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M001 - The Simple Pendulum[‡] (v1.0)

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AMS(MOS) subject classification: 65L80

Keywords: example collection, numerical integration, differential-algebraic equations

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The Simple Pendulum

Andreas Steinbrecher

November 11, 2015

Abstract

The considerations in this report *The Simple Pendulum* are part of the example collection which can be found in `http://www3.math.tu-berlin.de/multiphysics/Examples/`. The aim is to investigate different formulations, i.e., regularized formulations or also index reduced formulations, of the model equations in combination with different numerical solvers with respect to its applicability, efficiency, accuracy, and robustness.

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1 Introduction

The considerations in this report *The Simple Pendulum* are part of the example collection which can be found in `http://www3.math.tu-berlin.de/multiphysics/Examples/`. The aim is to investigate different formulations, i.e., regularized formulations or also index reduced formulations, of the model equations in combination with different numerical solvers with respect to its applicability, efficiency, accuracy, and robustness.

2 The Simple Pendulum

In this example we consider the movement of a simple pendulum. The simplified topology is illustrated in Figure 1.

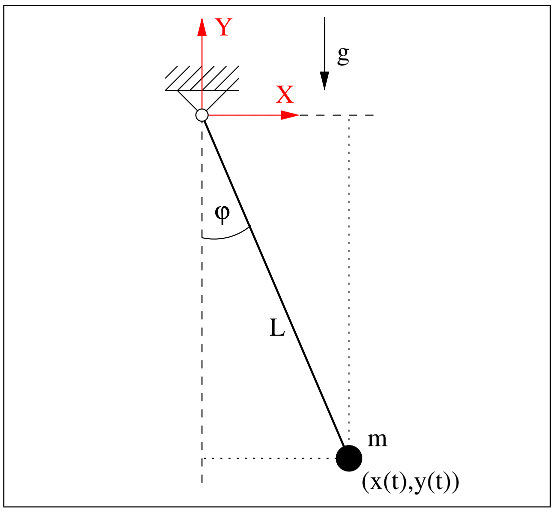

Figure 1: Topology

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2.1 Model equations

2.1.1 The Mathematical Model

The mathematical model corresponds to a semi-implicit DAE of strangeness index (s-index) $\nu_s = 2$, of differentiation index (d-index) $\nu_d = 3$, and of maximal constraint level (c-level) $\nu_c = 2$ consisting of 5 unknowns, 5 equations, comprising 4 differential equations and 1 algebraic equation. For details on the strangeness-index see [9], the differentiation index see [3, 8], and the maximal constraint level see [10].
The model equations for the simple pendulum have the form

$$\dot{x} = v, \quad (1a)$$

$$\dot{y} = w, \quad (1b)$$

$$m\dot{v} = -2x\lambda, \quad (1c)$$

$$m\dot{w} = -2y\lambda - m\mathfrak{g}, \quad (1d)$$

$$0 = x^2 + y^2 - L^2 \quad (1e)$$

for $t \in \mathbb{I}$ with the time domain $\mathbb{I} = [t_0, t_f]$. The unknown variables as well as the model parameters are listed in Tables 1 and 2, respectively.

variable	physical meaning	unit	dimension
x	x-position of the mass m	m	1
y	y-position of the mass m	m	1
v	velocity of the mass m in x-direction	m/s	1
w	velocity of the mass m in y-direction	m/s	1
λ	Lagrange-Multiplier	kg/s^2	1

Table 1: Unknown variables

parameter	physical meaning	unit	dimension
m	mass of the mass point	kg	1
L	length of the pendulum	m	1
$\mathfrak{g}$	gravitational acceleration	m/s^2	1

Table 2: Parameters

2.1.2 The Origin of the Problem

A mathematical pendulum of length $L > 0$ represents a point mass which moves without friction along a vertical circle of radius L under gravity.
Let us use absolute coordinates x and y denoting the position (x, y) of the mass m in the two dimensional space $\mathbb{R}^2$ for the description of the configuration of the pendulum. The forces acting on the mass m in x-direction are composed by the inertia force $-m\ddot{x}$ and the x-component of the constraint force, i.e., $-2x\lambda$ with the Lagrange multiplier λ. Furthermore, the forces acting on the mass point m in y-direction are composed by the inertia force $-m\ddot{y}$, the gravitational force $-m\mathfrak{g}$, and the y-component of the constraint force, i.e., $-2y\lambda$ with the Lagrange multiplier λ. From the force equilibrium we get the *dynamic equations of motion* of second order

$$0 = -m\ddot{x} - 2x\lambda,$$

$$0 = -m\ddot{y} - m\mathfrak{g} - 2y\lambda.$$

Together with the introduced velocity variables $v = \dot{x}$ and $w = \dot{y}$ as well as with the constraint $0 = g(x, y) = x^2 + y^2 - L^2$ forcing the position of the mass m in a fixed distance to the origin, we get the equations of motion for the simple pendulum in the form (1) with the *kinematic equations of motion* (1a),(1b), the *dynamic equations of motion* (1c), (1d), and the *holonomic constraint* (1e).
Since the pendulum is only influenced by the gravitational field of forces, i.e., by a conservative field of forces, and since it is not affected by other applied forces, it represents a mechanical system which conserves the total energy. This total energy is given by

$$E(x, y, v, w) = \frac{1}{2}m(v^2 + w^2) + m\mathfrak{g}y$$

and is conserved such that we get the *constraint of energy conservation*

$$\begin{aligned} 0 = e(x,y,v,w) &= E(x,y,v,w) - E(x_0,y_0,v_0,w_0) \\ &= (\frac{1}{2}m(v^2+w^2) + m\mathfrak{g}y) - (\frac{1}{2}m(v_0^2+w_0^2) + m\mathfrak{g}y_0) \end{aligned} \tag{2}$$

for $t \in \mathbb{I}$ and every solution of the equations of motion (1) with initial values x_0, y_0, v_0, w_0.
The unknown variables as well as the model parameters are listed in Tables 1 and 2, respectively. The values of the parameters, the initial values, and the time domain are specified in detail in the scenarios below.

2.1.3 Regularizations and used Formulations

Solutions of the model equations are restricted by so called *hidden constraints* which, in particular, are responsible for the difficulties in the numerical treatment. In particular, as one hidden constraint we have the *holonomic constraints of velocity level*

$$0 = 2xv + 2yw \tag{3a}$$

obtained from the total time derivative of the holonomic constraints (1e), where the derivatives $\dot{x}$ and $\dot{y}$ are replaced by (1a) and (1b), respectively. The constraint (3a) is also called *hidden constraint of level 1* since this constraint is obtained after differentiation of (certain) model equations once. A further hidden constraint is the *holonomic constraints of acceleration level*

$$0 = 2v^2 + 2w^2 - 2y\mathfrak{g} - \frac{4}{m}(x^2+y^2)\lambda. \tag{3b}$$

This is obtained from the total time derivative of the holonomic constraint on velocity level (3a), where the derivatives $\dot{x}$, $\dot{y}$, $\dot{v}$, and $\dot{w}$ are replaced by (1a)-(1d), respectively. The constraint (3b) is also called *hidden constraint of level 2* since this constraint is obtained after differentiation of (certain) model equations twice.

