Discussion of two Case Studies on DAEs using Different Approaches for Regularisation

Carina Pöll[1*], Irene Hafner[2], Bernhard Heinzl[3]

[1] Institute of Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria; *carina.poell@tuwien.ac.at

[2] dwh GmbH, Simulation Services, Neustiftgasse 57-59, Vienna, Austria

[3] Institute of Computer Aided Automation, Vienna University of Technology, Treitlstraße 3, 1040 Vienna, Austria

Simulation Notes Europe SNE 24(3-4), 2014, 179 - 184
DOI: 10.11128/sne.24.tn.102267
Received: July 15, 2014; Revised September 14, 2014;
Accepted: October 20, 2014;

Abstract. The object-oriented model description of physical or mechanical systems leads to differential-algebraic equations. In general the numerical solution of such equation systems is very complex, numerically extensive or may even be impossible. Therefore it is important to find methods for solving given equation system, this leads to the so-called index reduction and regularization methods. This paper gives a short overview of common methods of index reduction. Additionally a classification of these different approaches is made. Afterwards each approach is presented in detail and the advantages and disadvantages of the different methods are discussed. In order to compare the different index reduction methods, the methods described above are demonstrated by various examples. For the comparability of the different methods the obtained numerical solutions and the deviation from the constraint equations are displayed graphically. Therefore the distinct approaches can be compared with regard to their numerical solutions. The two examples are mechanical systems with differential index three. The equations of motion of a pendulum on a circular path in Cartesian coordinates and the motion of the double pendulum in Cartesian coordinates, which shows a chaotic behaviour, are used as case studies.

Introduction

An object-oriented acausal model description for physical or mechanical systems, such as Modelica or MATLAB/Simscape, leads to differential-algebraic equations with non-trivial differential index.

The numerical solution of these equations with methods for ordinary differential equations is generally very complex and therefore numerically extensive or may even be impossible. This problem leads to the so-called index reduction or regularisation methods. These methods transform the given differential-algebraic equation into a differential-algebraic equation with lower differential index or into an ordinary differential equation. Due to the large differences (structure, properties, etc.) of differential-algebraic equations, in the literature there can be found a number of different approaches and methods for the reduction of the differential index and the regularisation. Some of these approaches will be compared in this paper and evaluated by means of case studies. These approaches can be split into three topics, see [1]:

- index reduction using differentiation
- stabilization by projections
- methods based on local state space transformations

Each of these topics is discussed in detail in Section 2.

1 Basic Definitions

In this section some basic definitions, which are used in the following, are presented. A differential-algebraic equation (DAE), see [2], is given by an implicit equation,

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

with $F: I \times D_x \times D_{\dot{x}} \to \mathbb{R}^n$ ($n \in \mathbb{N}$), where I is a real interval, $\dot{x}$ denotes the derivative of x with respect to t and D_x, $D_{\dot{x}}$ are open subsets of $\mathbb{R}^n$. A differential-algebraic equation consists of differential as well as algebraic variables and equations.

The algebraic equations of the given differential-algebraic equation have the form

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

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

Equation (1) has differential index $m \in \mathbb{N}$, if m is the minimal number of derivatives such that from the system

$$F(t,x,\dot{x}) = 0, \frac{dF(t,x,\dot{x})}{dt} = 0, \dots, \frac{d^mF(t,x,\dot{x})}{dt^m} = 0 \tag{3}$$

an ordinary differential equation system can be extracted via algebraic manipulations, see [1]. After these algebraic calculations the given system can be transformed into an ordinary differential equation $\dot{x} = \varphi(t,x)$ with $\varphi: I \times D_x \to \mathbb{R}^n$. In the following the differential index is also called only index.

2 Regularisation Methods

In the following six regularization approaches are discussed, see [1].

