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Index Reduction and Regularisation Methods for Multibody Systems

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Abstract: This paper presents regularisation methods for differential–algebraic equations of mechanical systems. These systems can be described via systems of differential and algebraic equations that usually have differential index three. Such systems are typically gained by the use of multibody simulation tools, where the system is composed of connected rigid and flexible bodies and different joints and the underlying equations are derived automatically by the software. The considered methods in this paper are applicable to differential–algebraic equations of index three and are divided into three basic approaches: index reduction with differentiation, stabilisation by projection and methods based on state space transformation. The methods using differentiation are the substitution of the constraint equations by derivatives, the Baumgarte–Method and the Pantelides–Algorithm with the use of Dummy Derivatives. Furthermore two methods using projection are considered: the orthogonal projection method and the symmetric projection method. The next approach uses a local coordinate transformation to reduce the index. Lastly the Gear–Gupta–Leimkuhler formulation is considered. At the end the advantages and disadvantages of all these methods are discussed and a basic outline on the functionality and the requirements for the implementation of each method is given.

Keywords: DAE, Differential Index, Index Reduction, Mechanical Systems, Regularisation

1. INTRODUCTION

In general the numerical solution of differential–algebraic equation systems with high index by conventional solution methods for ordinary differential equations is very complex or may even be impossible. Therefore methods for solving this problem are necessary, which leads to the so–called index reduction. The aim of index reduction is to convert a system of differential–algebraic equations into a system of differential–algebraic equations of lower index or a system of ordinary differential equations.

This paper aims to provide an overview of common regularisation methods that are applicable for differential–algebraic equations which are derived from mechanical systems. Additionally, a classification of these different approaches is made. This classification divides the different approaches into three areas, see Hairer, and Wanner (2002): index reduction with the use of differentiation, stabilization of the numerical solution by projection and (local) transformation of the state space. Three different methods of index reduction with the use of differentiation are considered: replacement of the constraint by its derivative, the Baumgarte–Method and the Pantelides–Algorithm. There are two different methods using projections, called the orthogonal projection method and the symmetric projection method. The idea of the method using transformation of the state space is to obtain a system of ordinary differential equations on a manifold. Additionally the Gear–Gupta–Leimkuhler formulation is considered. According to the classification each approach is presented and explained in detail. In conclusion the advantages and disadvantages of the different regularisation methods are discussed.

2. BASIC DEFINITIONS

This section provides a collection of fundamental defintions, which will be needed subsequently. A differential–algebraic equation (abbreviated DAE), see Kunkel, and Mehrmann (2006), is given by an implicit equation

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

with a function $F\colon I \times D_x \times D_{\dot{x}} \to \mathbb{R}^n$, where $I \subseteq \mathbb{R}$ is a real interval and D_x, $D_{\dot{x}} \subseteq \mathbb{R}^n$ are open sets, $n \in \mathbb{N}$ and $x\colon I \to \mathbb{R}^n$ is a differentiable function, where $\dot{x}$ is the derivative of x with respect to t. According to the implicit function theorem F can be solved for $\dot{x}$ if the matrix $\frac{\partial F}{\partial \dot{x}}$ is regular.

Variables and equations can be categorised with the following definitions:

- algebraic variable: no derivatives of an algebraic variable may occur in the DAE.
- differential variable: derivatives of a differential variable occur in the DAE.
- algebraic equation: an algebraic equation is an equation where no derivatives occur.
- differential equation: a differential equation is an equation where derivatives occur.

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The algebraic equations of the differential–algebraic equation system $F(t, x, \dot{x}) = 0$ are of the form

$$g(x) = 0, \tag{2}$$

where $g\colon \mathbb{R}^n \to \mathbb{R}^m$ is a function with $m < n$, and they are called constraints or constraint equations.

A differential–algebraic equation has differential index $k \in \mathbb{N}_0$ (see Hairer, and Wanner (2002)) if k is the minimal number of derivatives, so that an ODE can be extracted from the system

$$F(t,x,\dot{x}) = 0,\ \frac{\mathrm{d}F(t,x,\dot{x})}{\mathrm{d}t} = 0,\ \ldots,\ \frac{\mathrm{d}^k F(t,x,\dot{x})}{\mathrm{d}t^k} = 0. \tag{3}$$

This generated ODE can (by algebraic transformations) be written in the form $\dot{x} = \varphi(t, x)$ with a function $\varphi\colon I \times D_x \to \mathbb{R}^n$. In the following the differential index will sometimes be only called index.