For the numerical treatment we will use the following formulations.

d-index 2 formulation (rcd1) The *d-index 2 formulation* has the form

$$\begin{aligned} \dot{x} &= v, && (4a)\\ \dot{y} &= w, && (4b)\\ m\dot{v} &= -2x\lambda, && (4c)\\ m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (4d)\\ 0 &= 2xv + 2yw && (4e) \end{aligned}$$

and belongs to the classical index reduction, where in the model equations (1) the holonomic constraint (1e) is replaced by the holonomic constraint on velocity level (3a). This formulation has d-index 2, s-index 1, and maximal constraint level 1 and contains (3b) as hidden constraint of level 1 while the constraint (1e) is removed. Therefore, in its numerical treatment slight instabilities due to the higher index, i.e., the existence of hidden constraints, and linear drift from the holonomic constraint (1e) is expected due to the loss of this constraint on position level. For more details we refer to [8, 10].

d-index 1 formulation (rcd0) The *d-index 1 formulation* has the form

$$\begin{aligned} \dot{x} &= v, && (5a)\\ \dot{y} &= w, && (5b)\\ m\dot{v} &= -2x\lambda, && (5c)\\ m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (5d)\\ 0 &= 2v^2 + 2w^2 - 2y\mathfrak{g} - \frac{4}{m}(x^2+y^2)\lambda && (5e) \end{aligned}$$

and belongs to the classical index reduction, where in the model equations (1) the holonomic constraint (1e) is replaced by holonomic constraint on acceleration level (3b). This formulation has d-index 1, s-index 0, and maximal constraint level 0 and contains no hidden constraint while the constraints (1e) and (3a) are removed. Therefore, in its numerical treatment no instabilities but quadratic drift from the holonomic constraint (1e) and linear drift from the holonomic constraint on velocity level (3a) is expected due to the loss of the constraint on position level (1e) and the constraint on velocity level (3a). For more details we refer to [8, 10].

overdetermined c-level 1 formulation (ovd1) The *overdetermined c-level 1 formulation* has the form

$$
\begin{aligned}
\dot{x} &= v, && (6a)\\
\dot{y} &= w, && (6b)\\
m\dot{v} &= -2x\lambda, && (6c)\\
m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (6d)\\
0 &= x^2 + y^2 - L^2, && (6e)\\
0 &= 2xv + 2yw, && (6f)
\end{aligned}
$$

where the holonomic constraint on velocity level (3a) is added to the model equations (1). This formulation has s-index 1, and maximal constraint level 1 while the d-index is not defined. Furthermore, this formulation contains (3b) as hidden constraint of level 1 while no constraint is removed. Therefore, in its numerical treatment slight instabilities due to the higher c-level, i.e., the existence of hidden constraints, but no drift are expected. The direct numerical integration needs adapted numerical methods suited for overdetermined DAEs. For more details we refer to [4, 10].

overdetermined c-level 0 formulation (ovd0) The *overdetermined c-level 0 formulation* has the form

$$
\begin{aligned}
\dot{x} &= v, && (7a)\\
\dot{y} &= w, && (7b)\\
m\dot{v} &= -2x\lambda, && (7c)\\
m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (7d)\\
0 &= x^2 + y^2 - L^2, && (7e)\\
0 &= 2xv + 2yw, && (7f)
\end{aligned}
$$

$$0 = 2v^2 + 2w^2 - 2y\mathfrak{g} - \frac{4}{m}(x^2 + y^2)\lambda, \qquad (7g)$$

where the holonomic constraint on velocity level (3a) and the holonomic constraint on acceleration level (3b) are added to the model equations (1). This formulation has s-index 1, and maximal constraint level 0 while the d-index is not defined. Furthermore, this formulation contains no hidden constraint while no constraint is removed. Therefore, in its numerical treatment no instabilities and no drift are expected. The direct numerical integration needs adapted numerical methods suited for overdetermined DAEs. For more details we refer to [4, 10].

Gear-Gupta-Leimkuhler formulation (GGL) (ggl1) The *Gear-Gupta-Leimkuler formulation* is suited for the regularization of equations of motion for multibody systems and has the form

$$
\begin{aligned}
\dot{x} &= v - 2x\eta, && (8a)\\
\dot{y} &= w - 2y\eta, && (8b)\\
m\dot{v} &= -2x\lambda, && (8c)\\
m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (8d)\\
0 &= x^2 + y^2 - L^2, && (8e)\\
0 &= 2xv + 2yw, && (8f)
\end{aligned}
$$

where the holonomic constraint on velocity level (3a) is added to the model equations (1) and an additional Lagrange multiplier η with $\eta(t_0) = 0$ is introduced. Therefore, the number of unknowns is increased. This formulation has d-index 2, s-index 1, and maximal constraint level 1 and contains (3b) as hidden constraint of level 1 while no constraint is removed. Therefore, in its numerical treatment slight instabilities due to the higher index but no drift are expected. For more details we refer to [6].

projected s-index 1 formulation (psi1) The *projected s-index 1 formulation* has the form

$$\begin{aligned} y\dot{x} - x\dot{y} &= yv - xw, && (9a) \\ m\dot{v} &= -2x\lambda, && (9b) \\ m\dot{w} &= -2y\lambda - m\mathfrak{g}, && (9c) \\ 0 &= x^2 + y^2 - L^2, && (9d) \\ 0 &= 2xv + 2yw, && (9e) \end{aligned}$$

where the holonomic constraint on velocity level (3a) is added to the model equations (1) and the redundancies between the constraints and the differential equations, i.e., the so called strangeness, are eliminated by applying the selector

$$S(x, y) = \begin{bmatrix} y & -x & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

to the differential equations (1a)-(1d) from the left. This formulation has d-index 2, s-index 1, and maximal constraint level 1 and contains (3b) as hidden constraint of level 1 while no constraint is removed. Therefore, in its numerical treatment slight instabilities due to the higher c-level, i.e., the existence of hidden constraints, but no drift are expected. For more details we refer to [9, 10].

projected s-index 0 formulation (psi0) The *projected s-index 0 formulation*, also called *projected strangeness-free formulation*, has the form

$$\begin{aligned} y\dot{x} - x\dot{y} &= yv - xw, && (10a) \\ m(y\dot{v} - x\dot{w}) &= y(-2x\lambda) - x(-2y\lambda - m\mathfrak{g}), && (10b) \\ 0 &= x^2 + y^2 - L^2, && (10c) \\ 0 &= 2xv + 2yw, && (10d) \\ 0 &= 2v^2 + 2w^2 - 2y\mathfrak{g} - \frac{4}{m}(x^2 + y^2)\lambda, && (10e) \end{aligned}$$

where the holonomic constraint on velocity level (3a) and the holonomic constraint on acceleration level (3b) are added to the model equations (1) and the redundancies between the constraints and the differential equations are eliminated by applying the selector

$$S(x, y) = \begin{bmatrix} y & -x & 0 & 0 \\ 0 & 0 & y & -x \end{bmatrix}$$

to the differential equations (1a)-(1d) from the left. This formulation has d-index 1, s-index 0 (strangeness-free), and maximal constraint level 0 and contains no hidden constraint while no constraint is removed. Therefore, in its numerical treatment no instabilities and no drift are expected. For more details we refer to [9, 10].

2.2 Numerical Results

For the numerical computations we use the following solvers combined with the original model equations (1) (denoted by (ori2)) and different (regularized) formulations, see Section 2.1.3.

`DASPK` (Version 2.0 from 12.Jul.2000) [13] is suited for nonlinear DAEs of d-index 1 and uses BDF-methods of order 1 up to 5 as discretization scheme.

`DASSL` (Version from 24.Jun.1991) [3] is suited for nonlinear DAEs of d-index 1 and uses BDF-methods of order 1 up to 5 as discretization scheme.

`GEOMS` (Version 1.3 from 17.Nov.2014) [10, 11] is suited for equations of motion for multibody systems and its regularizations based on overdetermined formulations and uses the Runge-Kutta method of type RADAU IIa of order 5 as discretization scheme.

`MEBDF` (Version from 20.Jan.2006) [1] is suited for quasi-linear DAEs with constant leading matrix and uses the extended multistep methods of Cash of order 1 up to 8 as discretization scheme.

`ODASSL` (Version from 03.Jan.1990) [4, 5] is suited for (possibly overdetermined) nonlinear DAEs with maximal c-level 0 and uses an adaption of the BDF-methods of order 1 up to 5 as discretization scheme.

OVDBDF (Version 0.2 from 09.Nov.2015) [2] is suited for (possibly overdetermined) nonlinear DAEs with maximal c-level 0 and uses an adaption of the BDF-methods of order 1 up to 5 as discretization scheme.

QUALIDAES (Version 0.1 from 09.Sep.2015) [12] is suited for (possibly overdetermined) quasi-linear DAEs with maximal c-level 1 and uses an adaption of the Runge-Kutta method of type RADAU IIa of order 5 as discretization scheme.