2.1 Differentiation and substitution of the constraint

A first idea for the reduction of the index is to differentiate the constraint equations and substitute the constraint equations by its derivatives. This procedure is repeated until the differential-algebraic equation has differential index 1. For example, let a DAE with differential index 3 be given, the constraint equations are substituted by the second derivative with respect to the time, i.e. the new constraint equation is

$$\ddot{g}(x) = 0. \tag{4}$$

The resulting system has index 1. A problem of this method is that due to the derivation there is a loss of information. Therefore the necessary initial values for the integration are unknown. This fact causes a numerical "drift-off", i.e. the numerical solution departs from the solution manifold.

2.2 Baumgarte-Method

Another approach using differentiation is the Baumgarte-Method, see [3]. This method substitutes the constraint equation (2) by a linear combination of $g, \dot{g}$ and $\ddot{g}$, i.e. instead of (2) the equation

$$\ddot{g} + 2\alpha\dot{g} + \beta^2 g = 0 \tag{5}$$

is used. This approach is motivated by the special form of the new constraint equation.

The shape of equation (5), i.e. the appearance of g and $\dot{g}$, ensures that there is no loss of information like in the approach explained above.

The parameters α and β in equation (5) have to be chosen such that the ordinary differential equation (5) is asymptotically stable. Therefore the zeros of the characteristic polynomial

$$\lambda^2 + 2\alpha\lambda + \beta^2 \tag{6}$$

of the ordinary differential equation have to be computed, which results in

$$\lambda_{1,2} = -\alpha \pm \sqrt{\alpha^2 - \beta^2}. \tag{7}$$

Therefore follows $\alpha > 0$. A problem of this approach is the choice of the two parameters.

2.3 Pantelides Algorithm

The procedure of the Pantelides-Algorithm has a fixed routine for every constraint equation. This algorithm is given by the following steps, see [4].

- The constraint equation has to be differentiated.
- The differentiated constraint has to be added to the system of equations. If there is an algebraic variable in the constraint equation, then the derivative of this variable becomes a so-called dummy derivative, for example the derivative of the algebraic variable y is written as dy, which is called dummy derivative.
- An integrator which has a connection to the constraint equation 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.
- By differentiation of the constraint it can occur that a new variable is generated, i.e. for example through differentiation y, which is an algebraic variable, becomes dy and there is an equation where y can be computed in the system (otherwise the constraint equation would not be a constraint equation).
- Therefore the equation of which y can be computed also has to be differentiated.
- The procedure of the last two points has to be repeated until no new variables are created.

A problem of this method is that during the procedure of the algorithm a lot of variables and equations may be created. Therefore the system of the resulting equations is getting large and can be unclear. Compared with the other methods which are discussed in this paper, this is the only approach where it is not necessary to compute the differential index.

2.4 Orthogonal Projection method

General assumptions:

- A DAE with differential index $k > 1$ is given.
- The algebraic variables can be expressed by the $(k-1)^{th}$ derivative of the constraint equation with respect to t.

The solution manifold M is given by the constraint equation and the first till the $(\mathrm{k}-2)^{\mathrm{th}}$ derivative of the constraint equation with respect to t, i.e.

$$M = \{x \in \mathbb{R}^n : g(x) = 0, \frac{d^i g}{dt^i} = 0,\ i \in I\}, \quad (8)$$

where $I = \{1, \ldots, k-2\}$.

The idea of the orthogonal projection method is to project orthogonally onto the solution manifold M, if the numerical solution does not fulfil the constraints.

For one step the procedure of this method is given as follows, see [6]:

- $\hat{y}_{n+1} = \Phi(y_n)$, where Φ is a numerical integrator.
- y_{n+1} is the orthogonal projection of $\hat{y}_{n+1}$ onto the solution manifold M.

In Figure 1 one step of this approach is shown.

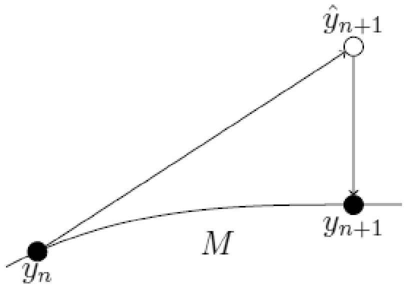

Figure 1: Schematic illustration of the orthogonal projection method.