3. DAES OF INDEX THREE

A general differential–algebraic equation system of index 3 is given as

$$\begin{aligned} \dot{y} &= f(y,z) \\ \dot{z} &= k(y,z,u) \\ g(y) &= 0, \end{aligned} \tag{4}$$

where $f\colon U \times V \to \mathbb{R}^n$, $k\colon U \times V \times W \to \mathbb{R}^m$, $g\colon U \to \mathbb{R}^p$ and $U \subset \mathbb{R}^n$, $V \subset \mathbb{R}^m$, $W \subset \mathbb{R}^p$ open. The variables y and z are differential variables and u represents an algebraic variable. Differentiation of $g(y) = 0$ with respect to t gives

$$g_y \dot{y} = g_y f = 0. \tag{5}$$

The second derivative of $g(y) = 0$ with respect to t yields

$$\begin{aligned} & f^T \otimes g_{yy} \otimes f + g_y f_y \dot{y} + g_y f_z \dot{z} = \\ & \quad = f^T \otimes g_{yy} \otimes f + g_y f_y f + g_y f_z k = 0, \end{aligned} \tag{6}$$

where $\otimes$ stands for the tensor product. Differentiating $g(y) = 0$ three times with respect to t results in a term containing $g_y f_z k_u \dot{u}$. If $g_y f_z k_u$ can be inverted, the given DAE has index 3 and the DAE

$$\begin{aligned} \dot{y} &= f(y,z) \\ \dot{z} &= k(y,z,u) \\ f^T \otimes g_{yy} \otimes f + g_y f_y f + g_y f_z k &= 0 \end{aligned} \tag{7}$$

is of index 1. If $g_y(y) f_z(y,z) k_u(y,z,u)$ can be inverted, $g_y(y) f_z(y,z) k(y,z,u) = 0$ can be solved for u with the use of the implicit function theorem, i.e. there exists a function $h\colon \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^p$ with $u = h(y,z)$.

In conclusion we can say that if $g_y(y) f_z(y,z) k_u(y,z,u)$ is invertible, the DAE (4) has index 3 and the algebraic variable u can be extracted from the second derivative of the constraint $g(y) = 0$.

This method is used in several of the approaches described in sections 5 to 7.

4. DAES IN CONNECTION TO MECHANICAL SYSTEMS

In this section the DAE of mechanical systems is derived, where q are the generalised coordinates and $\dot{q}$ the generalised velocities. Additionally the function $L\colon \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, which depends on t, q and $\dot{q}$, is given. In the following the variational problem

$$\int_{t_1}^{t_2} L\left(t, q(t), \dot{q}(t)\right)\, \mathrm{d}t \quad \to \quad \min! \tag{8}$$

is considered. The Euler–Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \quad i = 1, \ldots, n. \tag{9}$$

In the given case of mechanical systems L can be calculated via

$$L = E_{kin} - E_{pot}, \tag{10}$$

where E_{kin} stands for the kinetic energy and E_{pot} for the potential energy, see Hairer, and Wanner (2002).

Therefore the variational problem has the form

$$\int_{t_1}^{t_2} \left(E_{kin} - E_{pot}\right)\, \mathrm{d}t \quad \to \quad \min!. \tag{11}$$

The next step is to include auxilary conditions or constraint equations. This can be achieved with two approaches:

- Calculus of Variations:
  The Euler–Lagrange equations result in

  $$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial\left(L + \sum_{j=1}^{m} \lambda_j g_j\right)}{\partial q_i} = 0, \quad i = 1, \ldots, n, \tag{12}$$

  where g_j, $j = 1, \ldots, m$ are the constraint equations. These are furthermore added to the equations in 12, therefore a system of $n + m$ equations is obtained. These equations can be transformed into

  $$\begin{aligned} & \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\left(E_{kin} - E_{pot}\right)}{\partial \dot{q}_i}\right) - \\ & - \frac{\partial\left(\left(E_{kin} - E_{pot}\right) + \sum_{j=1}^{m} \lambda_j g_j\right)}{\partial q_i} = 0 \end{aligned} \tag{13}$$

  and the constraint equations yield the $(n+1)^{th}$ till $(n+m)^{th}$ equation.
- Lagrange–Formalism of the Classical Mechanics:
  For the consideration of the constraint equations $g_1(q) = 0, \ldots, g_m(q) = 0$ these are included directly in the function L, i.e.