RADAU5 (Version with small correction from April 14, 2000) [7, 8] is suited for quasi-linear DAEs with constant leading matrix up to d-index 2 and for Hessenberg systems up to d-index 3 and uses the Runge-Kutta method of type RADAU IIa of order 5 as discretization scheme.

The numerical integrations are done on an AMD Phenom(tm) II X6 1090T, 3210 MHz.

2.2.1 Scenario 01

The equations of motion are given in (1).

m	$= 1$ kg
L	$= 1$ m
$\mathfrak{g}$	$= 13.7503716373294544$ m/s^2

Table 3: Scenario 01: Parameters

In that scenario we will simulate the motion of the pendulum on $\mathbb{I} = [0\text{s}, 20\text{s}]$ with the parameters as depicted in Table 3 and the initial values

$$\begin{array}{llllll} x(t_0) = x_0 & = & 1 \quad v(t_0) = v_0 & = & 0 \quad \lambda(t_0) = \lambda_0 & = 0 \\ y(t_0) = y_0 & = & 0 \quad w(t_0) = w_0 & = & 0. & \end{array} \tag{11}$$

Let us note that we did modify the gravitational acceleration to $\mathfrak{g} = 13.7503716373294544\text{m/s}^2$ such that the exact solution has a period of 2s which allows the comparison of the accuracy every period.

Reference Solution Since this problem is not analytically solvable, we use the numerical solution obtained with QUALIDAES for the overdetermined c-level 0 formulation (ovd0) with a prescribed tolerance $TOL = 10^{-14}$ as reference solution for comparisons of the obtained precision. In Figure 2 the reference solution is illustrated, while in Table 4 the values of the analytical solution at the final time $t_f = 20$s are listed.

$x(t_f) =$	1.0E+00	$v(t_f) =$	0.0E+00	$\lambda(t_f) =$	0.0E+00
$y(t_f) =$	0.0E+00	$w(t_f) =$	0.0E+00		

Table 4: Scenario 01: Analytical solution at the final time point $t_f = 20$s.

Numerical Solution The used solver-formulation combinations and an overview of the success is illustrated in Table 5. For the numerical computations the tolerances RTOL=ATOL=10^{-i}, $i = 5, ..., 12$ are prescribed uniformly for all components of the state variables. Selected driver subroutines for the used solver-formulation combinations are available on the webpage
http://www3.math.tu-berlin.de/multiphysics/Examples/M001_SimplePendulum/.
In Figure 3 we have illustrated the solution of the numerical integration by use of a selection of solver-formulation combinations with a prescribed tolerance RTOL=ATOL=10^{-7}. Furthermore, in Figure 4 the obtained error of these numerical solutions is illustrated in logarithmic style. The largest deviation show the solutions MEBDF(rcd1) and DASSL(rcd0) which mainly comes from the higher index (4) and the drift due to the missing constraint (1e) of the d-index 2 formulation (rcd1) (4) as well as from the drift due to the missing constraints (1e) and (3a) in the d-index 1 formulation (rcd0) (5) which leads to up to quadratic drift from the constraints of position level (1e) and linear drift from the constraints of velocity level (3a), as illustrated in Figure 5. Similar results for DASPK(ggl1) and DASSL(ggl1) as well as for DASPK(rcd0) and MEBDF(rcd0) are obtained. The best accuracy for the prescribed tolerance is obtained by the usage of the solvers GEOMS(ovd0) and QUALIDAES(ovd0) and also for QUALIDAES(rcd0) and RADAU5(rcd0).
In Figure 5 we have illustrated the absolute residuals of the constraints, including the hidden constraints, as well as the energy conserving constraint for a selection of the numerical results. The numerical solutions

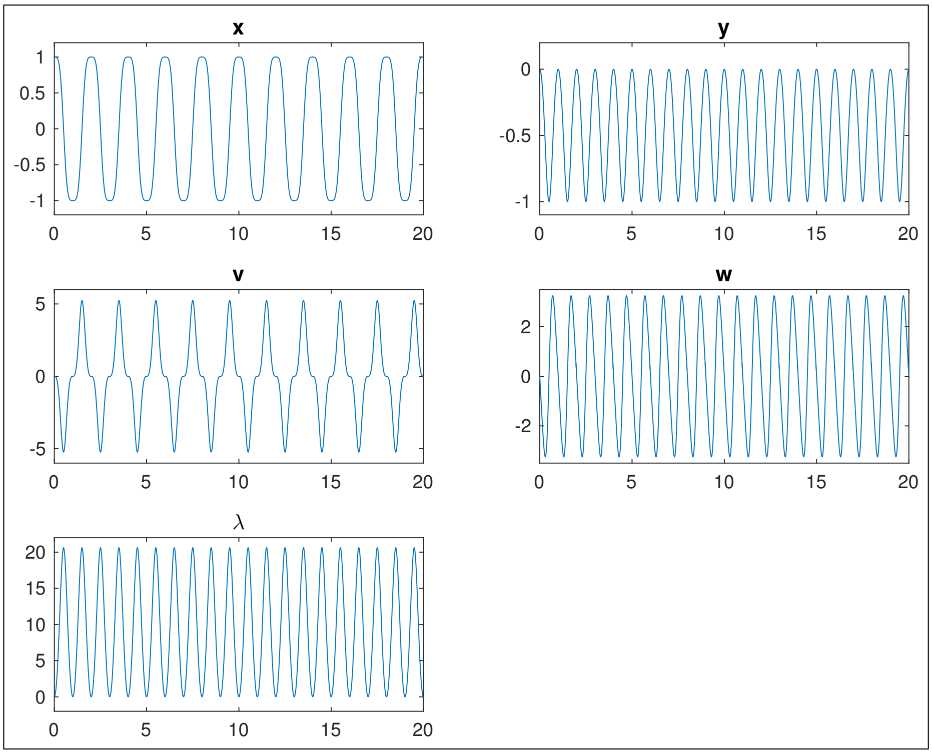

Figure 2: Scenario 01: Reference solution

	ori2	rcd1	rcd0	psi1	psi0	ggl1	ovd1	ovd0
DASPK	o[1]	o[1]	X	x[1]	X	o[1]	-[4]	-[4]
DASSL	o[1]	o[1]	X	x[1]	X	o[1]	-[4]	-[4]
GEOMS	-[5]	-[5]	-[5]	-[5]	-[5]	-[5]	X	X
MEBDF	X	X	X	-[6]	-[6]	X	-[4]	-[4]
ODASSL	o[1]	x[1]	X	x[1]	X	x[1]	x[1]	X
OVDBDF	o[1]	o[1]	X	o[1]	X	o[1]	o[1]	X
QUALIDAES	o[2]	x	X	X	X	X	X	X
RADAU5	x	X	X	-[6]	-[6]	X	-[4]	-[4]

'X' successful for every prescribed tolerance
'x' successful for some/few prescribed tolerances
'o' not successful for every prescribed tolerance
'-' formulation does not satisfy the structural requirements of the solver

[1] not suitable for DAEs consisting hidden constraints (c-level>0)
[2] not suitable for DAEs consisting hidden constraints of higher level than 1 (c-level>1)
[4] not suitable for overdetermined DAEs
[5] GEOMS is only suited for MBS structure including at least hidden constraints on velocity level
[6] the leading matrix of a quasi-linear DAE is required to be constant

Table 5: Scenario 01: Used solver-formulation combinations and an overview of the success

show the behavior depending on the used formulations as expected in the regulatrizations, see Section 2.1.3. So the constraint on position level is mainly violated with a large deviation from DASSL(rcd0), DASPK(rcd0), and MEBDF(rcd0) and a medium deviation from QUALIDAES(rcd0) and RADAU5(rcd0). The other violation of the constraints of position level for the other solver-formulation combinations fits into the prescribed tolerance of 10^{-7}. The constraints on velocity level are only significantly violated for DASSL(rcd0), DASPK(rcd0), and MEBDF(rcd0). The constraint on acceleration level only for the usage of (ggl1) and (ovd1) are violated significantly due to its c-level 1 and the existence of the constraint on acceleration as hidden constraints. The energy conservation is obtained very good for the numerical results obtained with GEOMS, QUALIDAES, and for the solver-formulation combination RADAU5(rcd0).
Details in the efficiency are listed in Table 6 for all successful computations and illustrated in Figure 6 for a selection of the numerical results. In particular, RADAU5(rcd0) offers the best efficiency for this scenario, in spite of the usage of the index-reduced formulation (rcd0), where the constraints on position level and on velocity level are lost. Furthermore, a very good performance is offered from QUALIDAES(rcd0) and QUALIDAES(ovd0) followed by ODASSL(psi0) while DASSL(rcd0), DASPK(rcd0), GEOMS(ovd0), MEBDF(rcd0), ODASSL(ovd0), and OVDBDF(ovd0) offer a good performance. The efficiency of QUALIDAES(ggl1) and