The problem of this method is to find the orthogonal projection. Another fact is, that the numeric integration has to be stopped after each step for checking whether the numerical solution fulfils the constraint equations and if it is not fulfilled, the orthogonal projection has to be applied.

2.5 Symmetric projection method

The idea of the symmetric projection method is to perturb y_n so that it is not on the solution manifold M and then apply a symmetric one-step-method. The distance of the new value (computed with the symmetric one-step-method) to the manifold corresponds to the absolute value of the perturbation.

For the general assumptions see section 2.4. The solution manifold is given by equation (8).

A one-step-method Φ_h (with step size h) is symmetric if $\Phi_h = {\Phi_{-h}}^{-1}$.
For one step the procedure of this method is: (see [7])

- $\hat{y}_n = y_n + \frac{d\tilde{g}}{dy}\mu$ where $\tilde{g}(y_n) = 0$.
- $\hat{y}_{n+1} = \Phi_h(\hat{y}_n)$, where Φ_h is a symmetric one-step-method.
- $y_{n+1} = \hat{y}_{n+1} + \frac{d\tilde{g}}{dy}\mu$ where $\tilde{g}(y_{n+1}) = 0$.

It is important that in the first and in the third step the same μ is used. Therefore the calculations described above have to be implemented with an iteration. The function $\tilde{g}$ consists of the constraint equations and of the derivatives of the constraint equations, which are used for describing the solution manifold.

In Figure 2 a schematic presentation of one step of this approach is shown.

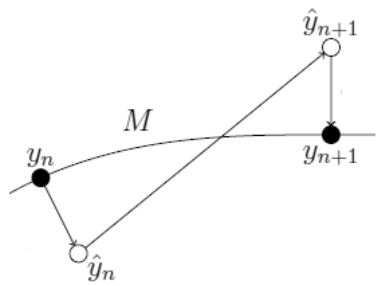

Figure 2. Schematic illustration of the symmetric projection method.

The disadvantage of this method is that the calculation has to be iterative and therefore the solution time is getting bigger in contrast to the methods where an ode-solver of MATLAB is used.

2.6 Methods based on local state space transformation

For the general assumptions see Section 2.4. The solution manifold is also given by (8).

The general idea of this approach is instead of solving the system on the whole state space only to solve it on a manifold, which is realized with an appropriate local coordinate transformation ψ.
For one step the procedure of this method is, see [6]:

- z_n is calculated with $\psi(z_n) = y_n$.
- $z_{n+1} = \Phi(z_n)$, where Φ is a numerical integrator.
- $\psi(z_{n+1}) = y_{n+1}$.

The local coordinatisation can be changed in every step. If there is a global coordinatisation, this method leads to a simple equation system. The difficulty of this approach is to find a suitable local or global coordinatisation.

3 Case Study 'Pendulum'

The first example is the motion of a pendulum in Cartesian coordinates, which is shown in Figure 3.

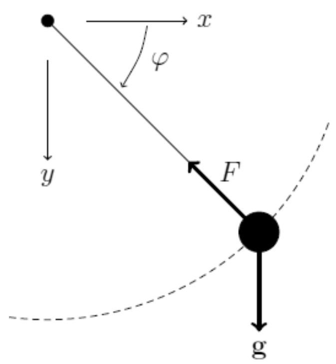

Figure 3: Schematic illustration of the motion of a pendulum in Cartesian coordinates.

The equations of motion of the pendulum are given by the following equations, see [5],

$$\dot{x} = v_x \tag{9}$$
$$\dot{y} = v_y \tag{10}$$
$$\dot{v}_x = -Fx \tag{11}$$
$$\dot{v}_y = g - Fy \tag{12}$$
$$x^2 + y^2 = 1, \tag{13}$$

where g is the gravitational acceleration and F is the force. Equation (13) is the constraint equation. The DAE (9)-(13) has differential index three, which can be seen from the third derivative with respect to t of equ. (13).