  $$L = E_{kin} - E_{pot} - \lambda_1 g_1 - \ldots - \lambda_m g_m, \tag{14}$$

  where λ_k, $k = 1, \ldots, m$ are Lagrange Multipliers. The Lagrange Multipliers λ_k are added to the generalised coordinates and $\dot{\lambda}_k$ is added to the generalised velocities. Therefore there are $n + m$ generalisied coordinates and velocities respectively instead of n. The Euler–Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0, \tag{15}$$

and can be transformed to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\left(E_{kin} - E_{pot} - \sum_{j=1}^m \lambda_j g_j\right)}{\partial \dot{q}_i}\right) - \\ -\frac{\partial\left(E_{kin} - E_{pot} - \sum_{j=1}^m \lambda_j g_j\right)}{\partial q_i} = 0.\end{aligned} \tag{16}$$

The constraint equation is independet of $\dot{q}$, the equations are transformed into

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\left(E_{kin} - E_{pot}\right)}{\partial \dot{q}_i}\right) - \\ -\frac{\partial\left(E_{kin} - E_{pot} - \sum_{j=1}^m \lambda_j g_j\right)}{\partial q_i} = 0.\end{aligned} \tag{17}$$

The Lagrange Multipliers are extracted from q and $\dot{q}$ and because of $\frac{\partial(\lambda_j g_j)}{\partial \lambda_j} = g_j$ the following equations are obtained

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\left(E_{kin} - E_{pot}\right)}{\partial \dot{q}_i}\right) - \\ -\frac{\partial\left(E_{kin} - E_{pot} - \sum_{j=1}^m \lambda_j g_j\right)}{\partial q_i} = 0\end{aligned} \tag{18}$$

and the m constraint equations.

The Lagrange–Multipliers of both approaches are equal except for the sign, i.e. $\lambda_{mech} = -\lambda_{var}$, so since the same $m + n$ equations are obtained it does not matter which method is chosen. In the following λ_{mech} is used, which leads to the equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\left(E_{kin} - E_{pot}\right)}{\partial \dot{q}_i}\right) - \\ -\frac{\partial\left(E_{kin} - E_{pot} - \sum_{j=1}^m \lambda_j g_j\right)}{\partial q_i} = 0 \\ g_j(q) = 0.\end{aligned} \tag{19}$$

Because of $E_{kin} = E_{kin}(q, \dot{q})$, $E_{pot} = E_{pot}(q, \dot{q})$ and using the linearity of differentiation the equations result in

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{kin}}{\partial \dot{q}_i}\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{pot}}{\partial \dot{q}_i}\right) - \\ -\frac{\partial E_{kin}}{\partial q_i} + \frac{\partial E_{pot}}{\partial q_i} + \frac{\partial \sum_{j=1}^m \lambda_j g_j}{\partial q_i} = 0 \\ g_j(q) = 0.\end{aligned} \tag{20}$$

Further calculations and

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{kin}}{\partial \dot{q}_i}\right) =: \frac{\mathrm{d}}{\mathrm{d}t}\left(m(q_i)\dot{q}_i\right), \quad i = 1, \ldots, n$$

lead to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(m(q_i)\dot{q}_i\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{pot}}{\partial \dot{q}_i}\right) - \\ -\frac{\partial E_{kin}}{\partial q_i} + \frac{\partial E_{pot}}{\partial q_i} + \sum_{j=1}^m \lambda_j \frac{\partial g_j}{\partial q_i} = 0 \\ g_j(q) = 0.\end{aligned} \tag{21}$$

After more calculations the equations

$$\begin{aligned}m(q_i)\ddot{q}_i + \frac{\mathrm{d}}{\mathrm{d}t}(m(q_i))\dot{q}_i - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{pot}}{\partial \dot{q}_i}\right) - \\ -\frac{\partial E_{kin}}{\partial q_i} + \frac{\partial E_{pot}}{\partial q_i} + \sum_{j=1}^m \lambda_j \frac{\partial g_j}{\partial q_i} = 0 \\ g_j(q) = 0\end{aligned} \tag{22}$$

are obtained.