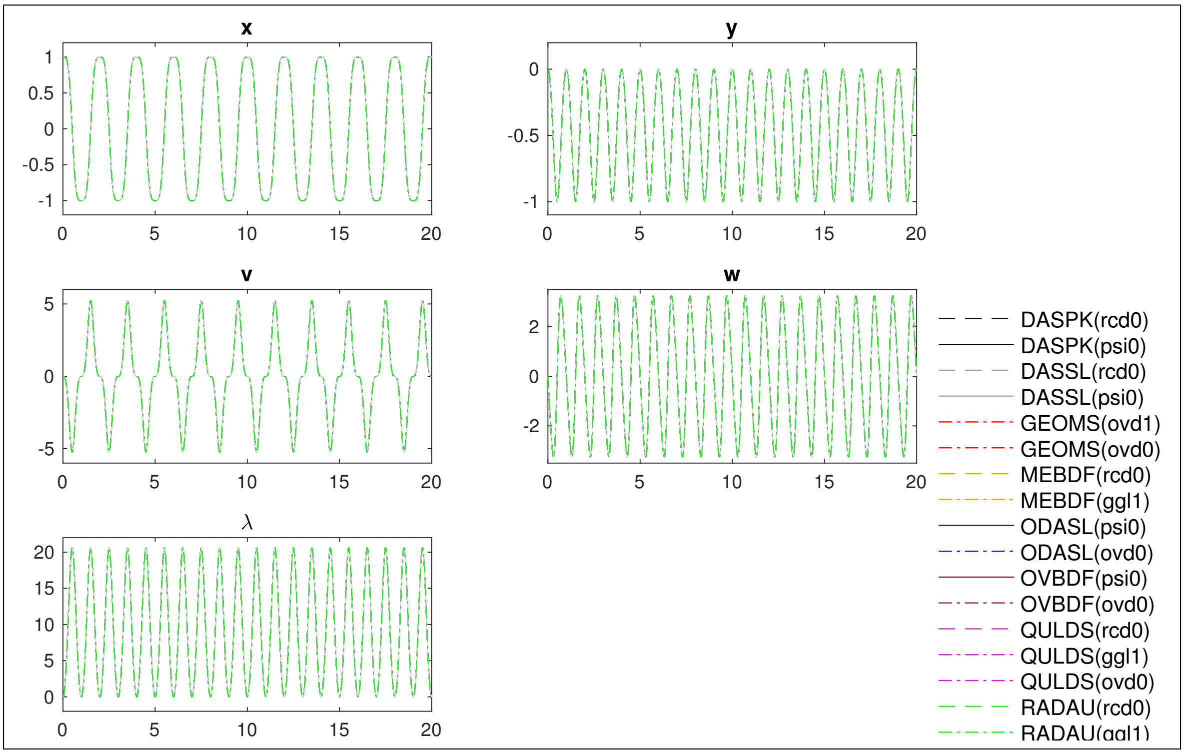

Figure 3: Scenario 01: Numerical solutions for a prescribed tolerance of RTOL=ATOL=10^{-7}

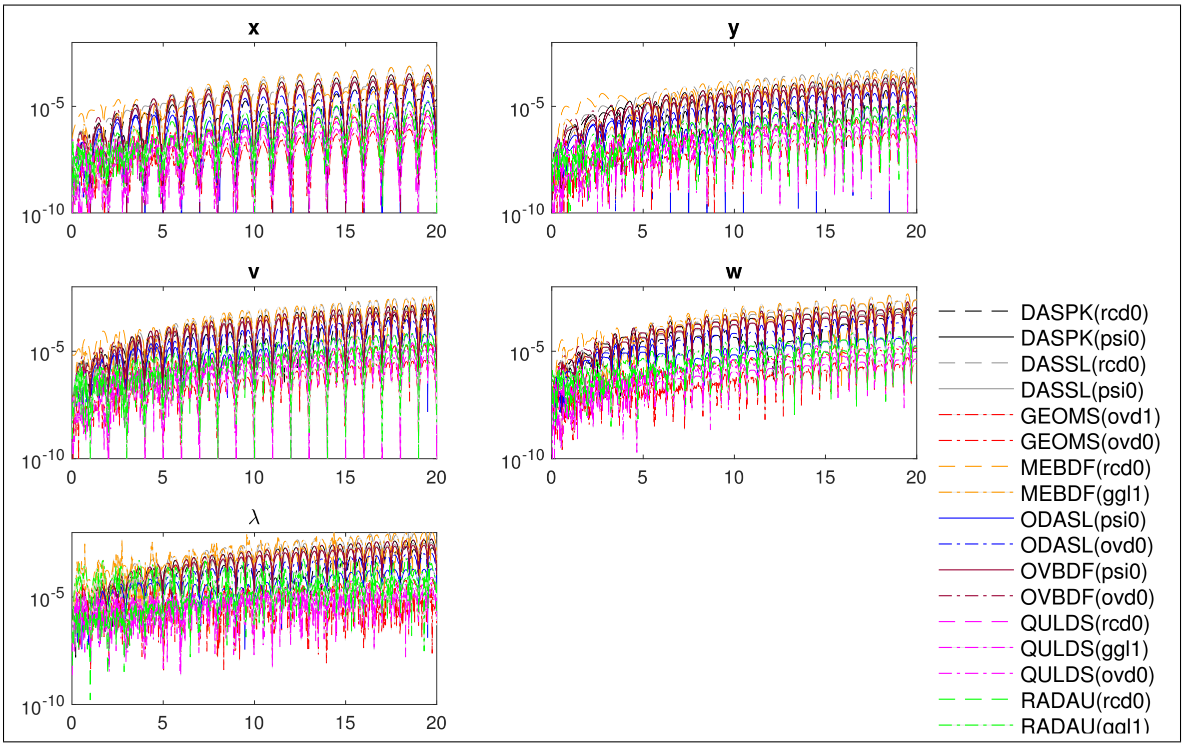

Figure 4: Scenario 01: Numerical error for a prescribed tolerance of RTOL=ATOL=10^{-7}

RADAU5(ggl1) is reduced due to the GGL formulation which is increased in its size and the efficiency of GEOMS(ovd1) is reduced due to the existence of hidden constraints in the formulation (ovd1). Nevertheless, the maximally obtained precision is excellent for the solvers GEOMS and QUALIDAES, and for the solver-formulation combination RADAU5(rcd0). For quantitative details in the efficiency, see Table 6.

