the condition (7) are of d-index $\nu_d = 1$.

2.2 Structural Analysis for DAEs

In this paper we restrict our investigations to the Signature Method (or Σ -method) [11] for the structural analysis of differential-algebraic systems. In contrast to the algebraic approach presented in the previous section the Σ -method analyzes the properties of the system based on its sparsity pattern. Other methods, in particular Pantelides Algorithm [10] are related to this method, see Section 3.1. Here, we only shortly review the basic steps of the Σ -method. For more details, see [8, 9, 11].

The Σ -method can be applied for general nonlinear DAEs of arbitrary high order p of the form

$$F(t, z, \dot{z}, \dots, z^{(p)}) = 0,$$
(8)

with $F : \mathbb{I} \times \mathbb{R}^n \times \cdots \times \mathbb{R}^n \to \mathbb{R}^n$ sufficiently smooth and $\mathbb{I} \subset \mathbb{R}$. We denote by F_i the *i*th component of the vector-valued function F and by z_j the *j*th component of the vector z. Then, the Σ -method consists of the following steps:

1. Building the signature matrix $\Sigma = [\sigma_{ij}]_{i,j=1,\dots,n}$ with

$$\sigma_{ij} = \begin{cases} \text{highest order of derivative of } z_j \text{ in } F_i, \\ -\infty \text{ if } z_j \text{ does not occur in } F_i. \end{cases}$$

2. Finding a highest value transversal (HVT) of Σ , i.e., a transversal T of Σ

$$T = \{(1, j_1), (2, j_2), \dots, (n, j_n)\}$$

where (j_1, \ldots, j_n) is a permutation of $(1, \ldots, n)$, with maximal value

$$Val(T) := \sum_{(i,j)\in T} \sigma_{ij}.$$

3. Computing the offsets vectors $c = [c_i]_{i=1,...,n}$ and $d = [d_j]_{j=1,...,n}$ with $c_i \ge 0$, $d_j \ge 0$ such that

$$d_j - c_i \ge \sigma_{ij}$$
 for all $i, j = 1, \dots, n$, (9a)

$$d_j - c_i = \sigma_{ij} \text{ for all } (i,j) \in T.$$
 (9b)

4. Forming the Σ -Jacobian $\mathfrak{J} = [\mathfrak{J}_{ij}]_{i,j=1,\dots,n}$, with

$$\mathfrak{J}_{ij} := \begin{cases} \frac{\partial F_i}{\partial z_j^{(\sigma_{ij})}} & \text{if } d_j - c_i = \sigma_{ij}, \\ 0 & \text{otherwise.} \end{cases}$$

(We call \mathfrak{J} the Σ -Jacobian since it is in general not equal to the analytical Jacobian, but defined by the offset vectors.)

5. Building the reduced derivative array

$$\mathcal{F}(t,\mathcal{Z}) = \begin{bmatrix} F_1(t,z,\dot{z},\dots,z^{(p)}) \\ \frac{d}{dt}F_1(t,z,\dot{z},\dots,z^{(p)}) \\ \vdots \\ \frac{d^{c_1}}{dt^{c_1}}F_1(t,z,\dot{z},\dots,z^{(p)}) \\ \vdots \\ F_n(t,z,\dot{z},\dots,z^{(p)}) \\ \frac{d}{dt}F_n(t,z,\dot{z},\dots,z^{(p)}) \\ \vdots \\ \frac{d^{c_n}}{dt^{c_n}}F_n(t,z,\dot{z},\dots,z^{(p)}) \end{bmatrix} = 0,$$
(10)

with

$$\mathcal{Z} = \begin{bmatrix} z_1 & \dot{z}_1 & \dots & z_1^{(d_1)} & \dots & z_n & \dot{z}_n & \dots & z_n^{(d_n)} \end{bmatrix}^T.$$

6. Success check: if the algebraic system $\mathcal{F}(t^*, \mathbb{Z}^*) = 0$ corresponding to (10) has a solution (t^*, \mathbb{Z}^*) with $t^* \in \mathbb{I}$ and

$$\mathcal{Z}^* = \begin{bmatrix} z_1 & w_1^1 & \dots & w_1^{d_1} & \dots & z_n & w_n^1 & \dots & w_n^{d_n} \end{bmatrix}^T \in \mathbb{R}^{n + \sum_i^n d_i}$$

and \mathfrak{J} is nonsingular at (t^*, \mathbb{Z}^*) , then (t^*, \mathbb{Z}^*) is a consistent point and the method succeeds.

If the Σ -method succeeds, it allows to determine the *structural index* of the DAE as

$$\nu_S := \max_i c_i + \begin{cases} 0 & \text{if all } d_j > 0, \\ 1 & \text{if some } d_j = 0, \end{cases}$$

and $Val(\Sigma)$ defined as the value of the highest value transversal T corresponds to the number of degrees of freedom of the system (i.e., the number of differential components d in Hypothesis 1).

The HVT defines a mapping between variables and equations of maximal value, but it is usually not uniquely determined. Also the offset vectors c and d are not uniquely defined by the conditions (9), since for any feasible solution c, d, also the vectors $[c_i + \theta]_i$, and $[d_j + \theta]_j$ for any $\theta > 0$ form a solution. A HVT as well as the offset vectors can be computed by solving a linear assignment problem (LAP), see [11], i.e., Σ is the matrix of the LAP where each assignment is specified by a transversal. This LAP (as a special kind of a linear programming problem) also has a dual problem, and the offset vectors c and d are the corresponding solutions of the dual problem. Since there exists a unique element-wise smallest solution of the dual problem, these so-called *canonical offsets* are also uniquely determined and independent of the chosen HVT.

Remark 2. Note that the definition of the signature matrix Σ can be generalized for rectangular systems with $F : \mathbb{I} \times \mathbb{R}^n \times \cdots \times \mathbb{R}^n \to \mathbb{R}^m$ and $m \neq n$ in an analogous way.

Example 3. The basic steps of the Σ -method are illustrated for the example of the simple pendulum of mass m = 1, length $\ell > 0$ under gravity \mathfrak{g} , see also [11]. The system equations are given by

$$F_{1}(z, \dot{z}) = \dot{p}_{1} - q_{1} = 0,$$

$$F_{2}(z, \dot{z}) = \dot{p}_{2} - q_{2} = 0,$$

$$F_{3}(z, \dot{z}) = \dot{q}_{1} + 2p_{1}\lambda = 0,$$

$$F_{4}(z, \dot{z}) = \dot{q}_{2} + 2p_{2}\lambda + \mathfrak{g} = 0,$$

$$F_{5}(z, \dot{z}) = p_{1}^{2} + p_{2}^{2} - \ell^{2} = 0,$$
(11)

where $z = \begin{bmatrix} p_1 & p_2 & q_1 & q_2 & \lambda \end{bmatrix}^T$. The signature matrix for the system (11) is given by

$$\Sigma = \begin{bmatrix} \mathbf{1} & - & \mathbf{0} & - & - \\ - & \mathbf{1} & - & \mathbf{0} & - \\ \mathbf{0} & - & \mathbf{1} & - & \mathbf{0} \\ - & \mathbf{0} & - & \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & - & - & - \end{bmatrix},$$
(12)

where the two possible HVTs are marked by gray and blue boxes. (Here, the entries – stand for $-\infty$.) The canonical offset vectors are given by c = [1, 1, 0, 0, 2] and d = [2, 2, 1, 1, 0], and $Val(\Sigma) = 2$ (independently of the chosen HVT). The corresponding Σ -Jacobian is given by

$$\mathfrak{J} = \begin{bmatrix} F_{1,\dot{p}_1} & 0 & F_{1,q_1} & 0 & 0 \\ 0 & F_{2,\dot{p}_2} & 0 & F_{2,q_2} & 0 \\ 0 & 0 & F_{3,\dot{q}_1} & 0 & F_{3,\lambda} \\ 0 & 0 & 0 & F_{4,\dot{q}_2} & F_{4,\lambda} \\ F_{5,p_1} & F_{5,p_2} & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 2p_1 \\ 0 & 0 & 0 & 1 & 2p_2 \\ 2p_1 & 2p_2 & 0 & 0 & 0 \end{bmatrix}$$

and the reduced derivative array (10) takes the form

$$\mathcal{F}(t,\mathcal{Z}) = \begin{vmatrix} \dot{p}_1 - q_1 \\ \ddot{p}_1 - \dot{q}_1 \\ \dot{p}_2 - q_2 \\ \ddot{p}_2 - \dot{q}_2 \\ \dot{q}_1 + 2p_1\lambda \\ \dot{q}_2 + 2p_2\lambda + \mathfrak{g} \\ p_1^2 + p_2^2 - \ell^2 \\ 2p_1\dot{p}_1 + 2p_2\dot{p}_2 \\ 2p_1\dot{p}_1 + 2p_2\dot{p}_2 + 2\dot{p}_2^2 \end{vmatrix} = 0,$$
(13)

with $\mathcal{Z} = \begin{bmatrix} p_1 & \dot{p}_1 & \ddot{p}_1 & p_2 & \dot{p}_2 & \ddot{p}_2 & q_1 & \dot{q}_1 & q_2 & \dot{q}_2 & \lambda \end{bmatrix}^T$. Thus, the Σ -Jacobian \mathfrak{J} is nonsingular at every consistent point and the Σ -method succeeds with $\nu_S = \max_i c_i + 1 = 3$.