With

$$M(q) := (E_{kin})_{\dot{q}\dot{q}}$$

and

$$(M(q))_{ii} = m(q_i),$$

rewriting $\left(\sum_{j=1}^m \lambda_j \frac{\partial g_j}{\partial q_i}\right)_i$ as matrix vector multiplication $\left(\frac{\partial g}{\partial q}\right)^T \lambda$ and

$$-F_i(t, q, \dot{q}) = \frac{\mathrm{d}}{\mathrm{d}t}(m(q_i))\dot{q}_i - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial E_{pot}}{\partial \dot{q}_i}\right) - \frac{\partial E_{kin}}{\partial q_i} + \frac{\partial E_{pot}}{\partial q_i}$$

the equations above are transformed into

$$\begin{aligned}M(q)\ddot{q} - F(t, q, \dot{q}) + \left(\frac{\partial g}{\partial q}\right)^T \lambda = 0 \\ g_j(q) = 0.\end{aligned} \tag{23}$$

Finally the general form of equations of mechanical systems is obtained. The equations of motion of mechanical systems are given by

$$\begin{aligned}M(q)\ddot{q} &= F(t, q, \dot{q}) - G^T(q)\lambda \\ g(q) &= 0,\end{aligned} \tag{24}$$

where $q \in \mathbb{R}^n$ are the generalised coordinates, $M \in \mathbb{R}^{n\times n}$ is the symmetric positive definite mass matrix, $F\colon \mathbb{R}\times\mathbb{R}^n\times\mathbb{R}^n \to \mathbb{R}^n$ are the forces, $g\colon \mathbb{R}^n \to \mathbb{R}^m$ is the constraint, $G = \frac{\partial g}{\partial q} \in \mathbb{R}^{m\times n}$ has full rank and $\lambda \in \mathbb{R}^m$ is the Lagrange Mulitplier, see Eich, and Hanke (1995).

Typically the differential index of DAEs of mechanical systems is three. In the following the differential index is calculated for the case $m = 1$. The equation $g(q) = 0$ of the DAE (24) is considered. The derivative of g with respect to t is

$$\dot{g}(q) = G(q)\dot{q}, \tag{25}$$

where $G(q) \in \mathbb{R}^n$. The second derivative of g with respect to t is

$$\ddot{g}(q) = \dot{q}^T G_q(q)\dot{q} + G(q)\ddot{q}, \tag{26}$$

where $G_q(q) \in \mathbb{R}^{n\times n}$. Because M is symmetric and positive definite, M is regular and therefore invertible. With the equation $M(q)\ddot{q} = F(t, q, \dot{q}) - G^T(q)\lambda$ of the DAE (24) $\ddot{q}$ can be expressed as

$$\ddot{q} = M(q)^{-1}(F(t, q, \dot{q}) - G^T(q)\lambda). \tag{27}$$

Inserting this in the equation $\ddot{g}(q) = 0$ and (26) leads to

$$\dot{q}^T G_q(q)\dot{q} + G(q)M(q)^{-1}(F(t, q, \dot{q}) - G^T(q)\lambda) = 0. \tag{28}$$

Further calculations give

$$\dot{q}^T G_q(q)\dot{q} + G(q)M(q)^{-1}F(t,q,\dot{q}) = G(q)M(q)^{-1}G^T(q)\lambda. \tag{29}$$

The real number $G(q)M(q)^{-1}G^T(q)$ does not equal zero because $M(q)^{-1}$ is a symmetric positive definite matrix, therefore it has n positive eigenvalues and the eigenvectors build a base of $\mathbb{R}^n$ (V is the matrix with the eigenvectors in the columns, V is orthogonal) and therefore $G(q)M(q)^{-1}G^T(q) = H(q)^T DH(q) = \sum_{i=1}^{n} \lambda_i (h_i)^2 > 0$ with $V^T G^T = H$, where D is the diagonal matrix with the eigenvalues as entries and h_i are the columns of H. Therefore it is possible to multiply with $\left(G(q)M(q)^{-1}G^T(q)\right)^{-1}$. This leads to

$$\begin{aligned} &(G(q)M(q)^{-1}G^T(q))^{-1}\cdot \\ &\cdot(\dot{q}^T G_q(q)\dot{q} + G(q)M(q)^{-1}F(t,q,\dot{q})) = \lambda. \end{aligned} \tag{30}$$

It is remarkable that from the second derivative of the constraint $\ddot{g}(q) = 0$ the Lagrange–Mulitplier λ can be expressed. With (30) one can see that the DAE (24) has index three.