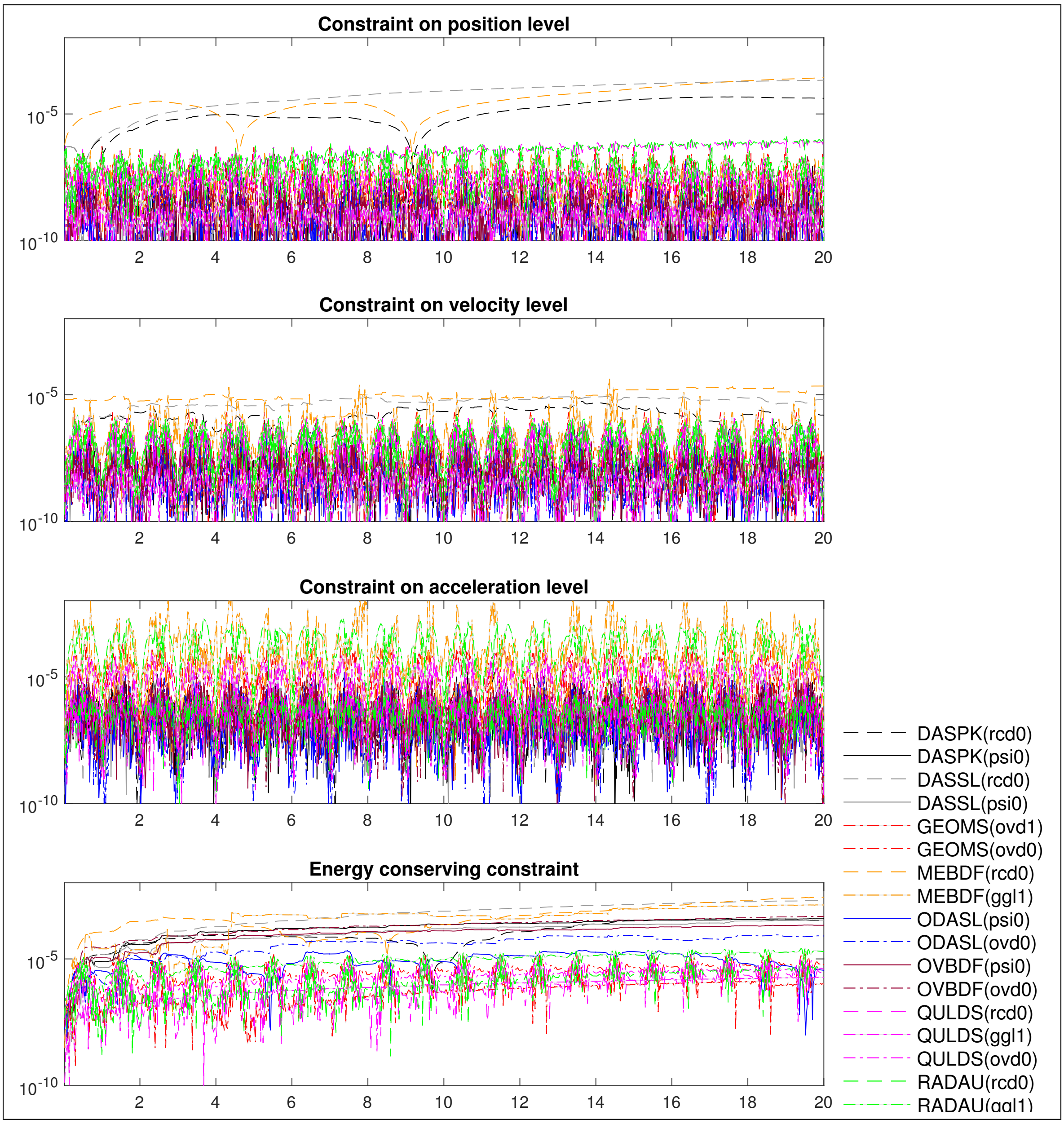

Figure 5: Scenario 01: Residuum of the constraints for a prescribed tolerance of RTOL=ATOL=10^{-7}

	Tol	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}	10^{-11}	10^{-12}
DASPK(rcd0)	Tsim	1.2e-02	1.6e-02	1.6e-02	2.0e-02	2.4e-02	3.2e-02	3.6e-02	5.2e-02
	ERR	5.4e-01	1.2e-02	2.8e-03	3.1e-03	6.6e-05	1.0e-05	3.2e-06	5.7e-07
DASPK(psi1)	Tsim	3.7e+00	-	-	-	-	-	-	-
	ERR	6.5e+00	-	-	-	-	-	-	-
DASPK(psi0)	Tsim	1.6e-02	2.0e-02	2.4e-02	3.2e-02	3.6e-02	4.4e-02	5.6e-02	8.0e-02
	ERR	2.9e-01	6.1e-02	7.7e-03	8.4e-04	8.1e-05	1.6e-06	3.3e-07	5.6e-08
DASSL(rcd0)	Tsim	1.2e-02	1.6e-02	2.0e-02	2.0e-02	2.8e-02	3.2e-02	4.4e-02	5.6e-02
	ERR	4.5e-01	3.9e-02	1.7e-02	8.6e-04	3.6e-05	4.3e-06	4.5e-06	8.5e-07
DASSL(psi1)	Tsim	3.9e+00	-	-	-	-	-	-	-
	ERR	6.6e+00	-	-	-	-	-	-	-
DASSL(psi0)	Tsim	1.6e-02	2.0e-02	2.4e-02	3.2e-02	4.0e-02	4.8e-02	6.4e-02	8.0e-02
	ERR	3.5e-01	2.4e-02	5.1e-03	8.4e-04	7.6e-05	6.9e-06	2.4e-07	3.8e-08
GEOMS(ovd1)	Tsim	2.4e-02	3.6e-02	4.8e-02	7.2e-02	1.3e-01	1.9e-01	3.4e-01	5.7e-01
	ERR	2.5e-03	3.6e-04	6.7e-05	1.4e-05	2.6e-06	7.4e-07	1.2e-07	2.3e-08
GEOMS(ovd0)	Tsim	2.0e-02	2.4e-02	3.2e-02	4.0e-02	5.2e-02	6.8e-02	1.0e-01	1.4e-01
	ERR	3.4e-03	7.4e-04	1.1e-04	1.2e-05	1.7e-06	2.5e-07	4.7e-08	9.3e-09
MEBDF(ori2)	Tsim	2.4e-02	2.4e-02	2.8e-02	2.8e-02	3.6e-02	4.0e-02	5.6e-02	6.0e-02
	ERR	8.9e-01	6.5e-02	2.6e-02	8.9e-03	9.3e-04	1.4e-04	2.1e-05	1.2e-05
MEBDF(rcd1)	Tsim	2.4e-02	2.4e-02	2.8e-02	3.2e-02	3.6e-02	4.4e-02	4.8e-02	6.0e-02
	ERR	2.3e+00	1.7e-01	6.7e-02	1.1e-02	1.5e-03	9.1e-05	2.0e-05	1.7e-06
MEBDF(rcd0)	Tsim	1.6e-02	2.0e-02	2.0e-02	2.4e-02	2.8e-02	2.8e-02	3.6e-02	3.6e-02
	ERR	1.2e+00	3.3e-02	6.6e-03	9.1e-03	5.9e-04	1.1e-04	3.3e-05	3.1e-06
MEBDF(ggl1)	Tsim	2.4e-02	2.8e-02	3.2e-02	3.6e-02	4.4e-02	4.8e-02	6.0e-02	6.8e-02
	ERR	1.0e-01	2.9e-02	1.7e-02	3.7e-04	1.5e-04	2.0e-05	3.0e-06	3.5e-07
ODASSL(rcd1)	Tsim	4.5e-01	-	-	-	-	-	-	-
	ERR	1.6e+00	-	-	-	-	-	-	-
ODASSL(rcd0)	Tsim	8.0e-03	1.2e-02	1.6e-02	1.6e-02	2.4e-02	3.6e-02	4.4e-02	6.0e-02
	ERR	9.8e-01	7.3e-02	9.7e-03	9.5e-04	1.5e-04	4.3e-06	1.2e-06	1.1e-07
ODASSL(psi1)	Tsim	7.4e-01	-	-	-	-	-	-	-
	ERR	1.2e+00	-	-	-	-	-	-	-
ODASSL(psi0)	Tsim	1.2e-02	1.6e-02	2.0e-02	2.4e-02	2.8e-02	3.6e-02	4.8e-02	6.8e-02
	ERR	4.0e-02	7.7e-03	3.5e-04	2.0e-05	8.7e-06	7.8e-07	3.4e-07	8.0e-08
ODASSL(ggl1)	Tsim	3.1e+00	-	-	-	-	-	-	-
	ERR	2.9e+00	-	-	-	-	-	-	-
ODASSL(ovd1)	Tsim	5.3e-01	-	-	-	-	-	-	-
	ERR	1.5e+00	-	-	-	-	-	-	-
ODASSL(ovd0)	Tsim	1.6e-02	2.0e-02	2.8e-02	3.2e-02	4.0e-02	5.2e-02	6.4e-02	9.6e-02
	ERR	1.2e-01	5.9e-03	1.8e-03	2.2e-04	1.7e-05	5.9e-07	3.3e-08	4.8e-08
OVDBDF(rcd0)	Tsim	1.2e-02	1.6e-02	1.6e-02	2.0e-02	2.4e-02	3.2e-02	4.0e-02	5.2e-02
	ERR	8.0e-01	2.2e-02	1.4e-02	4.0e-04	4.9e-04	5.3e-06	4.8e-06	4.9e-07
OVDBDF(psi0)	Tsim	1.6e-02	2.0e-02	2.4e-02	3.2e-02	4.0e-02	4.8e-02	6.4e-02	8.8e-02
	ERR	2.0e-01	2.6e-02	4.4e-03	3.9e-04	6.0e-05	4.0e-06	2.1e-07	1.8e-08
OVDBDF(ovd0)	Tsim	1.2e-02	1.6e-02	1.6e-02	2.4e-02	2.4e-02	3.6e-02	4.4e-02	5.2e-02
	ERR	3.2e-01	4.7e-02	7.8e-03	1.0e-03	7.0e-05	4.2e-06	6.6e-07	3.9e-08
QUALIDAES(rcd1)	Tsim	1.6e-02	2.4e-02	4.0e-02	7.2e-02	1.5e-01	-	-	-
	ERR	2.0e-03	3.1e-04	5.2e-05	9.1e-06	2.6e-06	-	-	-
QUALIDAES(rcd0)	Tsim	1.2e-02	1.6e-02	2.0e-02	2.4e-02	3.2e-02	4.0e-02	5.2e-02	6.8e-02
	ERR	1.3e-03	5.3e-04	1.3e-04	1.8e-05	2.6e-06	4.3e-07	5.7e-08	9.0e-09
QUALIDAES(psi1)	Tsim	2.4e-02	3.2e-02	4.0e-02	5.6e-02	8.4e-02	1.3e-01	2.0e-01	3.2e-01
	ERR	1.2e-03	2.4e-04	4.1e-05	9.3e-06	1.7e-06	4.3e-07	8.7e-08	2.1e-08
QUALIDAES(psi0)	Tsim	1.6e-02	1.6e-02	2.4e-02	2.8e-02	3.2e-02	4.8e-02	6.4e-02	8.4e-02
	ERR	2.0e-02	2.1e-03	2.5e-04	3.9e-05	5.2e-06	9.1e-07	1.4e-07	2.4e-08
QUALIDAES(ggl1)	Tsim	2.0e-02	2.8e-02	4.4e-02	6.4e-02	1.0e-01	1.6e-01	2.5e-01	4.0e-01
	ERR	2.6e-03	3.9e-04	3.9e-05	6.0e-06	1.1e-06	2.3e-07	5.2e-08	1.1e-08
QUALIDAES(ovd1)	Tsim	2.0e-02	2.8e-02	3.2e-02	4.8e-02	7.6e-02	1.0e-01	1.7e-01	2.7e-01
	ERR	3.2e-03	3.3e-04	4.7e-05	8.3e-06	1.9e-06	4.5e-07	8.3e-08	2.0e-08
QUALIDAES(ovd0)	Tsim	1.2e-02	1.6e-02	2.0e-02	2.4e-02	3.6e-02	4.4e-02	6.0e-02	8.4e-02
	ERR	3.7e-03	5.1e-04	7.0e-05	1.1e-05	1.6e-06	2.2e-07	3.9e-08	7.1e-09
RADAU5(ori2)	Tsim	1.6e-02	2.4e-02	3.2e-02	4.4e-02	6.8e-02	1.0e-01	1.6e-01	-
	ERR	3.9e-02	1.5e-02	5.4e-03	2.0e-03	6.8e-04	2.7e-04	9.6e-05	-
RADAU5(rcd1)	Tsim	1.2e-02	1.2e-02	1.6e-02	2.0e-02	2.4e-02	3.2e-02	4.8e-02	6.0e-02
	ERR	8.5e-03	1.8e-03	8.1e-04	2.1e-04	6.4e-05	2.0e-05	6.9e-06	2.0e-06
RADAU5(rcd0)	Tsim	1.2e-02	1.2e-02	1.6e-02	2.0e-02	2.4e-02	3.6e-02	4.4e-02	6.0e-02
	ERR	2.0e-03	7.5e-04	1.2e-04	1.9e-05	2.3e-06	3.3e-07	4.3e-08	7.1e-09
RADAU5(ggl1)	Tsim	1.2e-02	1.6e-02	1.6e-02	2.4e-02	2.8e-02	4.0e-02	5.6e-02	7.6e-02
	ERR	1.4e-02	2.7e-03	7.2e-04	2.1e-04	7.1e-05	2.1e-05	7.0e-06	2.0e-06