The crucial step in the Σ -method is the success check, i.e., verifying the regularity of the Σ -Jacobian at a consistent point. Systems for which the Σ -Jacobian is singular for all points (t, \mathcal{Z}) that solve the enlarged system (10) are called *structurally singular*^{*}. Accordingly, we will call systems for which the Σ -method succeeds *structurally regular*.

Lemma 4. Consider a nonlinear DAE of the form

$$F(t, z, \dot{z}) = 0, \tag{14}$$

with sufficiently smooth function $F : \mathbb{I} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ that satisfies Hypothesis 1. If the Σ -method succeeds (locally at a consistent point), then the DAE (14) is (locally) regular.

Proof. Let (14) satisfies Hypothesis 1 with μ , r, a, d, v and u = n - d - a and assume that the system is singular, i.e., u = v > 0. Thus, there are undetermined components of the solution vector z of dimension u and redundancies or inconsistencies in the system. If no equation can be assigned to be solved for an undetermined solution component, it means that there exists no HVT in the corresponding signature matrix and the Σ -method fails. The same is true if there are equations of the form $F_i(t) = 0$ in the system. On the other hand, redundancies in the system lead to linear dependent rows in the corresponding Σ -Jacobian \mathfrak{J} and the success check of the Σ -method will fail.

Remark 5. The sparsity structure of the system is essential for the success of the Σ -method. Consider e.g. the system

$$F(t, z, \dot{z}) = \begin{bmatrix} \dot{z}_1 - t\dot{z}_2 + f_1(t) \\ z_1 - tz_2 + f_2(t) \end{bmatrix}$$

which is regular and of d-index 2. For this system the success check of the Σ -method fails due to a singular Σ -Jacobian. However, a simple equivalence transformation of the system using the coordinate transformation

$$\begin{bmatrix} \tilde{z}_1\\ \tilde{z}_2 \end{bmatrix} := \begin{bmatrix} z_1 - tz_2\\ z_2 \end{bmatrix}$$

leads to the equivalent system

$$F(t, \tilde{z}, \dot{\tilde{z}}) = \begin{bmatrix} \dot{\tilde{z}}_1 + \tilde{z}_2 + f_1(t) \\ \tilde{z}_1 + f_2(t) \end{bmatrix},$$

for which the Σ -method succeeds.

It has been shown in [11] that the Σ -method works successfully for certain classes of DAE systems, amongst others for systems in Hessenberg form of size $r \geq 2$ given by

$$0 = \begin{bmatrix} G_1(z_1) & & & \\ -\dot{z}_1 & +G_2(z_1, z_2) & & \\ -\dot{z}_2 & +G_3(z_1, z_2, z_3) & & \\ \vdots & & & \\ -\dot{z}_{r-1} & +G_r(z_1, z_2, \dots, z_{r-1}, z_r) \end{bmatrix}$$
(of dimension n_1)
(of dimension n_2)
(of dimension n_3)
 \vdots
(of dimension n_r)

with $z_i \in C^1(\mathbb{I}, \mathbb{R}^{n_{i+1}})$, $i = 1, \ldots, r-1$, and $z_r \in C(\mathbb{I}, \mathbb{R}^{n_1})$ and

$$G_{1,z_1} \cdot G_{2,z_2} \cdot \ldots \cdot G_{r,z_r}$$
 is nonsingular (15b)

in a neighborhood of the solution. It is well known that systems in Hessenberg form have d-index $\nu_d = r$, see [1] (or s-index $\mu = r - 1$, and $a = rn_1$, d = n - a, $n = \sum_{i=1}^r n_i$, see [6]). In particular, Hessenberg systems include semi-explicit systems of d-index 2 and the equations of motion of constrained multibody systems.

^{*}Note that the term *structurally singular* is also used slightly different in the literature: on the one hand, it is used for systems that do not allow an assignment of the highest occurring derivative of each variables to an specific equation (i.e., systems that do not have an HVT), and on the other hand it is used for systems with singular Σ -Jacobian. Here, we use the term with respect to the second meaning.

Theorem 6 ([11]). Consider a DAE system in Hessenberg form (15a) (of size $r \ge 2$) that satisfies condition (15b). Then, the Σ -method applied to (15a) succeeds (locally at a consistent point) with $\nu_S = \max_i c_i + 1 = r = \nu_d$.

If the Σ -method succeeds the structural index determined by the offset vectors gives an upper bound for the d-index of the system, i.e., $\nu_d \leq \nu_S$, and only for specially structured systems as e.g. systems in Hessenberg form we have equality of the two indices. Examples where the structural index ν_S exceeds the d-index can be found in [12].

Another information that can be obtained from the structural analysis is a block triangular form of the signature matrix Σ or of the Σ -Jacobian \mathfrak{J} , respectively. We define

$$S_{\Sigma} := \{(i,j) \mid \sigma_{ij} > -\infty\}$$

as the sparsity pattern of Σ , and

$$S_{\mathfrak{J}} := \{(i,j) \mid d_j - c_i = \sigma_{ij}\}$$

as the sparsity pattern of \mathfrak{J} . $S_{\mathfrak{J}}$ depends on the offsets c and d obtained by the structural analysis, while S_{Σ} only depends on the structural information given by the DAE (8). In general, it holds that $S_{\mathfrak{J}} \subseteq S_{\Sigma}$ for any offset vectors c, d. A block triangular form based on a specific sparsity pattern is created by forming permutations of equations and variables. In the following, the permuted matrices are denoted by

$$\tilde{\Sigma} = \begin{bmatrix} \tilde{\Sigma}_{11} & \dots & \tilde{\Sigma}_{1p} \\ \vdots & \ddots & \vdots \\ \tilde{\Sigma}_{p1} & \dots & \tilde{\Sigma}_{pp} \end{bmatrix} \text{ and } \tilde{\mathfrak{J}} = \begin{bmatrix} \tilde{\mathfrak{J}}_{11} & \dots & \tilde{\mathfrak{J}}_{1p} \\ \vdots & \ddots & \vdots \\ \tilde{\mathfrak{J}}_{p1} & \dots & \tilde{\mathfrak{J}}_{pp} \end{bmatrix},$$

with blocks $\tilde{\Sigma}_{ij}$, $\tilde{\mathfrak{J}}_{ij}$ of size $N_i \times N_j$ with $N_i > 0$ and $\sum_{i=1}^p N_i = n$. The system is said to be in block lower triangular (BLT) form based on S_{Σ} , if the permuted signature matrix is in the form

$$\tilde{\Sigma} = \begin{bmatrix} \tilde{\Sigma}_{11} & -\infty & \dots & -\infty \\ \vdots & \tilde{\Sigma}_{22} & & \vdots \\ \vdots & & \ddots & -\infty \\ \tilde{\Sigma}_{p1} & \dots & \dots & \tilde{\Sigma}_{pp} \end{bmatrix},$$

and the system is said to be in *BLT form based on* S_3 , if the permuted Σ -Jacobian is in the form

$$\tilde{\mathfrak{J}} = \begin{bmatrix} \tilde{\mathfrak{J}}_{11} & 0 & \dots & 0 \\ \vdots & \tilde{\mathfrak{J}}_{22} & & \vdots \\ \vdots & & \ddots & 0 \\ \tilde{\mathfrak{J}}_{p1} & \dots & \dots & \tilde{\mathfrak{J}}_{pp} \end{bmatrix}.$$

Note that a BLT form based on $S_{\mathfrak{J}}$ is often finer than a BLT form based on S_{Σ} , since it puts \mathfrak{J} into BLT form but not necessarily Σ . However, a BLT form based on $S_{\mathfrak{J}}$ is only meaningful if the structural analysis succeeds. Furthermore, the values of \mathfrak{J} may change with time, so the results only hold locally.

3 Regularization for Structurally Regular DAEs

In order to obtain a regularized index reduced formulation of a given DAE system the information provided by the structural analysis, e.g., by the Σ -method can be used. If the Σ -method succeeds for a given system (8), the canonical offset vector c gives the required information which equations have to be differentiated and how many times in order to be able to extract all hidden constraints, similar as in the derivative array approach. The reduced derivative array can be obtained by adding the derivatives of F_i up to order c_i to the original system resulting in system (10). Note that this system is in general not the *minimal reduced derivative array* as considered e.g. in [5]. The extended system (10) consists of $M = \sum_i c_i + n$ equations in n unknowns z_1, \ldots, z_n , more precisely it depends on $z_1, \dot{z}_1, \ldots, z_1^{(d_1)}, \ldots, z_n, \dot{z}_n, \ldots, z_n^{(d_n)}$. Thus, we have to introduce $\sum_i c_i$ new variables to get the same number of equations and unknowns. For each equation $F_i, i = 1, \ldots, n$ we can select a variable z_{j_i} based on the information provided by the HVT, i.e., we choose the unique j_i such that $(i, j_i) \in T$. Then, in the case that $c_i > 0$, we introduce the following new variables:

$$w_{j_{i}}^{\sigma_{ij_{i}}+1} \quad \text{replacing} \quad z_{j_{i}}^{(\sigma_{ij_{i}}+1)},$$

$$\vdots \qquad (16)$$

$$w_{j_{i}}^{\sigma_{ij_{i}}+c_{i}} \quad \text{replacing} \quad z_{j_{i}}^{(\sigma_{ij_{i}}+c_{i})} = z_{j}^{(d_{j})}.$$

We collect these new variables into the vectors

$$w_{j_i} := \begin{bmatrix} w_{j_i}^{\sigma_{ij_i}+1} \\ \vdots \\ w_{j_i}^{\sigma_{ij_i}+c_i} \end{bmatrix} \quad \text{for } c_i > 0, \quad \text{and} \quad w_{j_i} = \begin{bmatrix} . \end{bmatrix} \quad \text{for } c_i = 0.$$

Note that this replacement of variables is not unique, since it depends on the chosen HVT. In order to choose the best suitable HVT, i.e., one that is valid in a maximal neighborhood of a consistent point, we use a weighting for the different possible HVTs. We define a (local) *weighting coefficient* for each possible HVT by

$$\kappa_T := \prod_{(i,j)\in T} |\mathfrak{J}_{ij}|.$$

If there is more than one possible HVT we choose one with largest value κ_T . In the following, we denote by T^* a HVT of Σ with $\kappa_{T^*} = \max_T(\kappa_T)$.