This procedure for calculating the differential index can be extended to the general case $m > 1$, which also leads to the same results.

5. INDEX REDUCTION WITH DIFFERENTIATION

In the following three different methods using differentiation are considered.

5.1 Differentiation and Substitution of the Constraint

In this approach the goal for reducing the index is to differentiate the constraint $g(x) = 0$ and substitute the constraint by its $(k-1)^{th}$ derivative $g^{(k-1)}(x) = 0$, given a DAE of index $k > 1$, until the system has differential index 1.

For the considered mechanical systems of index 3 this means that instead of the given system (4) the new system

$$\begin{aligned} \dot{y} &= f(y,z) \\ \dot{z} &= k(y,z,u) \\ \ddot{g}(y) &= 0 \end{aligned} \tag{31}$$

is obtained.

The problem with this method is that due to the differentiation there is a loss of information and so the necessary initial values for the back-integration are unknown. Therefore the numerical "drift–off" occurs, which means that the numerical solution departs from the exact solution.

5.2 Baumgarte–Method

The Baumgarte–Method can only be used for DAEs with differential index three. The initial point of this method is the index–1–formulation of the DAE with index three, i.e. the differential equations of the DAE and the second derivative with respect to t of the constraint equations of the DAE as in (31). The constraint $\ddot{g}(x) = 0$ is substituted by a linear combination of g, $\dot{g}$ and $\ddot{g}$ of the form (see Eich, and Hanke (1995))

$$\ddot{g} + 2\alpha\dot{g} + \beta^2 g = 0, \tag{32}$$

which yields the total system

$$\begin{aligned} \dot{y} &= f(y,z) \\ \dot{z} &= k(y,z,u) \\ \ddot{g} + 2\alpha\dot{g} + \beta^2 g &= 0. \end{aligned} \tag{33}$$

Because of the consideration of the constraint $(g(x) = 0)$ in the resulting DAE (33) there is no loss of information. The parameters α and β have to be chosen so that the differential equation is asymptotically stable. This means that the real part of the eigenvalues of the characteristical polynomial of (32),

$$\lambda^2 + 2\alpha\lambda + \beta^2, \tag{34}$$

have to be strictly negative, i.e. $Re(\lambda_{1,2}) < 0$. The eigenvalues are calculated by

$$\lambda_{1,2} = -\alpha \pm \sqrt{\alpha^2 - \beta^2}, \tag{35}$$

therefore follows

$$\alpha > 0. \tag{36}$$

The problem of this approach is the exact choice of the constants α and β. In Ascher, Chin, and Reich (1994) the choice of the parameters is discussed.

5.3 Pantelides–Algorithm

For each constraint equation of the given DAE the following procedure has to be followed.

(1) Each constraint has to be differentiated.
(2) The differentiated constraint equation has to be added to the DAE. If there has been an algebraic variable in the constraint, then the derivative of this variable in the differentiated equation is replaced by a so–called dummy derivative, for example the algebraic variable y results in dy after differentiation.
(3) An integrator of a differential variable which occurs in the constraint and the derivative of the constraint respectively is eliminated, i.e. for example $\dot{x}$ is eliminated and instead of $\dot{x}$ a new variable called dx is used.
(4) By differentiation of the constraint it is possible that a new variable is generated, i.e. for example through differentiation y (algebraic variable) becomes dy and there is an equation where y can be computed in the system, because if there would be no such equation for y the constraint equation would not be a constraint equation because y could be computed from this equation.
(5) Therefore this equation also has to be differentiated and added to the system.
(6) The proceeding of the points 4–5 continues until no new variables are created.

On the one hand this algorithm may create a lot of variables and equations during the procedure and therefore the system of the resulting equations can get very large.

On the other hand side the differential index has not to be known in advance for using this method.

6. STABILISATION BY PROJECTION

A DAE with differential index $k > 1$ is given. If the numerical solution does not fulfill the constraint, the numerical solution is projected onto a manifold, which is given by the constraint $g(x) = 0$ and the $1^{st}, \ldots, (k-2)^{th}$ derivatives with respect to t of the constraint. The solution manifold is

$$M = \left\{ x(t)\colon g(x(t)) = 0, \frac{\mathrm{d}^i g(x(t))}{\mathrm{d}t^i} = 0, \forall\, i \in I \right\}, \quad (37)$$

with $I = \{1, \ldots, k-2\}$. The algebraic variables can be expressed by the $(k-1)^{th}$ derivative of the constraint and are inserted into the differential equations of the DAE. This procedure leads to a system of differential equations $\dot{y} = f(t, y)$ on the manifold M.