All simulations are realized with MATLAB R2012b. The first approach leads to the numerical 'drift-off'. Therefore this approach is not suitable for the simulation of the given DAE. This can be seen in Figure 4, where the result of the simulation with the ode-solver `ode15s` is shown.

The orthogonal projection method uses an explicit *Euler* method for the integration. The numerical solution of this method is not correct due to the increasing speed, which is shown in Figure 5.

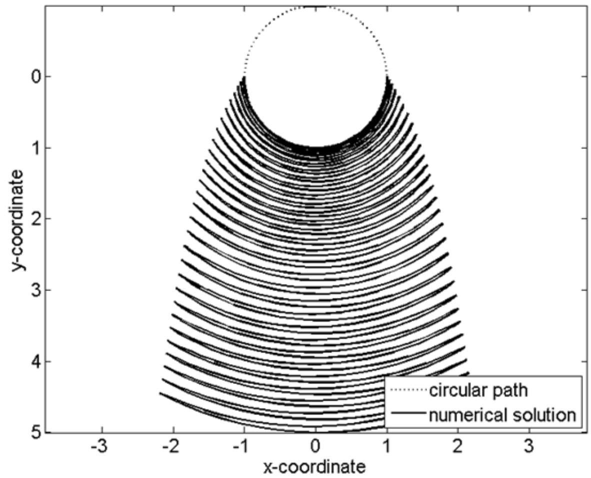

Figure 4: Result of the simulation using differentiation and substitution of the constraint.

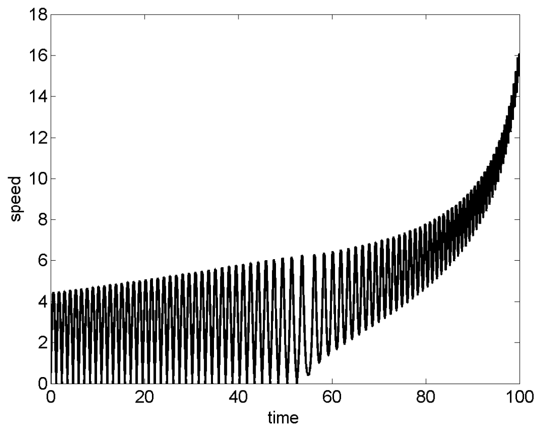

Figure 5: Speed of the numerical solution obtained with the orthogonal projection method.

The Baumgarte-Method leads to a system of ordinary differential equations, which is solved with the ode-solver `ode45`.

The Pantelides-Algorithm leads to four equation systems because of equation (13), which are used for four different regions of the unit circle. For solving these four equation systems the ode-solver `ode15i` is used.

The symmetric projection method is solved iteratively, where the trapezoidal rule, which is a symmetric one-step-method, is used. In contrast to the orthogonal projection method, this method does not show increasing speed.

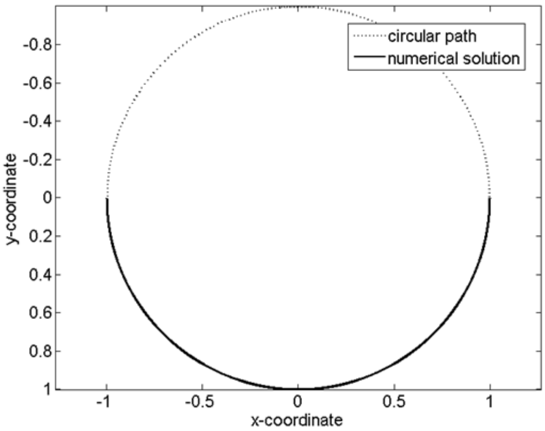

Figure 6: Result of the phase space trajectory.

The state space transformation is solved using polar coordinates for the coordinatisation. This coordinatisation is global, which is a great advantage of this method. This method leads to a two-dimensional system of ordinary differential equations, which is solved with `ode45`.