Theorem 7. Consider a nonlinear DAE

$$F(t, z, \dot{z}) = \begin{bmatrix} F_1(t, z, \dot{z}) \\ \vdots \\ F_n(t, z, \dot{z}) \end{bmatrix} = 0$$
(17)

with sufficiently smooth function $F : \mathbb{I} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ that satisfies Hypothesis 1 and for which the Σ -method succeeds with canonical offsets vectors $c = [c_1, \ldots, c_n]$ and $d = [d_1, \ldots, d_n]$. Let T^* be a HVT of the corresponding signature matrix with $\kappa_{T^*} = \max_T(\kappa_T)$. The augmented system

$$\mathcal{F}(t, z, \dot{z}, w) = 0, \tag{18}$$

with

$$w = \begin{bmatrix} w_1^T & \dots & w_n^T \end{bmatrix}^T$$

is obtained by appending the differentiated equations

$$\frac{d^{\ell}}{dt^{\ell}}F_i(t,z,\dot{z}) = 0, \quad \ell = 1,...,c_i,$$
(19)

for each equation with $c_i > 0$, i = 1, ..., n to the DAE (17) and introducing new variables

$$w_{j_i} = \begin{bmatrix} w_{j_i}^{\sigma_{ij_i}+1} & \dots & w_{j_i}^{\sigma_{ij_i}+c_i} \end{bmatrix}^T$$

for $z_{j_i}^{(\sigma_{ij_i}+1)}, \ldots, z_{j_i}^{(\sigma_{ij_i}+c_i)}$ for the unique j_i such that $(i, j_i) \in T^*$ whenever $c_i > 0$, and $w_{j_i} = [.]$ for $c_i = 0$. Then the augmented system (18) is (locally) a regular system of d-index 1 (or s-index $\mu = 0$).

Proof. We show that for the augmented system (18) the Σ -method succeeds with $\nu_S = 1$. Then, from Lemma 4 it follows that (18) is (locally) regular and of d-index $\nu_d = 1$.

We start with a stepwise construction of the signature matrix for the augmented system (18). At first we construct the signature matrix for the reduced derivative array (10) on the basis of the given signature matrix Σ of (17). W.l.o.g. we can assume that the HVT T^* is on the diagonal of Σ (otherwise we can permute the rows of Σ). For each row $\sigma_i = [\sigma_{i1} \quad \sigma_{i2} \quad \ldots \quad \sigma_{in}]$ of Σ corresponding to an equation with offset $c_i > 0$ we add c_i rows of the form

$$\tilde{\sigma}_i^1 = \begin{bmatrix} \sigma_{i1} + 1 & \sigma_{i2} + 1 & \dots & \sigma_{in} + 1 \end{bmatrix}$$

$$\vdots$$

$$\tilde{\sigma}_i^{c_i} = \begin{bmatrix} \sigma_{i1} + c_i & \sigma_{i2} + c_i & \dots & \sigma_{in} + c_i \end{bmatrix}$$

to the original signature matrix Σ (using the convention that $-\infty + k = -\infty$ for all $k \in \mathbb{N}$). Permuting the rows of the resulting signature matrix such that the first *n* rows correspond to the original matrix Σ followed by the rows $\tilde{\sigma}_1^1, \ldots, \tilde{\sigma}_1^{c_1}$ up to $\tilde{\sigma}_n^1, \ldots, \tilde{\sigma}_n^{c_n}$, the signature matrix of the reduced derivative array can be written as

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \dots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \dots & \sigma_{nn} \\ \hline \sigma_{j_11} + 1 & \sigma_{j_12} + 1 & \dots & \sigma_{j_1n} + 1 \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{j_11} + c_{j_1} & \sigma_{j_12} + c_{j_1} & \dots & \sigma_{j_1n} + c_{j_1} \\ \hline \vdots & & & \vdots \\ \sigma_{j_m1} + 1 & \sigma_{j_m2} + 1 & \dots & \sigma_{j_mn} + 1 \\ \vdots & & \vdots & \ddots & \vdots \\ \sigma_{j_m1} + c_{j_m} & \sigma_{j_m2} + c_{j_m} & \dots & \sigma_{j_mn} + c_{j_m} \end{bmatrix} =: [\tilde{\sigma}_{ij}]_{i=1,\dots,M,j=1,\dots,n}, \quad (20)$$

with distinct $j_1, \ldots, j_m \in \mathcal{I} := \{i \in \{1, \ldots, n\} | c_i > 0\}$. To construct the augmented system (18), for each equation F_i of (17) with corresponding offset $c_i > 0$ new variables $w_i = [w_i^{\sigma_{ii}+1}, \ldots, w_i^{\sigma_{ii}+c_i}]^T$ are introduced and every occurrence of $z_i^{(\sigma_{ii}+1)}$ in (10) is replaced by $w_i^{\sigma_{ii}+1}$, every occurrence of $z_i^{(\sigma_{ii}+c_i)}$ is replaced by $w_i^{\sigma_{ii}+2}$, and so on, up to $z_i^{(\sigma_{ii}+c_i)} = z_i^{(d_i)}$ that is replaced by $w_i^{\sigma_{ii}+c_i}$ in all equations of the reduced derivative array. Note that since T^* is assumed to be on the diagonal of Σ we always have $(i, i) \in T^*$ for $i = 1, \ldots, n$.

Then, the signature matrix for the augmented system (18) can be constructed as follows: for each equation F_i with $i \in \mathcal{I}$ we consecutively add new columns to the signature matrix (20) corresponding to the newly introduced variables $w_i^{\sigma_{ii}+1}, \ldots, w_i^{\sigma_{ii}+c_i}$. Additionally, we update the entries in *i*-th column of the signature matrix (20) (since T^* is on the diagonal). In detail this process can be described as follows. We append a new column for the variable $w_i^{\sigma_{ii}+1}$ to the matrix (20). The entries $\tilde{\sigma}_{\ell i}$ in the *i*-th column of (20) are replaced by

$$\bar{\sigma}_{\ell i} := \begin{cases} \tilde{\sigma}_{\ell i} & \text{if} \quad \tilde{\sigma}_{\ell i} \leq \tilde{\sigma}_{i i} \\ \tilde{\sigma}_{\ell i} - 1 & \text{if} \quad \tilde{\sigma}_{\ell i} > \tilde{\sigma}_{i i} \end{cases}$$
(21)

for all $\ell = 1, \ldots, M$. In the newly introduced column for the variable $w_i^{\sigma_{ii}+1}$, lets say column n+1, we set $\sigma_{\ell,n+1} = 0$ whenever $\tilde{\sigma}_{\ell i} > \tilde{\sigma}_{ii}$ for all $\ell = 1, \ldots, M$ (see (21)), otherwise we set $\sigma_{\ell,n+1} = -\infty$. We proceed in the same way for the next variable $w_i^{\sigma_{ii}+2}$ until we reach $w_i^{\sigma_{ii}+c_i}$. This process is repeated for all equations F_i with $i \in \mathcal{I}$. Finally, we obtain a signature matrix of

the form

σ_{11}	$\tilde{\sigma}_{12}$		$ ilde{\sigma}_{1n}$	≤ 0			≤ 0		≤ 0		•••	≤ 0	
$ ilde{\sigma}_{21}$	σ_{22}		:	÷	≤ 0		÷		÷	≤ 0		÷	
:		۰.	:	:		·	:		:		·	÷	
$ ilde{\sigma}_{n1}$	•••		σ_{nn}	≤ 0	•••	•••	≤ 0		≤ 0	•••	•••	≤ 0	
$\tilde{\sigma}_{n+1,1}$	• • •	• • • •	$\tilde{\sigma}_{n+1,n}$	0	≤ 0		≤ 0		≤ 0	•••		≤ 0	
÷	·		:	÷	·	·	÷		:	·.		÷	
•		·	•	÷		·	≤ 0		÷		·	÷	.
$\tilde{\sigma}_{n+c_{j_1},1}$			$\tilde{\sigma}_{n+c_{j_1},n}$	0	• • •		0		≤ 0			≤ 0	
:			:		÷			·			:		
$\tilde{\sigma}_{M-c_{j_m}+1,1}$	•••	• • • •	$\tilde{\sigma}_{M-c_{j_m}+1,n}$	≤ 0			≤ 0		0	≤ 0		≤ 0	
:	·		•	÷	·.		÷		÷	·.	·	÷	
:		۰.	:	÷		۰.	÷		÷		·	≤ 0	
•			•					1					
$\tilde{\sigma}_{M1}$			$ ilde{\sigma}_{Mn}$	≤ 0			≤ 0		0			0	ļ

Note that the signature matrix obtained in this way might overestimate the real signature matrix of the augmented system (18) since derivatives of lower order, e.g., of order $\sigma_{ij} - 1$, might not actually occur in the corresponding equation. However, as mentioned in [11], this overestimation does not influence the result of the signature method.