For a DAE with differential index three the manifold M is given by

$$M = \left\{ x(t)\colon g(x(t)) = 0, \frac{\mathrm{d}g(x(t))}{\mathrm{d}t} = 0 \right\} \quad (38)$$

and the algebraic variables can be expressed by the second derivative of the constraint with respect to t.

6.1 Orthogonal Projection Method

One step $y_n \mapsto y_{n+1}$ of the Orthogonal Projection Method is calculated in the following way, see Hairer (2001):

- $\hat{y}_{n+1} = \Phi_h(t_n, y_n)$ is calculated, where Φ_h is a numerical integrator with step size h applied to $\dot{y} = f(t, y)$ (for example a Runge–Kutta method).
- To obtain $y_{n+1} \in M$, $\hat{y}_{n+1}$ is projected orthogonally onto the manifold M.

In Fig. 1 the Orthogonal Projection Method is represented.

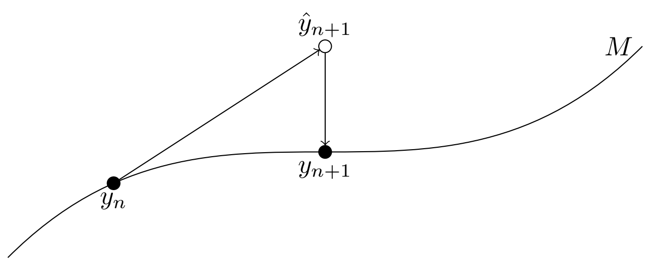

Fig. 1. Illustration of the Orthogonal Projection Method

This method is also called Standard Projection Method. The problem with this method is to find the orthogonal projection.

6.2 Symmetric Projection Method

First the definition of a symmetric one–step–method is necessary. A one–step–method Φ_h is called *symmetric*, if $\Phi_h = \Phi_{-h}^{-1}$ where h stands for the step size of the method.

One step $y_n \mapsto y_{n+1}$ of the Symmetric Projection Method is calculated in the following way, see Hairer (2000):

- $\hat{y}_n = y_n + \frac{\partial \tilde{g}}{\partial y}^T (y_n)\mu$ with $\tilde{g}(y_n) = 0$.
- $\hat{y}_{n+1} = \Phi_h(\hat{y}_n)$ is calculated, where Φ_h is a symmetric one–step–method applied to $\dot{y} = f(y)$.
- $y_{n+1} = \hat{y}_{n+1} + \frac{\partial \tilde{g}}{\partial y}^T (y_{n+1})\mu$ with μ such that $\tilde{g}(y_{n+1}) = 0$.

It is important that the same μ is used in every part of the step $y_n \to y_{n+1}$, which means that μ has to be iterated. $\tilde{g} = 0$ stands for all equations describing the solution manifold which consists of the "obvious" constraints $g = 0$ of the given DAE as well as "hidden" constraints obtained by derivation.

In Fig. 2 the Symmetric Projection Method is shown.

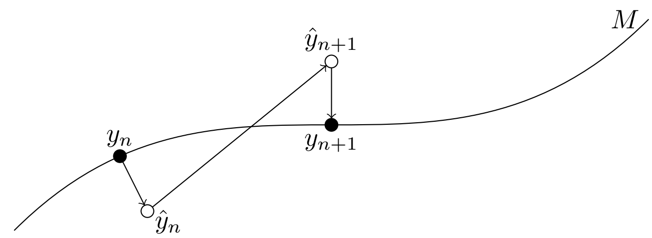

Fig. 2. Illustration of the Symmetric Projection Method

7. METHODS BASED ON LOCAL STATE SPACE TRANSFORMATION

The given DAE is not solved on the whole state space, but on a manifold, see Hairer (2001). The manifold is implicitly given by the constraint $g(x) = 0$ and the $1^{st}, \ldots, (k-2)^{th}$ derivatives with respect to t of the constraint, where k denotes the differential index of the DAE. The manifold M is once again given by equation (37). The algebraic variables can be expressed by the $(k-1)^{th}$ derivative of the constraint and are inserted into the differential equations of the DAE. This procedure leads to a system of differential equations $\dot{y} = f(t, y)$ on the manifold M. This ODE on the manifold M is solved by the introduction of local coordinate transformations.