Tsim - Simulation time in seconds, ERR - error w.r.t. reference solution, '-' numerical integration was not successful

Table 6: Scenario 01: Efficiency

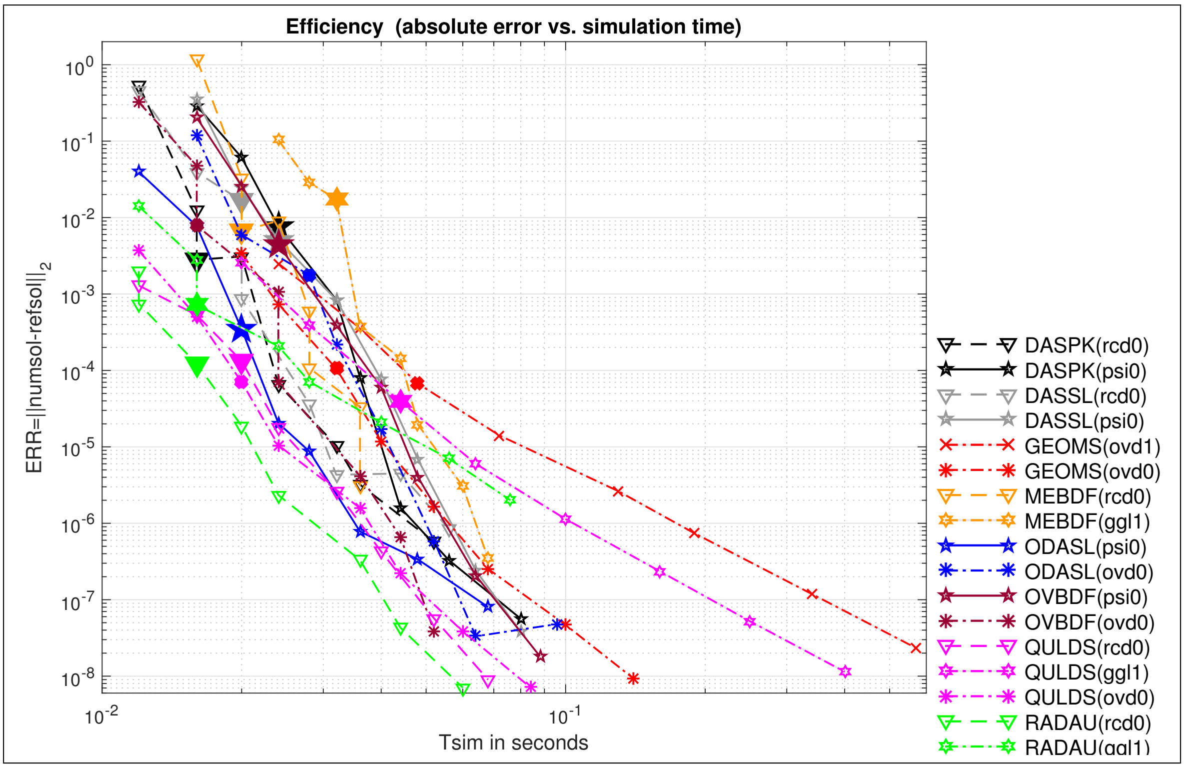

Figure 6: Scenario 01: Efficiency

2.2.2 Scenario 02

This Scenario 02 is the same as Scenario 01 except the time domain is extended to $\mathbb{I} = [0\text{s}, 2000\text{s}]$. Therefore, we have the equations of motion given in (1), the parameters as depicted in Table 3, and the initial values (11). Let us note again that we did modify the gravitational acceleration to $\mathfrak{g} = 13.7503716373294544\text{m/s}^2$ such that the exact solution has a period of 2s which allows the comparison of the accuracy every period.