The first *n* diagonal entries are not changed during this construction and all other entries in the first upper left block (the original signature matrix Σ) are either decreased or unchanged. Also, all entries in the first *n* columns are either smaller than the entries in the HVT position or of the same magnitude. Furthermore, in the newly added columns only values $\sigma_{ij} \leq 0$ are introduced. Thus, for the signature matrix (22) we have again a HVT on the diagonal. The canonical offset vectors are given by $c = [0, \ldots, 0]$ and $d = [\sigma_{11}, \ldots, \sigma_{nn}, 0 \ldots, 0]$ (the values in the position of the HVT). The Σ -Jacobian corresponding to the augmented system is still regular since by adding the derivatives of equations and introducing the new algebraic variables no linear dependencies are introduced and the Σ -Jacobian of the original systems has been regular. Thus, the Σ -method succeeds (locally at a consistent point) with structural index $\nu_S = 1$.

Theorem 7 allows us to compute a regularization for a nonlinear DAE (17) whenever the Σ -method can be successfully applied. Thus, from Theorem 7 we can obtain a system of d-index 1 that is much better suited for numerical computations. In the following, we call (18) the *regularized system* and the proceeding as in Theorem 7 will be denoted as the *structural approach* for regularization.

Example 8. To clarify the above described regularization process we consider again the pendulum equations (11) given in Example 3. The system (11) is regular and of d-index $\nu_d = 3$ and s-index $\mu = 2$. It is well-known that the algebraic constraint is given by $F_5(z, \dot{z}) = 0$ and this equation has to be differentiated twice to obtain an d-index 1 system (using some algebraic manipulations of the resulting equations). The extended system (13) consists of 9 equations in 5 unknowns. If we choose the HVT $T^* = T_1$ marked by the blue boxes in the signature matrix (12) (assuming that $\kappa_{T_1} = 2p_2^2 \ge \kappa_{T_2} = 2p_1^2$), then we introduce the new variables

$$\begin{array}{lll} w_3^1 & {\rm for} & \dot{q}_1 \ (\hat{=} \dot{z}_3) \\ w_2^2 & {\rm for} & \ddot{p}_2 \ (\hat{=} \ddot{z}_2) \\ w_1^1 & {\rm for} & \dot{p}_1 \ (\hat{=} \dot{z}_1) \\ w_1^2 & {\rm for} & \ddot{p}_1 \ (\hat{=} \ddot{z}_1) \end{array}$$

and we get the augmented system

$$\begin{bmatrix} w_1^1 - q_1 \\ w_1^2 - w_3^1 \\ \dot{p}_2 - q_2 \\ w_2^2 - \dot{q}_2 \\ w_3^1 + 2p_1 \lambda \\ \dot{q}_2 + 2p_2 \lambda + \mathfrak{g} \\ p_1^2 + p_2^2 - \ell^2 \\ 2p_1 w_1^1 + 2p_2 \dot{p}_2 \\ 2p_1 w_1^2 + 2(w_1^1)^2 + 2p_2 w_2^2 + 2\dot{p}_2^2 \end{bmatrix} = 0$$
(23)

with unknowns $p_1, p_2, q_1, q_2, \lambda, w_1^1, w_1^2, w_2^2, w_3^1$. If we apply the Σ -method to the augmented system (23) (with $z = \begin{bmatrix} p_1 & p_2 & q_1 & q_2 & \lambda & w_1^1 & w_1^2 & w_2^2 & w_3^1 \end{bmatrix}^T$) we get the signature matrix

Γ-	_	0	_	_	0	_	_	-]
-	_	_	_	_	_	0	_	0
-	1	_	0	_	_	_	_	-
-	_	_	1	_	_	_	0	_
0	—	—	—	0	—	—	—	0
-	0	—	1	0	—	—	—	-
0	0	—	—	—	—	—	—	-
0	1	_	_	_	0	_	—	—
0	1	—	—	—	0	0	0	

with HVT of value $Val(\Sigma) = 2$ and c = [0, ..., 0], d = [0, 1, 0, 1, 0, 0, 0, 0, 0]. The corresponding Σ -Jacobian is given by

	0	0	-1	0	0	1	0	0	0
	0	0	0	0	0	0	1	0	-1
	0	1	0	0	0	0	0	0	0
	0	0	0	-1	0	0	0	1	0
$\mathfrak{J} =$	2λ	0	0	0	$2p_1$	0	0	0	1
	0	0	0	1	$2p_2$	0	0	0	0
	$2p_1$	0	0	0	0	0	0	0	0
	$2w_1^1$	$2p_2$	0	0	0	$2p_1$	0	0	0
	$2w_1^2$	$4\dot{p}_2$	0	0	0	$4w_{1}^{1}$	$2p_1$	$2p_2$	0

which is nonsingular (at a consistent point) and the structural analysis succeeds with structural index $\nu_S = 1$.

Theorem 7 can also be applied if the Σ -method overestimates the d-index as can be seen in the following example.

Example 9. We consider the simple RC-circuit example from [12] depicted in Figure 1. The modified nodal analysis results in a DAE system of the form

$$\begin{bmatrix} C & -C & 0 \\ -C & C & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_3 \\ \dot{\iota} \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & -G & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_3 \\ \iota \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ V(t) \end{bmatrix}$$

of d-index 1, where ι denotes the current in the voltage source, C denotes the capacitance of the capacitor and G denotes the conductance of the resistor, V(t) is a function describing the voltage at the voltage source, and η_1, η_3 are the node potentials at node 1 and 3. The signature matrix



Figure 1: Simple electrical RC-circuit

and Σ -Jacobian are given by

$$\Sigma = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & - \\ 0 & - & - \end{bmatrix}, \quad \mathfrak{J} = \begin{bmatrix} C & -C & -1 \\ -C & C & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

and the Σ -method succeeds with c = [0, 0, 1], d = [1, 1, 0] and structural index $\nu_S = 2 > \nu_d = 1$. The extended system is obtained by differentiating the last equation once, and introducing w_1^1 for $\dot{\eta}_1$ results in the augmented system

This system is still regular and of d-index 1, but now the Σ -method succeeds with structural index $\nu_S = 1$.

3.1 Relation to Pantelides Algorithm and the Dummy Derivative Approach

Our approach of reducing the index of a DAE based on the structural analysis formulated in Theorem 7 is similar to the *Method of Dummy Derivatives* [7], where *Pantelides Algorithm* [10] is used to determine the number of times each equation has to be differentiated in order to obtain a reduced derivative array. It has been shown in [11] that Pantelides Algorithm and the Signature Method are essentially equivalent in the sense that if they both can be applied and they both succeed (or converge) they result in the same structural index and the offset vector $c = [c_i]$ corresponds to the number of differentiations for each equation F_i as determined by Pantelides algorithm.

However, while in the dummy derivative method an algorithm (described in [7]) that is based on selecting certain columns of the Jacobian to obtain a regular submatrix is described and the selection of the variables which derivatives are replaced are based on this algorithm, in our method the selection of variables is directly prescribed by the HVT T^* and the offset vectors. This selection of variables is much easier to achieve and requires no further numerical computations once the structural analysis has been done. As a result, the selected variables are not necessarily the same and the two approaches might result in a different d-index-1 system.

A further great advantage of the signature method is the direct success check (i.e., checking the regularity of the Σ -Jacobian) that clarifies if the structural analysis has been successful. In contrast, Pantelides Algorithm will not converge for structurally singular systems. Another difference between the methods is that while the signature method can directly be applied to higher order DAE systems Pantelides method cannot. Note that Pantelides algorithm might call for unnecessary differentiations in the same way as the signature method (see Example 9).

Both approaches, the dummy derivative method and Theorem 7, only work for regular (uniquely solvable) systems. However, the advantage of using the signature method as in Theorem 7 is the direct success check that allows to use the results for further treatment, see Section 4.