The numerical solutions obtained with the Baumgarte-Method, Pantelides-Algorithm, symmetric projection method and the state space transformation result in quite similar results with respect to the phase space trajectory. Therefore only one of these solutions is shown graphically, see Figure 6. While the phase space trajectory looks similar, the deviations of the numerical solutions obtained with the different methods show big differences.

The state space transformation has the smallest deviation from the numerical solution to the circular path and is easy to implement. Therefore this method would be the recommended approach for the given DAE.

4 Case Study 'Double Pendulum'

The second case study treats a double pendulum. The equations of motion of the pendulum are given by the following equations,

$$\dot{x}_1 = v_{x_1} \tag{14}$$

$$\dot{y}_1 = v_{y_1} \tag{15}$$

$$\dot{x}_2 = v_{x_2} \tag{16}$$

$$\dot{y}_2 = v_{y_2} \tag{17}$$

$$\dot{v}_{x_1} = -F_1 x_1 - F_2(x_1 - x_2) \tag{18}$$

$$\dot{v}_{y_1} = g - F_1 y_1 - F_2(y_1 - y_2) \tag{19}$$

$$\dot{v}_{x_2} = -F_2(x_2 - x_1) \tag{20}$$

$$\dot{v}_{y_1} = g - F_2(y_2 - y_1) \tag{21}$$

$${x_1}^2 + {y_1}^2 = 1 \tag{22}$$

$$(x_1 - x_2)^2 + (y_1 - y_2)^2 = 1 \tag{23}$$

Where g is the gravitational acceleration and $F_1$and F_2 are forces. Equations (22) and (23) are the constraint equations. The DAE (14)-(23) has differential index three, which can be seen from the third derivative with respect to t of equations (22) and (23). Like before all simulations are realized with MATLAB R2012b.

The approach using differentiation and substitution of the constraint is, like for the first case study, not suitable for the numerical simulation of the given DAE.

The orthogonal projection method has unbounded speed, which leads to 'wrong' positions on the solution manifold. Therefore this method cannot lead to reasonable results.

The Baumgarte-Method leads to very different results for different values of the parameters. In Figure 7 one result with the Baumgarte-Method is shown, where the red line is the numerical solution of the second pendulum until 10 seconds and from 10 till 100 seconds the numerical solution of this pendulum is shown in black.

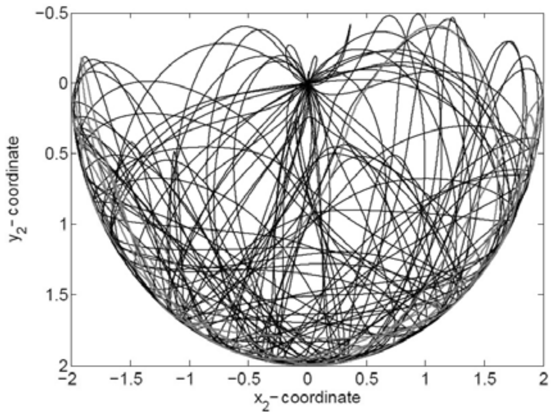

Figure 7: Result of the pendulum (x_2, y_2) with the Baumgarte-Method with $\alpha = 100$ and $\beta = 1000$.

The simulation of the Pantelides-Algorithm leads to a problem. The ode-solver has problems to solve the equations, which leads to too small step sizes. Therefore the ode-solver `ode15i` has to be stopped and restarted with new values. Furthermore there are sixteen different equation systems which are a little complex to implement.

The symmetric projection method again has a long simulation time because of the iterative calculation, but with this approach the speed is bounded in contrast to the orthogonal projection method.