Analytical Solution With the choosen gravitational acceleration $\mathfrak{g} = 13.7503716373294544\text{m/s}^2$ we know the analytical solution after every period, i.e., for all $t = i \cdot 2\text{s},\ i \in \mathbb{N}$ as

$$\begin{array}{rclrclrcl} x(t) & = & x_0, & v(t) & = & v_0, & \lambda(t) & = & \lambda_0, \\ y(t) & = & y_0, & w(t) & = & w_0, & & & \text{for all } t = i \cdot 2\text{s},\ i \in \mathbb{N}. \end{array}$$

So we use as reference solution the values of the exact solution on the time points $t_i = i \cdot 2\text{s}$ for i=0,...1000 for comparisons.

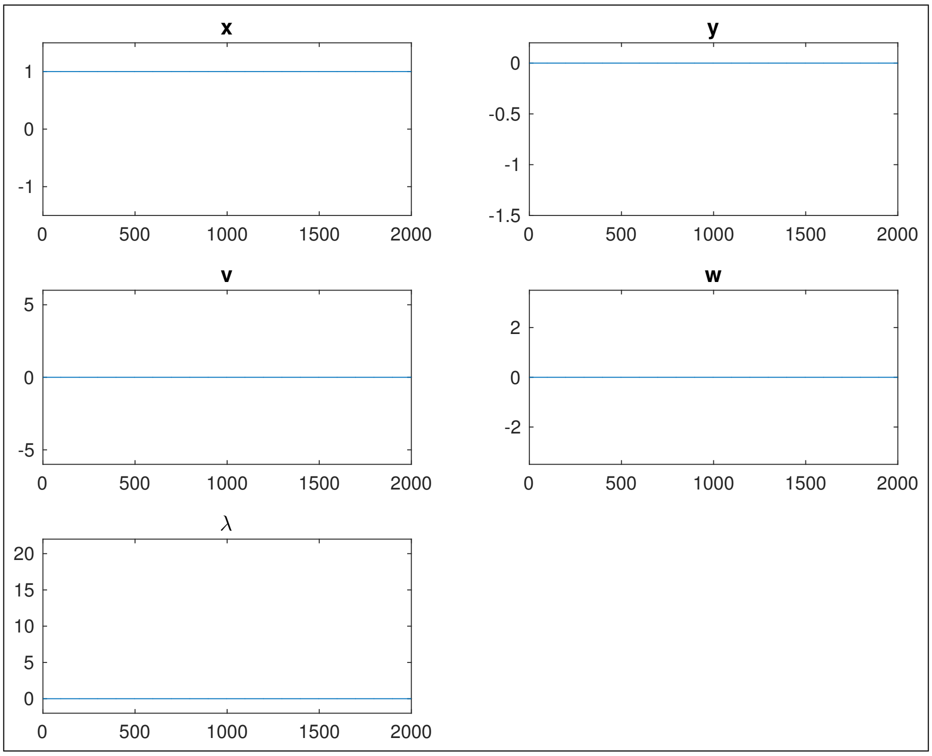

Figure 7: Scenario 02: Analytical solution

In Figure 7 the analytical solution for $t = 2i,\ i \in \{0, 1, ..., 1000\}$ is illustrated. In this figure only the positions after every period are plotted such that the curves are illustrated to be constant. Furthermore, in Figure 8 the analytical solution is illustrated for the first 10 periods, i.e., in $\mathbb{I} = [0\text{s}, 20\text{s}]$. In Table 7 the values of the analytical solution at the final time $t_f = 2000\text{s}$ are listed.

$x(t_f) =$	1.0E+00	$v(t_f) =$	0.0E+00	$\lambda(t_f) =$	0.0E+00
$y(t_f) =$	0.0E+00	$w(t_f) =$	0.0E+00		

Table 7: Scenario 02: Analytical solution at the final time point $t_f = 2000\text{s}$.

Numerical Solution The used solver-formulation combinations and an overview of the success is illustrated in Table 8. For the numerical computations the tolerances `RTOL`=`ATOL`=10^{-i}, $i = 5, ..., 12$ are prescribed uniformly for all components of the state variables. Selected driver subroutines for the used solver-formulation combinations are available on the webpage
`http://www3.math.tu-berlin.de/multiphysics/Examples/M001_SimplePendulum/`.

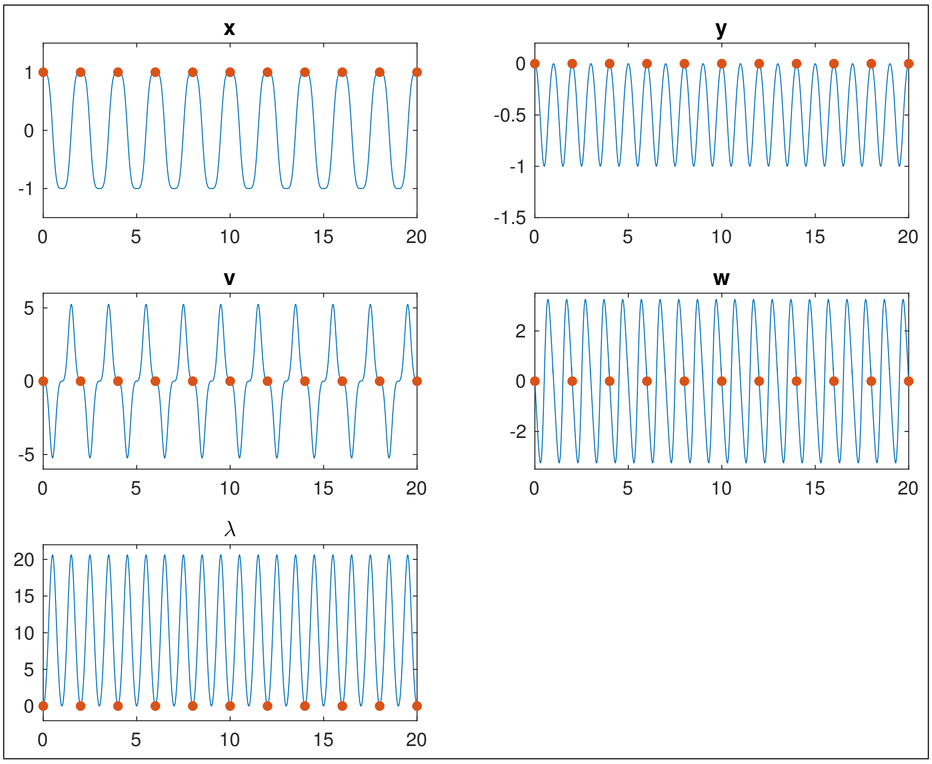

Figure 8: Scenario 02: Analytical solution for the first ten periods only, i.e., $\mathbb{I} = [0\text{s}, 20\text{s}]$

	ori2	rcd1	rcd0	psi1	psi0	ggl1	ovd1	ovd0
`DASPK`	o[1]	o[1]	x	o[1]	x	o[1]	-[4]	-[4]
`DASSL`	o[1]	o[1]	x	o[1]	x	o[1]	-[4]	-[4]
`GEOMS`	-[5]	-[5]	-[5]	-[5]	-[5]	-[5]	X	X
`MEBDF`	o	o	x	-[6]	-[6]	o	-[4]	-[4]
`ODASSL`	o[1]	o[1]	x	o[1]	X	o[1]	o[1]	X
`OVDBDF`	o[1]	o[1]	x	o[1]	x	o[1]	o[1]	X
`QUALIDAES`	o[2]	x	X	X	X	X	X	X
`RADAU5`	x	X	X	-[6]	-[6]	X	-[4]	-[4]

'X' successful for every prescribed tolerance
'x' successful for some/few prescribed tolerances
'o' not successful for every prescribed tolerance
'-' formulation does not satisfy the structural requirements of the solver