4 Structural-Algebraic Approach for Coupled Systems

From now on we want to consider coupled systems of DAEs where in each subsystem S_i the dynamics are given by a semi-explicit DAE of the form

$$S_i: \begin{cases} \dot{x}^i &= f^i(t, x^i, y^i, u^i), \\ 0 &= g^i(t, x^i, y^i, u^i), \end{cases}$$
(24)

with differential state variables $x^i \in \mathbb{R}^{n_x^i}$, algebraic state variables $y^i \in \mathbb{R}^{n_y^i}$ and inputs $u^i \in \mathbb{R}^{n_u^i}$. We assume that for given input u^i each of these subsystems is of d-index 1. By condition (7) this means that the Jacobian $g_{y^i}^i$ is nonsingular for all points (t, x^i, y^i, \dot{x}^i) in the solution manifold

$$\mathbb{L}_{0}^{i} := \{ (t, x^{i}, y^{i}, \dot{x}^{i}) \in \mathbb{I} \times \mathbb{R}^{n_{x}^{i}} \times \mathbb{R}^{n_{y}^{i}} \times \mathbb{R}^{n_{x}^{i}} | \dot{x}^{i} = f^{i}(t, x^{i}, y^{i}, u^{i}), \ g^{i}(t, x^{i}, y^{i}, u^{i}) = 0 \}$$

of the corresponding subsystem (assuming that u^i is given). This assumption is justified by considering a separate regularization of each (uni-physical) subsystem in a pre-processing step as described in Section 2. Hereby, the special structure of each uni-physical subsystem can be taken into account. Moreover, for reasons of clarity and readability we restrict to cyclic coupling of two subsystems S_1 and S_2 via coupling conditions given by

$$u^{i} = G_{ij}(t, x^{j}, y^{j}), \quad i, j = 1, 2, \ i \neq j,$$
(25)

see Figure 2. The functions $G_{ij} \in C(\mathbb{I} \times \mathbb{R}^{n_x^j} \times \mathbb{R}^{n_y^j}, \mathbb{R}^{n_u^i})$, describing the connection of the states



Figure 2: Cyclic coupling of two subsystems.

of subsystem S_j to the input of subsystem S_i , are assumed to be sufficiently smooth. With this considerations the coupled system that we will consider is given by

$$\begin{bmatrix} \dot{x}^{1} \\ \dot{x}^{2} \end{bmatrix} = \begin{bmatrix} f^{1}(t, x^{1}, y^{1}, G_{12}(x^{2}, y^{2})) \\ f^{2}(t, x^{2}, y^{2}, G_{21}(x^{1}, y^{1})) \end{bmatrix},$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} g^{1}(t, x^{1}, y^{1}, G_{12}(x^{2}, y^{2})) \\ g^{2}(t, x^{2}, y^{2}, G_{21}(x^{1}, y^{1})) \end{bmatrix},$$

$$(26)$$

or, equivalently, by

$$\dot{x} = f(t, x, y),$$

 $0 = g(t, x, y)$
(27)

using the notation

$$x = \begin{bmatrix} x^1 \\ x^2 \end{bmatrix} \in \mathbb{R}^{n_x}, \ y = \begin{bmatrix} y^1 \\ y^2 \end{bmatrix} \in \mathbb{R}^{n_y}, \ f = \begin{bmatrix} f^1 \\ f^2 \end{bmatrix}, \ g = \begin{bmatrix} g^1 \\ g^2 \end{bmatrix},$$
(28)

with $n_x = n_x^1 + n_x^2$ and $n_y = n_y^1 + n_y^2$. Even if both subsystems S_1 and S_2 are of d-index 1, a cyclic coupling as in (26) can easily lead to a high index system as can been seen in the following example.

Example 10. Consider the two d-index 1 systems (for given u^i)

$$S_{i}: \begin{cases} \dot{x}^{i} = \alpha^{i}y^{i} + b^{i}(t), \\ 0 = y^{i} + u^{i} + c^{i}(t), \end{cases} \quad i = 1, 2$$

with non-zero coefficients $\alpha^i \in \mathbb{R}$ and coupling conditions

$$u^{1} = \delta x^{2} + \epsilon y^{2}, \quad u^{2} = \gamma x^{1} + \beta y^{1}, \quad \delta, \epsilon, \gamma, \beta \in \mathbb{R}.$$
 (29)

The coupled system is given by

If $\epsilon \cdot \beta \neq 1$, the coupled system (30) is regular and of d-index $\nu_d = 1$. However, if $\epsilon \cdot \beta = 1$, the Jacobian $g_{,y}$ of (30) is singular and depending on the parameter $\alpha^1, \alpha^2, \delta, \gamma$ different scenarios can occur. If $\delta = \gamma = 0$ the system is non-regular (i.e., the d-index is not defined), but strangenessfree, i.e., the s-index is $\mu = 0$, and for the solvability of the system the consistency condition $\beta c^1(t) = c^2(t)$ for all t has to be satisfied. For other choices of the parameters an increase in the index and/or redundancies occur, e.g., if we chose $\beta = \epsilon = 1$ as well as $\alpha^1 = \alpha^2 = \delta = 1$ and $\gamma = -1$ we get a regular system of d-index 3. <

In general, it holds that the system (27) is regular and of d-index 1 if and only if the Jacobian

$$g_{,y}(t,x,y) = \begin{bmatrix} g_{,y^1}^1 & g_{,u^1}^1 \cdot G_{12,y^2} \\ g_{,u^2}^2 \cdot G_{21,y^1} & g_{,y^2}^2 \end{bmatrix}$$
(31)

is nonsingular for all points $(t, x, y) \in \mathbb{M} = \{(t, x, y) \in \mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \mid g(t, x, y) = 0\}$ (cp. with (7)). If the *index-1-condition* (31) is not satisfied, then an increase in the index can occur (that can be arbitrary high) and/or equations of the form $0 = 0 + \gamma(t)$ are included in the system that lead to redundancies or inconsistencies, i.e., the DAE is not or not uniquely solvable anymore. In the latter case the concept of the d-index cannot be applied anymore and one has to consider the more general strangeness-index concept.

In the following, we want to investigate the use of the structural analysis, in particular of the Σ -method as presented in Section 2.2 and 3, for the regularization of coupled systems (27).

4.1 The Signature Method for Coupled Systems

We apply the Σ -method presented in Section 2.2 to the coupled system (27). At first we review the system of Example 10.

Example 11. If we apply the Σ -method to the coupled system (30) (with $\alpha^1, \alpha^2, \delta, \gamma, \epsilon, \beta \neq 0$), we get the signature matrix

$$\Sigma = \begin{bmatrix} \mathbf{1} & - & 0 & - \\ - & \mathbf{1} & - & 0 \\ - & 0 & \mathbf{0} & 0 \\ 0 & - & 0 & \mathbf{0} \end{bmatrix}$$
(32)

with marked HVT on the diagonal and canonical offset vectors c = [0, 0, 0, 0] and d = [1, 1, 0, 0]. The corresponding Σ -Jacobian is given by

$$\mathfrak{J} = \begin{bmatrix} 1 & 0 & -\alpha^1 & 0\\ 0 & 1 & 0 & -\alpha^2\\ 0 & 0 & -1 & -\epsilon\\ 0 & 0 & -\beta & -1 \end{bmatrix},\tag{33}$$

and \mathfrak{J} is singular if $\epsilon \cdot \beta = 1$, i.e., the success check of the Σ -method fails. However, we have seen in Example 10 that for the choice $\epsilon \cdot \beta = 1$ the system can be regular but of d-index larger than 1, i.e., the system is uniquely solvable, and from this perspective perfectly good-natured. Otherwise, i.e., if $\epsilon \cdot \beta \neq 1$, the Σ -Jacobian is nonsingular, and the structural index is determined to be $\nu_S = 1$ which corresponds to the d-index.

The same observations as in Example 11 can be made for general coupled systems of the form (26) with

$$F(t, x^{1}, x^{2}, y^{1}, y^{2}, \dot{x}^{1}, \dot{x}^{2}) = \begin{bmatrix} \dot{x}^{1} - f^{1}(t, x^{1}, y^{1}, G_{12}(x^{2}, y^{2})) \\ \dot{x}^{2} - f^{2}(t, x^{2}, y^{2}, G_{21}(x^{1}, y^{1})) \\ g^{1}(t, x^{1}, y^{1}, G_{12}(x^{2}, y^{2})) \\ g^{2}(t, x^{2}, y^{2}, G_{21}(x^{1}, y^{1})) \end{bmatrix} = 0.$$
(34)

At first we can formulate the following Lemma.

Lemma 12. Consider a coupled system of the form (34) which is composed by coupling two semiexplicit d-index 1 subsystems (24), i.e., $g_{,y^i}^i$ is nonsingular for i = 1, 2. Then, the Σ -method applied to (34) yield the canonical offset vectors c = [0, ..., 0] and $d = [d_i]_{i=1,...,n}$ with

$$d_i = \begin{cases} 1 & \text{for } i \le n_x, \\ 0 & \text{for } i > n_x, \end{cases}$$

where $n_x = n_x^1 + n_x^2$.

Proof. The signature matrix of (34) is of the form

$$\Sigma = \begin{bmatrix} 1 & \leq 0 & \cdots & \leq 0 \\ \leq 0 & 1 & \ddots & \vdots & \leq 0 \\ \vdots & \ddots & \ddots & \leq 0 \\ \leq 0 & \cdots & \leq 0 & 1 \\ \hline & & & & \leq 0 & \cdots & \leq 0 \\ \leq 0 & & & \vdots & \ddots & \vdots \\ \leq 0 & & & & \leq 0 \end{bmatrix}$$
(35)

Since the Jacobians $g_{y^i}^i$, i = 1, 2 of (34) are assumed to be nonsingular, we can permute the algebraic equations such that there are non-zero values on the diagonal of the lower right block matrix in (35), i.e., the signature matrix of the permuted system is of the form

$$\tilde{\Sigma} = \begin{bmatrix} \mathbf{1} & \leq 0 & \cdots & \leq 0 \\ \leq 0 & \mathbf{1} & \ddots & \vdots & \leq 0 \\ \vdots & \ddots & \ddots & \leq 0 \\ \leq 0 & \cdots & \leq 0 & \mathbf{1} \end{bmatrix}$$
(36)
$$\begin{bmatrix} \mathbf{0} & \leq 0 & \cdots & \leq 0 \\ \leq 0 & \cdots & \leq 0 \\ \vdots & \ddots & \ddots & \leq 0 \\ \leq 0 & \cdots & \leq 0 & \mathbf{0} \end{bmatrix}$$

with HVT on the main diagonal. Thus, the canonical offsets are given by $\tilde{c}_i = 0$ for i = 1, ..., n, $\tilde{d}_j = 1$ for $j = 1, ..., n_x$, and $\tilde{d}_j = 0$ for $j = n_x + 1, ..., n$. Since only the algebraic equations have been permuted we get the same canonical offset vectors for the original system.