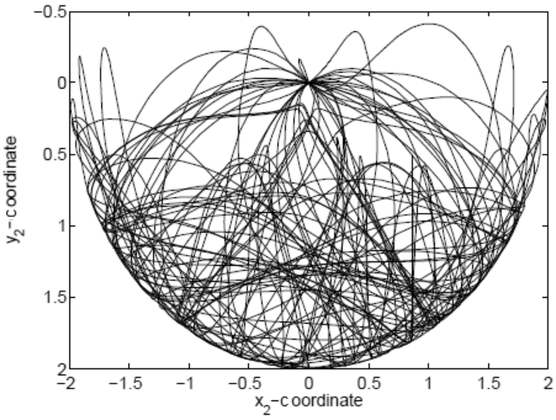

Figure 8: Result of the pendulum (x_2, y_2) with the state space transformation.

Using the state space transformation the given DAE can be transformed into a system of four ordinary differential equations with the use of a coordinatisation using cosine and sine. Simulating this approach using ode45 or `ode23t` for example leads to different results, which can be explained by the chaotic behaviour of the double pendulum, see [8]. In Figure 8 the result for the second pendulum with the state space transformation is shown. Comparing Figure 7 and Figure 8 it is obvious that the numerical solution using Baumgarte-Method and state space transformation is not equal. Still one can observe that until 10 seconds the results of most of the approaches are similar, but from 10 till 100 seconds the numerical solutions show big differences.

In general it is a fact that for this case study one cannot say whether a simulation result is the "right" or the "best" because there exists no analytical solution and the double pendulum shows a chaotic behaviour.

5 Conclusion and Outlook

After analysing the presented methods with the two examples some facts can be observed.

The method using differentiation and substitution of the constraint equations and the orthogonal projection method do not lead to suitable results. Using the first method leads to the numerical 'drift-off'. The second method does not show the numerical 'drift-off', which means that the numerical solution stays on the solution manifold, but due to the increasing speed the positions are not correct.

- The Baumgarte-Method results in small deviations to the constraint equations for a suitable choice for the two parameters.
- The implementation of the Pantelides-Algorithm is a little complex because of the many equations and unknowns and for the second case study the ode-solver had to be stopped an restarted because of too small step sizes.
- The symmetric projection method has a long simulation time because there is iteration, but the results stay close to the solution manifold.
- The last method is the state space transformation, which can be done global for the two used case studies. This is a very important fact, because therefore the resulting equations where the most simple.

For further research it would be interesting to study DAEs with a differential index unequal to three and analyse the use of the methods for such DAEs. Furthermore an improvement with respect to the implementation for the Pantelides-Algorithm would be to write an own solver.For the simulation of the orthogonal projection method it would be interesting to use another numerical integration method for investigating whether the speed is increasing too.

Another further study would be to test the state space transformation for DAEs where no global transformation can be used.

References

[1] Hairer E, Wanner G. *Solving Ordinary Differential Equations II.* Germany: Springer; 2002. 491 p.

[2] Kunkel P, Mehrmann V. *Differential-Algebraic Equations: Analysis and Numerical Solution.* Finland: European Mathematical Society; 2006. 385 p.

[3] Eich E, Hanke M. Regularization Methods for Constrained Mechanical Multibody Systems. *ZAMM - Journal of Applied Mathematics and Mechanics*. 1995; 75(10): 761-773. doi: 10.1002/zamm.19950751013

[4] Cellier FE. *The Structural Singularity Removal Algorithm by Pantelides*. http://www:inf:ethz:ch/personal/fcellier/Lect/MMPS/Ppt/mmps_6_engl:ppt, date: 10.02.2014.

[5] Cellier FE, Kofman E. *Continuous System Simulation.* USA: Springer; 2006. 658 p.

[6] Hairer E. Geometric Integration of Ordinary Differential Equations on Manifolds. *BIT Numerical Mathematics.* 2001; 41(5): 996-1007. doi: 10.1023/A:1021989212020

[7] Hairer E. Symmetric Projection Methods for Ordinary Differential Equations on Manifolds. *BIT Numerical Mathematics*. 2000; 40(4): 726-734. doi: 10.1023/A:1022344502818

[8] Stolze J. *Einführung in die nichtlineare Dynamik*. http://t1:physik:tu-dortmund:de/stolze/teaching/TNF/tnf_chaos:pdf, date: 24.06.2014.