Let a local coordinate function $\psi\colon U \to \mathbb{R}^n$, $U \subset \mathbb{R}^m$ open, $\psi(U) \subset M \subset \mathbb{R}^n$ be given on the m–dimensional manifold M. The transformation $y = \psi(z)$ transforms the differential equation $\dot{y} = f(t, y)$ into

$$\frac{\partial \psi(z)}{\partial z}\dot{z} = f(t, \psi(z)). \quad (39)$$

With the assumption $f(t, y) \in T_y M$, where $T_y M$ is the tangent space in a fixed point $y \in M$ and has dimension m, the differential equation (39) is equivalent to

$$\dot{z} = F(t, z) := \frac{\partial \psi(z)}{\partial z}^{+} f(t, \psi(z)), \quad (40)$$

where $\frac{\partial \psi(z)}{\partial z}^{+} = \left(\frac{\partial \psi(z)}{\partial z}^T \frac{\partial \psi(z)}{\partial z} \right)^{-1} \frac{\partial \psi(z)}{\partial z}^T$ denotes the Moore–Penrose–pseudoinverse matrix of $\frac{\partial \psi(z)}{\partial z}$.

One step $y_n \mapsto y_{n+1}$ using local coordinates is calculated in the following way:

- Local coordinates are chosen and z_n is calculated with $y_n = \psi(z_n)$.

- $z_{n+1} = \Phi_h(t_n, z_n)$ is calculated with a numerical method Φ_h applied to (40).
- $y_{n+1} = \psi(z_{n+1})$

The coordinates $y = \psi(z)$ can be changed in each step. The difficulty of this method is to find suitable coordinates. The choice of the local coordinates can be realised via the Generalised Coordinate Partitioning (see Wehage, and Haug (1982)) or the Tangent Space Parametrisation (see Potra, and Rheinboldt (1991)).

8. GEAR–GUPTA–LEIMKUHLER FORMULATION

The Gear–Gupta–Leimkuhler formulation aims to include the description of the solution manifold by the constraint equations into the equation system. As this would lead to an overdetermined system, a correction term is introduced, see (41), where v denotes the generalized velocities. It can be shown that every solution of this system with $\mu = 0$ provides a solution of the original system.

$$\begin{aligned} \dot{q} &= v - G^T(q)\mu \\ M(q)\dot{v} &= F(t, q, v) - G^T(q)\lambda \\ g(q) &= 0 \\ G(q)v &= 0 \end{aligned} \tag{41}$$

(41) represents an equation system of differential index two for which a solution not leaving the manifold can be obtained using BDF methods, implicit Runge–Kutta methods or the solver ODASSL (see Arnold, Burgermeister, Führer, Hippmann, and Rill (2011)), which has been developed especially for this formulation.

9. COMPARISION OF THE REGULARISATION METHODS

Each method presented above has advantages as well as disadvantages. These are listed in Tables 1 and 2 respectively. The abbreviations used in Tables 1 and 2 are declared as follows:

DS C ... differentiation and substitution of the constraint
B–M ... Baumgarte–Method
P–A ... Pantelides–Alogrithm
OP ... orthogonal projection method
SP ... symmetric projection method
T ... methods based on state space transformation.

Table 1. Advantages of the Approaches

Approach	Advantages
DS C	easy to apply
B–M	no drift-off in contrary to DS C
P–A	knowledge of index not necessary
OP	solution stays on the manifold
SP	solution stays on the manifold
T	accurate and easy to apply if global

Table 2. Disadvantages of the Approaches

Approach	Disadvantages/Problems
DS C	loss of information (drift–off)
B–M	choice of parameters
P–A	many unknowns and equations
OP	finding the orthogonal projection
SP	iterative calculation
T	finding of a global transformation

10. CONCLUSION AND OUTLOOK

In this paper, all in all seven methods for the regularisation of DAEs with differential index three were presented. Every method can be applied to solve the differential–algebraic equations resulting from the equations of motion of mechanical systems, which usually have index three.

In further studies these methods will be tested by means of several case studies and compared regarding the distance of the numerical solution to the solution manifold, their numerical accuracy and applicability for different tasks. Additionally, methods suitable for DAEs of arbitrary index will be tried out on other than mechanical systems.

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