From Lemma 12 we immediately get that the structural index of the coupled system (34) determined by the canonical offset vectors of Σ -method is given by

$$\nu_S = \max c_i + 1 = 1.$$

Furthermore, the corresponding Σ -Jacobian of the coupled system (34) is given by

$$\mathfrak{J} = \begin{bmatrix} 1 & & & \\ & \ddots & & * \\ & & 1 & \\ & & 0 & & \frac{\partial g}{\partial \tilde{y}} \end{bmatrix}.$$
(37)

Thus, \mathfrak{J} is nonsingular at a consistent point if and only if the Jacobian $g_{,y}$ is nonsingular at this point, which means that the coupled system (34) is of d-index $\nu_d = 1$. Otherwise, the success check of the Σ -method fails due to singularity of the Σ -Jacobian. Altogether, we have shown the following key result.

Theorem 13. The Σ -method applied to a coupled system of the form (27) that is composed by coupling two semi-explicit d-index 1 systems (24) succeeds if and only if the the coupled system (27) is again of d-index 1. If the Σ -method succeeds the structural index of (27) is determined to be $\nu_S = \nu_d = 1$.

As a consequence of Theorem 13, if $g_{,y}$ is singular, i.e., the coupled system (34) is of higher index and/or non-regular, the success check of the Σ -method fails and the structural analysis cannot handle the problem. In this case, even if the coupled system (34) is regular and well-posed a regularization using the structural approach is not possible. We want to emphasize that this is not a weakness that occurs only for the Σ -method, but a problem that occurs for all structural methods, cf. Section 3.1. Thus, in the following, we will present a new combined structuralalgebraic approach that allows to handle these kind of coupled problems in the cases where the structural analysis fails.

Remark 14. For coupled systems of the form (27) that are composed of semi-explicit d-index-1 subsystems, the coupled system can only be of higher index if the system is structurally singular, i.e., the signature method fails. It is not possible that the coupled system (27) is of higher index and nevertheless the signature method can be applied successfully.

4.2 The Combined Structural-Algebraic Approach

A way out for structurally singular system is a combination of the structural approach presented in Section 3 with the algebraic approach presented in Section 2 that will be discussed in the following. We assume that the Σ -method applied to the coupled system (26) with appropriate reordering of equations and variables yields a signature matrix of the form

$$\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \hline \Sigma_{21} & \Sigma_{22} \end{bmatrix} := \begin{bmatrix} \tilde{\mathcal{I}}_{n_x} & \leq 0 \\ \hline \leq 0 & \tilde{0}_{n_y} \end{bmatrix}$$
(38)

using the notation

$$\tilde{\mathcal{I}}_n := \begin{bmatrix} 1 & \leq 0 \\ & \ddots & \\ \leq 0 & & 1 \end{bmatrix} \in \mathbb{R}^{n \times n}, \quad \tilde{0}_n := \begin{bmatrix} 0 & \leq 0 \\ & \ddots & \\ \leq 0 & & 0 \end{bmatrix} \in \mathbb{R}^{n \times n}.$$
(39)

Thus, we have a HVT on the main diagonal and the corresponding Σ -Jacobian is given by

$$\begin{bmatrix} \mathbf{\tilde{J}}_{11} & \mathbf{\tilde{J}}_{12} \\ \mathbf{\tilde{J}}_{21} & \mathbf{\tilde{J}}_{22} \end{bmatrix} := \begin{bmatrix} I_{n_x} & * \\ 0 & g_{,y} \end{bmatrix}.$$
(40)

If the Jacobian $g_{,y} = \mathfrak{J}_{22}$ is singular the success check of the Σ -method fails. A singular Jacobian $g_{,y}$ means that the coupled system (26) is either regular but of d-index larger than 1, or non-regular (in particular, if the Jacobian $g_{,x}$ vanishes identically) with also possibly higher s-index.

Our aim now is to use as much information as possible from the structural analysis in order to classify the coupled system as regular or non-regular and, consequently, to compute a regularized formulation that can be used for numerical computations. Therefore, we first have to identify the equations and differential variables that are responsible for a d-index higher than 1. In a second step, we have to differentiate these equations and add the differentiated equations to the original system. For this enlarged system we can introduce new algebraic variables (for the identified differential variables) and replace certain derivatives. We will see that, if the resulting system is still of high index, we can repeat this process iteratively.

In order to reduce the numerical effort we first transform the block Σ_{22} of the signature matrix (38) into BLT form, i.e., by row/column permutation we compute a block partitioning such that

$$\tilde{\Sigma}_{22} = \begin{bmatrix} \Sigma_{22}^{11} & -\infty & \dots & -\infty \\ \tilde{\Sigma}_{22}^{21} & \tilde{\Sigma}_{22}^{22} & \ddots & \vdots \\ \vdots & & \ddots & -\infty \\ \tilde{\Sigma}_{22}^{p1} & \dots & \tilde{\Sigma}_{22}^{p,p-1} & \tilde{\Sigma}_{22}^{pp} \end{bmatrix}$$

with square diagonal blocks $\tilde{\Sigma}_{22}^{ii} = \tilde{0}_{\tilde{N}_i}$ of size $\tilde{N}_i \times \tilde{N}_i$ in the form (39) with $\sum_{i=0}^p \tilde{N}_i = n_y$. The blocks $\tilde{\Sigma}_{22}^{ij}$ below the block diagonal only have entries ≤ 0 . Note, that we still have an HVT on the diagonal after permutation. The block \mathfrak{J}_{22} of the Σ -Jacobian (40) is permuted accordingly to the form

$$\tilde{\mathfrak{J}}_{22} = \begin{bmatrix} \mathfrak{J}_{22}^{11} & 0 & \cdots & 0\\ \tilde{\mathfrak{J}}_{22}^{21} & \tilde{\mathfrak{J}}_{22}^{22} & \ddots & \vdots\\ \vdots & & \ddots & 0\\ \tilde{\mathfrak{J}}_{22}^{p1} & \cdots & \tilde{\mathfrak{J}}_{22}^{p,p-1} & \tilde{\mathfrak{J}}_{22}^{pp} \end{bmatrix}$$

In the following, the coupled system permuted and partitioned according to the BLT form of Σ and \Im is denoted by

$$\begin{aligned} \dot{x} &= f(t, x, \tilde{y}_1, \dots, \tilde{y}_p), \\ 0 &= \tilde{g}_1(t, x, \tilde{y}_1, \dots, \tilde{y}_p), \\ \vdots \\ 0 &= \tilde{g}_p(t, x, \tilde{y}_1, \dots, \tilde{y}_p), \end{aligned}$$

and $\tilde{y} = \begin{bmatrix} \tilde{y}_1^T & \dots & \tilde{y}_p^T \end{bmatrix}^T$, $\tilde{g} = \begin{bmatrix} \tilde{g}_1^T & \dots & \tilde{g}_p^T \end{bmatrix}^T$. Note, that we have only permuted the algebraic variables and algebraic equations. Now, the singularity of \mathfrak{J} corresponds to the singularity of some of the diagonal blocks $\tilde{\mathfrak{J}}_{22}^{ii}$ of $\tilde{\mathfrak{J}}_{22}$ and we denote by

$$\mathbb{J} := \{ i \in \{1, \dots, q\} \mid \det(\tilde{\mathfrak{J}}_{22}^{ii}) = 0 \}$$

the index set of singular blocks $\tilde{\mathfrak{J}}_{22}^{ii}$. Using this information we can proceed as follows:

Procedure 1. Given a coupled system (27) with signature matrix $\Sigma =: \Sigma^0$, canonical offset vectors c and d, and Σ -Jacobian $\mathfrak{J} =: \mathfrak{J}^0$, i = 0.

- 1. Transformation to BLT form: We transform the blocks Σ_{22}^i and \mathfrak{J}_{22}^i to the BLT forms $\tilde{\Sigma}_{22}^i$ and $\tilde{\mathfrak{J}}_{22}^i$ and determine the set \mathbb{J}^i of singular blocks in $\tilde{\mathfrak{J}}_{22}^i$. If $\mathbb{J}^i = \emptyset$ the Σ -method succeeds with $\nu_S = 1$ and we proceed with Step 7.
- 2. Selection of equations: We need to identify the equations that are responsible for nonregularity or high index. For each block $\tilde{\mathfrak{J}}_{22}^{jj}$ with $j \in \mathbb{J}^i$ we compute a smooth matrix function $U_j(t, x, \tilde{y})$ of pointwise full rank such that the columns of $U_j(t, x, \tilde{y})$ form a basis of the null space of $(\tilde{\mathfrak{J}}_{22}^{jj})^T$. Let $U_j(t, x, \tilde{y})$ be of size $\tilde{N}_j \times k_j$, i.e., $k_j = \dim(\operatorname{kernel}((\tilde{\mathfrak{J}}_{22}^{jj})^T))$.
- 3. Construction of the enlarged system: For each $j \in \mathbb{J}^i$ we have to differentiate the equations determined by

$$U_j(t, x, \tilde{y})^T \tilde{g}_j(t, x, \tilde{y}) = 0.$$

Defining

$$h_j(t, x, \tilde{y}, \dot{x}, \dot{\tilde{y}}) := \frac{d}{dt} \left(U_j(t, x, \tilde{y})^T \tilde{g}_j(t, x, \tilde{y}) \right) \quad \text{for all } j \in \mathbb{J}^t$$

we can built up the enlarged system

$$\begin{bmatrix} \dot{x} - f(t, x, \tilde{y}) \\ \tilde{g}(t, x, \tilde{y}) \\ h(t, x, \tilde{y}, \dot{x}, \dot{\tilde{y}}) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$
(41)

where

$$h(t, x, \tilde{y}, \dot{x}, \dot{\tilde{y}}) := [h_j(t, x, \tilde{y}, \dot{x}, \dot{\tilde{y}})]_{j \in \mathbb{J}^d}$$

collects all added differentiated equations.

4. Introduction of new variables: For each $j \in \mathbb{J}^i$ we have to introduce k_j new variables and replace the derivatives of selected differential variables. The differential variables are selected based on the sparsity pattern of the signature matrix of the enlarged system (41). Let

$$\tilde{\Sigma}_E^i = \begin{bmatrix} \Sigma_{11}^i & \tilde{\Sigma}_{12}^i \\ \tilde{\Sigma}_{21}^i & \tilde{\Sigma}_{22}^i \\ \tilde{\Sigma}_{31}^i & \tilde{\Sigma}_{32}^i \end{bmatrix}$$

denote the signature matrix of the enlarged system (41). For the block $\tilde{\Sigma}_{31}^i$ of size $K_i \times n_x$ with $K_i = \sum_{j \in \mathbb{J}^i} k_j$, we determine a transversal

$$T_h = \{(1, \ell_1), (2, \ell_2), \dots, (K_i, \ell_{K_i})\},\$$

where $\{\ell_1, \ldots, \ell_{K_i}\}$ is a disjoint subset of $\{1, \ldots, n_x\}$ and the value of T_h is

$$Val(T_h) = \sum_{(i,j)\in T_h} \tilde{\sigma}_{ij} = K_i.$$

In addition, the condition that the Jacobian $h_{[\dot{x}_{\ell_1},...,\dot{x}_{\ell_{K_i}}]}$ is nonsingular has to be satisfied.

If we cannot find a transversal T_h with $Val(T_h) = K_i$ and nonsingular $h_{[\dot{x}_{\ell_1},...,\dot{x}_{\ell_{K_i}}]}$ the system is non-regular and we stop the procedure. Otherwise, each occurrence of \dot{x}_{ℓ_m} in (41) is replaced by a new variable w_{ℓ_m} for $m = 1, ..., K_i$ leading to the augmented system

$$F^{i}(t, \dot{x}, x, \tilde{y}, w) = 0, \quad w = \begin{bmatrix} w_{\ell_{1}} & \dots & w_{\ell_{m}} \end{bmatrix}^{T}.$$
 (42)

5. Transformation to semi-explicit form: We transform the augmented system (42) again to semi-explicit form by permuting the remaining differential variables to the front positions and the remaining differential equations to the top, while replacing the (possibly occurring) differential variables in the newly added equations. Thus, we get a semi-explicit augmented system of the form

$$\dot{\hat{x}} = \hat{f}(t, \hat{x}, \hat{y}),$$

 $0 = \hat{g}(t, \hat{x}, \hat{y}),$
(43)

with reduced number of differential variables \hat{x} and increased number of algebraic variables \hat{y} .

- 6. Application of Σ -method to the augmented system: We apply the Σ -method to the augmented semi-explicit system (43) and obtain the signature matrix Σ^{i+1} and Σ -Jacobian \mathfrak{J}^{i+1} . If the Σ -method succeeds with $\nu_S \geq 1$ we proceed with Step 7. Otherwise, i.e., if the Σ -method fails, we go to Step 1 and proceed iteratively with $i \leftarrow i + 1$.
- 7. Index reduction: If the Σ -method succeeds we can use the index reduction proposed in Theorem 7, if $\nu_S = 1$ we are done and we have constructed a regularized system.

Remark 15. If the Σ -Jacobian has been nonsingular in the beginning, the Steps 2.-6. are omitted since $\mathbb{J}^0 = \emptyset$. In this case, the semi-explicit augmented system (43) is just the original system (27) and the Σ -method can be applied successfully. In each iterative step of Procedure 1 the newly introduced variables are purely algebraic, i.e., the number of differential equations is reduced after each iteration and, thus, the procedure terminates after finitely many steps.

Theorem 16. Consider a coupled system (27) of differential-algebraic equations. If we apply Procedure 1, then the process terminates after finitely many steps, either with a resulting regularized system for which the Σ -method succeeds, or due to observed redundancies in the system (43).

Proof. If the Σ -Jacobian \mathfrak{J} has been regular in the beginning, the procedure finishes in the 0th iteration and the Σ -method can be applied successfully. Then, the index reduction proposed in Theorem 7 can be applied resulting in a regularized system.

Otherwise, if at least one block of $\tilde{\mathfrak{J}}_{22}^i$ is singular in the *i*-th step of the iterative procedure, i.e., $\mathbb{J}^i \neq \emptyset$, for each singular block $\tilde{\mathfrak{J}}_{22}^{jj}$, $j \in \mathbb{J}^i$ of dimension $\tilde{N}_j \times \tilde{N}_j$ the dimension of kernel $(\tilde{\mathfrak{J}}_{22}^{jj})^T$ is $k_j > 0$. Thus in the enlarged system (41) $K_i > 0$ equations are added to the system. The newly introduced variables are purely algebraic, i.e., in the augmented system the number of differential variables is reduced after each iteration of the procedure and Procedure 1 terminates after finitely many steps. If no transversal T_h can be found with $Val(T_h) = K_i$ and $h_{[\dot{x}_{\ell_1},...,\dot{x}_{\ell_{K_i}}]}$ nonsingular, the system (41) is non-regular. Otherwise, introducing new algebraic variables for derivatives of some of the differential variables does not influence the regularity of the system, but eliminates some of the coupling of algebraic variables into differential equations (causing the higher index of the problem). If, after transformation to semi-explicit form, the Σ -method can be applied successfully the regularization procedure of Theorem 7 can be applied. Otherwise, iteratively applying the procedure either reveals non-regularities or results in a system for which the Σ -method succeeds.

Example 17. We apply Procedure 1 to the system (30) for the case that $\epsilon \cdot \beta = 1$ and $\gamma \neq 0$, i.e., in the case where the success check fails (see Example 11). The lower right block of the signature matrix (32) is already given in BLT form, i.e., there is just one 2-by-2 block $\tilde{\Sigma}_{22}^0$ and $\tilde{\mathfrak{J}}_{22}^0$ is given by

$$\tilde{\mathfrak{J}}_{22}^{0} = \begin{bmatrix} -1 & -\epsilon \\ -\beta & -1 \end{bmatrix}.$$

Therefore, we only need to compute the null space of $\tilde{\mathfrak{J}}_{22}^0 = \begin{bmatrix} -1 & -\epsilon \\ -\beta & -1 \end{bmatrix}$. We get $U_1^0 = \begin{bmatrix} -\beta \\ 1 \end{bmatrix}$ as a basis of kernel $((\tilde{\mathfrak{J}}_{22}^0)^T)$. Thus, we have to differentiate the equation

$$0 = \gamma x^1 - \beta \delta x^2 - \beta c^1 + c^2,$$

yielding

$$0 = \gamma \dot{x}^1 - \beta \delta \dot{x}^2 - \beta \dot{c}^1 + \dot{c}^2.$$

Appending this equation to the original system (30) yields the enlarged system

The signature matrix of this enlarged system is given by

$$\tilde{\Sigma}_{E}^{0} = \begin{bmatrix} 1 & - & 0 & - \\ - & 1 & - & 0 \\ \hline - & 0 & 0 & 0 \\ 0 & - & 0 & 0 \\ \hline 1 & 1 & - & - \end{bmatrix}$$
(45)

and we can find e.g. the transversal

$$T_h = \{(1,1)\}$$

with $h_{\dot{x}_1} = [-\gamma]$ nonsingular. Thus, each occurrence of \dot{x}_1 is replaced by the new variable w_1 and we get

The augmented system (46) again transformed to semi-explicit form

Now, the Σ -method applied to this new system yields

$$\Sigma^{1} = \begin{bmatrix} 1 & - & - & 0 & - \\ - & - & 0 & - & 0 \\ 0 & - & 0 & 0 & - \\ - & 0 & 0 & 0 & - \\ - & - & - & 0 & 0 \end{bmatrix}$$

with c = [0, 0, 0, 0, 0], d = [1, 0, 0, 0, 0], and the Σ -Jacobian is given by

$$\mathfrak{J}^{1} = \begin{bmatrix} 1 & 0 & 0 & -\alpha^{2} & 0 \\ 0 & 0 & -\alpha^{1} & 0 & 1 \\ 0 & 0 & -1 & -\epsilon & 0 \\ 0 & -\gamma & -\beta & -1 & 0 \\ 0 & 0 & 0 & -\beta\delta\alpha^{2} & \gamma \end{bmatrix}.$$

The BLT form is given by

$$\tilde{\Sigma}^{1} = \begin{bmatrix} 1 & - & - & 0 & - \\ - & 0 & 0 & 0 & - \\ - & - & 0 & - & 0 \\ 0 & - & 0 & 0 & - \\ - & - & - & 0 & 0 \end{bmatrix}, \quad \tilde{\mathfrak{J}}^{1} = \begin{bmatrix} 1 & 0 & 0 & -\alpha^{2} & 0 \\ 0 & -\gamma & -\beta & -1 & 0 \\ 0 & 0 & -\alpha^{1} & 0 & 1 \\ 0 & 0 & -1 & -\epsilon & 0 \\ 0 & 0 & 0 & -\beta\delta\alpha^{2} & \gamma \end{bmatrix}.$$

The regularity of

$$\tilde{\mathfrak{J}}_{22}^{1} = \begin{bmatrix} \frac{-\gamma & -\beta & -1 & 0}{0 & -\alpha^{1} & 0 & 1} \\ 0 & -1 & -\epsilon & 0 \\ 0 & 0 & -\beta\delta\alpha^{2} & \gamma \end{bmatrix}$$

depends on the given parameter. If $\det(\tilde{\mathfrak{J}}_{22}^1) \neq 0$, the success check of the Σ -method succeeds and the procedure terminates, otherwise we have $\det(\tilde{\mathfrak{J}}_{22}^1) = -\gamma(\gamma\alpha^1\epsilon + \beta\delta\alpha^2) = 0$. In the second case, since $\gamma \neq 0$, we have $\gamma\alpha^1\epsilon + \beta\delta\alpha^2 = 0$ and a basis for the kernel of $(\tilde{\mathfrak{J}}_{22}^1)^T$ is given by

$$U_1^1 = \begin{bmatrix} 0\\ -\gamma\\ \alpha^1 \gamma\\ 1 \end{bmatrix}$$

We have to differentiate the equation

$$0 = \alpha^1 \gamma \delta x^2 - \gamma b^1 + \alpha^1 \gamma c^1 + \beta \dot{c}^1 - \dot{c}_2 + \beta \delta b^2,$$

giving

$$0 = \alpha^1 \gamma \delta \dot{x}^2 - \gamma \dot{b}^1 + \alpha^1 \gamma \dot{c}^1 + \beta \ddot{c}^1 - \ddot{c}_2 + \beta \delta \dot{b}^2$$

The extended system is given by

The signature matrix for the extended system is given by

$$\tilde{\Sigma}_{E}^{1} = \begin{bmatrix} 1 & - & - & 0 & - \\ - & - & 0 & - & 0 \\ 0 & - & 0 & 0 & - \\ - & 0 & 0 & 0 & - \\ - & - & - & 0 & 0 \\ \hline 1 & - & - & - & - \end{bmatrix}$$
(48)

and we can find the only transversal

$$T_h = \{(1,1)\}$$

and $h_{\dot{x}_2} = \left[-\alpha^1 \gamma \delta\right]$. If $-\alpha^1 \gamma \delta \neq 0$ this Jacobian is is nonsingular (otherwise the system is non-regular) and each occurrence of \dot{x}_2 is replaced by the new variable w_2 and we get the purely algebraic system

 \triangleleft

Now, for this system the Σ -method succeeds with structural index $\nu_S = 1$.

Remark 18. In each iteration of Procedure 1 the signature matrix for the augmented system can be obtained efficiently from the signature matrix of the previous step. Furthermore, the information on the HVT and on the offsets can be used to speed up the structural analysis for the augmented system. Also the regularity of \mathfrak{J} has to be verified already during the success check of the Σ -method, thus, the required null space information of \mathfrak{J} is already (partially) available. Thus, the described procedure requires relatively low additional computational effort.

5 Numerical Examples

Various kinds of simulation software packages uses some kind of structural analysis to treat DAE systems. In this section we compare the behavior of three different simulation environments that uses the modeling language MODELICA for the system formulation for the numerical solution of a coupled system of the form (27). In particular, we consider the simple coupled system given in Example 10 that is regular but of higher index and compare the behavior of the simulation environments OPENMODELICA (Version 1.6.0), DYMOLA (Version 2012) and MAPLESIM (Version 6.01).

We use two different models for describing the problem: the formulation as one system with system equations given by (30) (Model (A)), and the formulation as interconnected system consisting of the two subsystems S_1 and S_2 connected by Modelica *connectors* that define the given coupling conditions (29) (Model (B)), see Figure 3. For all computation we choose the parameters $\alpha^1 = \alpha^2 =$



Figure 3: Interconnection of subsystems

 $\delta = \epsilon = 1$ and vary β with $\beta \in \{1.0 - 10^{-4}, 1.0, 1.0 + 10^{-4}\}$. As simulation parameters we use the stopping time T = 1.0 and we prescribe consistent initial values $x_1(0) = -2$, and $x_2(0) = 3$ for the differential variables. Note that using DYMOLA only two initial conditions can be fixed. The right hand side of equation (30) is given by the functions $b^1(t) = \frac{1}{100}e^t$, $c^1(t) = \sin(3t)$, $b^2(t) = \frac{1}{1000}e^{-2t}$,

 $c^{2}(t) = \cos(t)$. Furthermore, we use the default DAE solvers of each environment, i.e., the BDFsolver Dassl in OPENMODELICA and DYMOLA, and the Cash-Karp 4(5) Runge-Kutta method in MAPLESIM. Table 1 summarizes the behavior of the different simulation environments.

	Model (A)					
Simulation environment	$\beta = 1.0 - 10^{-4}$	$\beta = 1.0$	$\beta=1.0+10^{-4}$			
OpenModelica	ok	fail*	$fail^{\dagger}$			
Dymola	ok	$fail^{\ddagger}$	$fail^{\S}$			
MAPLESIM	ok	ok	ok			

	Model (B)					
Simulation environment	$\beta = 1.0 - 10^{-4}$	$\beta = 1.0$	$\beta=1.0+10^{-4}$			
OpenModelica	ok	fail*	$fail^{\dagger}$			
Dymola	ok	$fail^{\ddagger}$	$fail^{\S}$			
MAPLESIM	ok	ok	fail¶			

Table 1: Comparison of different simulation environments for Example 10

The simulation environments DYMOLA and OPENMODELICA are not able to simulate the system if $\beta \in \{1.0, 1.0 + 10^{-4}\}$ due to the failure of the underlying structural analysis. However, MAPLESIM is able to simulate the system of Example 10 if it is formulated as Model (A), but fails also for Model (B) with $\beta = 1.0 + 10^{-4}$. Thus, even for a very simple problems simulation environments relying on a structural analysis can fail to simulate the DAE system. The simulation results for $\beta = 1.0$ are depicted in Figure 4 for Model (A) and in Figure 5 for Model (B). We see that the solver OPENMODELICA computes clearly wrong results while throwing an error message. The solver DYMOLA does not provide any results in this case.

Next, we compare the behavior of the different simulation environments for the reduced formulation (49) of (30) implemented as Model (C). Table 2 summarizes the behavior of the different simulation environments using the same simulation parameter as before. The simulation results for $\beta = 1.0$

	Model (C)				
Simulation environment	$\beta = 1.0 - 10^{-4}$	$\beta = 1.0$	$\beta=1.0+10^{-4}$		
OpenModelica	ok	ok	ok		
Dymola	ok	ok	ok		
MAPLESIM	ok	ok	ok		

Table 2: Comparison of different simulation environments for Example 10

are depicted in Figure 6 together with the plots of the absolute errors in Figure 7. We can see that now for all simulation environments the simulation succeeds yielding similar results. Thus, the reformulation of the DAE system using a combined structural-algebraic regularization technique allows the solvers to handle coupled DAE systems that are otherwise classified as structural singular problem that cannot be solved.

^{*}Error message: "Error solving linear system of equations. System is singular."

[†]Error message: "Error, simulation stopped at time: 7.14067 with idid: -3" (Dassl)

[‡]Error message: "Scalar system is always singular"

 $^{^{\}S}$ Integration is terminated at T=7.17 (local error test failure)

[¶]Error message: "Cannot evaluate the solution further right of 7.1223287, probably a singularity"



Figure 4: Simulation Results for Model (A)

6 Conclusions

The consideration of simple coupled systems (27) of semi-explicit d-index-1 DAEs has revealed that an index reduction based only on structural information cannot reliably handle these kind of systems if the system (27) is of higher index or non-regularities occur due to coupling, i.e., if the coupled system (27) is *structurally singular*. Even if the system is regular and well-posed a regularization and/or index reduction is not possible based on a structural analysis. Unfortunately, various kinds of structural algorithms as, e.g., Pantelides algorithm in combination with the dummy derivative method are used in many simulation environments as e.g. DYMOLA, OPENMODELICA or MAPLESIM.

The results of Theorem 7 show how we can compute a regularization for systems for which the Σ -method succeeds. However, in the case of coupled systems (27) this only covers d-index-1 systems. Our new combined structural-algebraic approach allows to handle structurally singular systems and thus improves the treatment of high-index DAEs. Here, the somewhat expensive computation of projections onto the corresponding subspaces is only required if the structural analysis cannot handle the problem, and then only for small subproblems using a BLT partitioning. Using additional information from the structural analysis, even if the success check fails, allows to select equations and variables more efficiently. Moreover, we can detect non-regularities in the system.

Still under investigation are the questions if we can use a similar approach if the system is not in semi-explicit form, e.g., for quasilinear DAE system, and how this approach can be most efficiently integrated into existing solvers or simulation environments.

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Figure 5: Simulation Results for Model (B)

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Figure 6: Simulation Results for reduced formulation



Figure 7: Absolute errors of the simulation results for reduced formulation