[1] not suitable for DAEs consisting hidden constraints (c-level>0)
[2] not suitable for DAEs consisting hidden constraints of higher level than 1 (c-level>1)
[4] not suitable for overdetermined DAEs
[5] `GEOMS` is only suited for MBS structure including at least hidden constraints on velocity level
[6] the leading matrix of a quasi-linear DAE is required to be constant

Table 8: Scenario 02: Used solver-formulation combinations and an overview of the success

In Figure 9 we have illustrated the solution of the numerical integration by use of a selection of solver-formulation combinations with a prescribed tolerance `RTOL`=`ATOL`=10^{-7}.
Furthermore, in Figure 10 the obtained error of these numerical solutions with a prescribed tolerance `RTOL`=`ATOL`=10^{-7} is illustrated in logarithmic style.
The largest deviation show the solutions obtained with solvers based on BDF methods, i.e., `DASPK`, `DASSL`, `MEBDF`, and `OVDBDF`, but except `ODASSL`. The numerical solution obtained with solvers based on Runge-Kutta methods, i.e., `GEOMS`, `QUALIDAES`, and `RADAU5` and in addition `ODASSL` offer a good precision in its numerical solutions.
In Figure 11 we have illustrated the absolute residuals of the constraints, including the hidden constraints, as well as the energy conserving constraint for a selection of the numerical results. The numerical solutions show the behavior depending on the used formulations as expected in the regulatrizations, see Section 2.1.3. So the d-index 1 formulation (rcd0) (5) offers a quadratic drift from the constraints of position level and a linear drift from the constraints of velocity level. Note that the drift obtained with BDF methods (`DASPK`, `DASSL`, `MEBDF`) for (rcd0) (5) is larger than the drift obtained with Runge-Kutta methods (`QUALIDAES`, `RADAU5`). The energy conservation is unacceptable for the numerical results

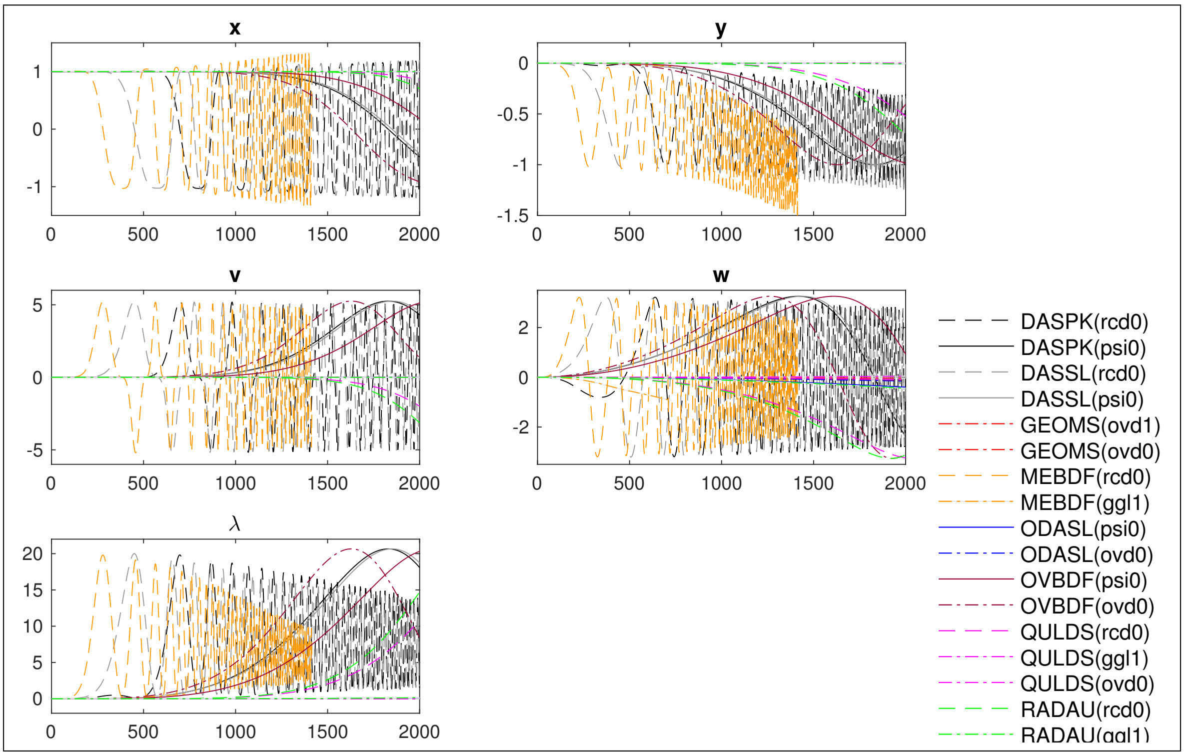

Figure 9: Scenario 02: Numerical solutions for a prescribed tolerance of RTOL=ATOL=10^{-7} (The solution is plotted every 2s only.)

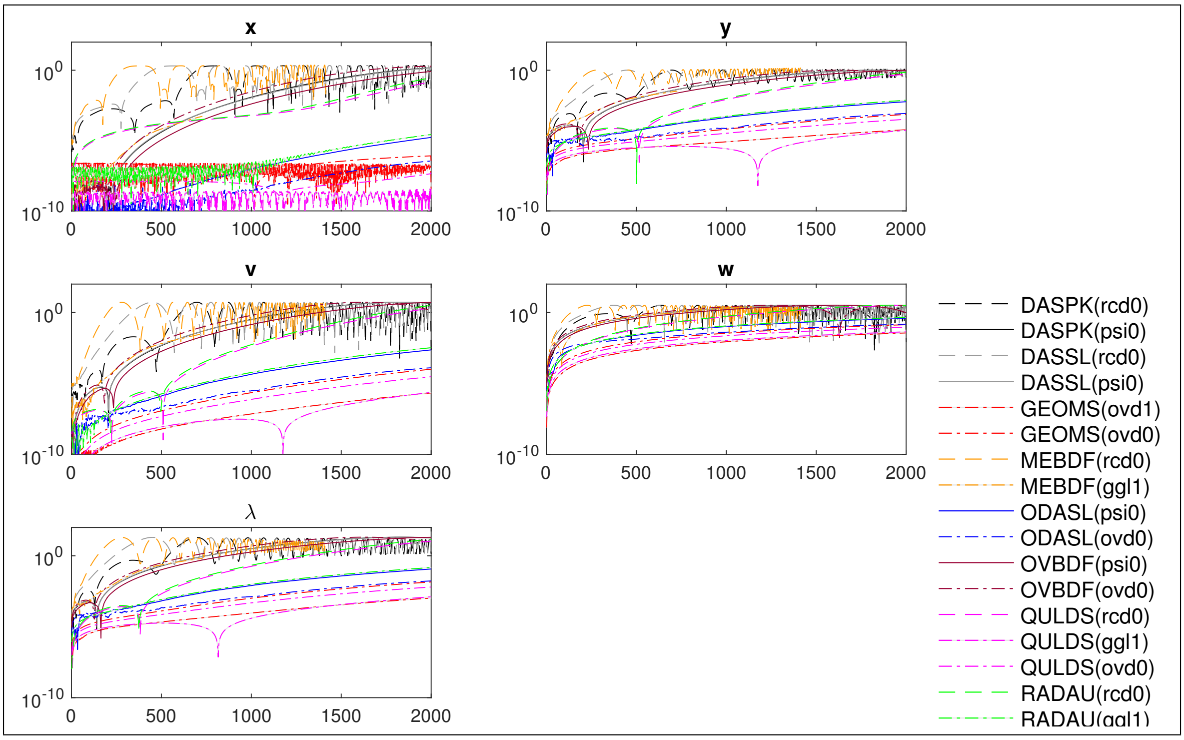

Figure 10: Scenario 02: Numerical error for a prescribed tolerance of RTOL=ATOL=10^{-7} (The error is plotted every 2s only.)

obtained from the d-index 1 formulation (rcd0) (5). The energy conservation is more precise for the usage of the projected strangeness-free formulation (psi0) (10) even for BDF methods while the energy is good preserved for the usage of solvers based on Runge-Kutta methods as well as for ODASSL. In particular, the

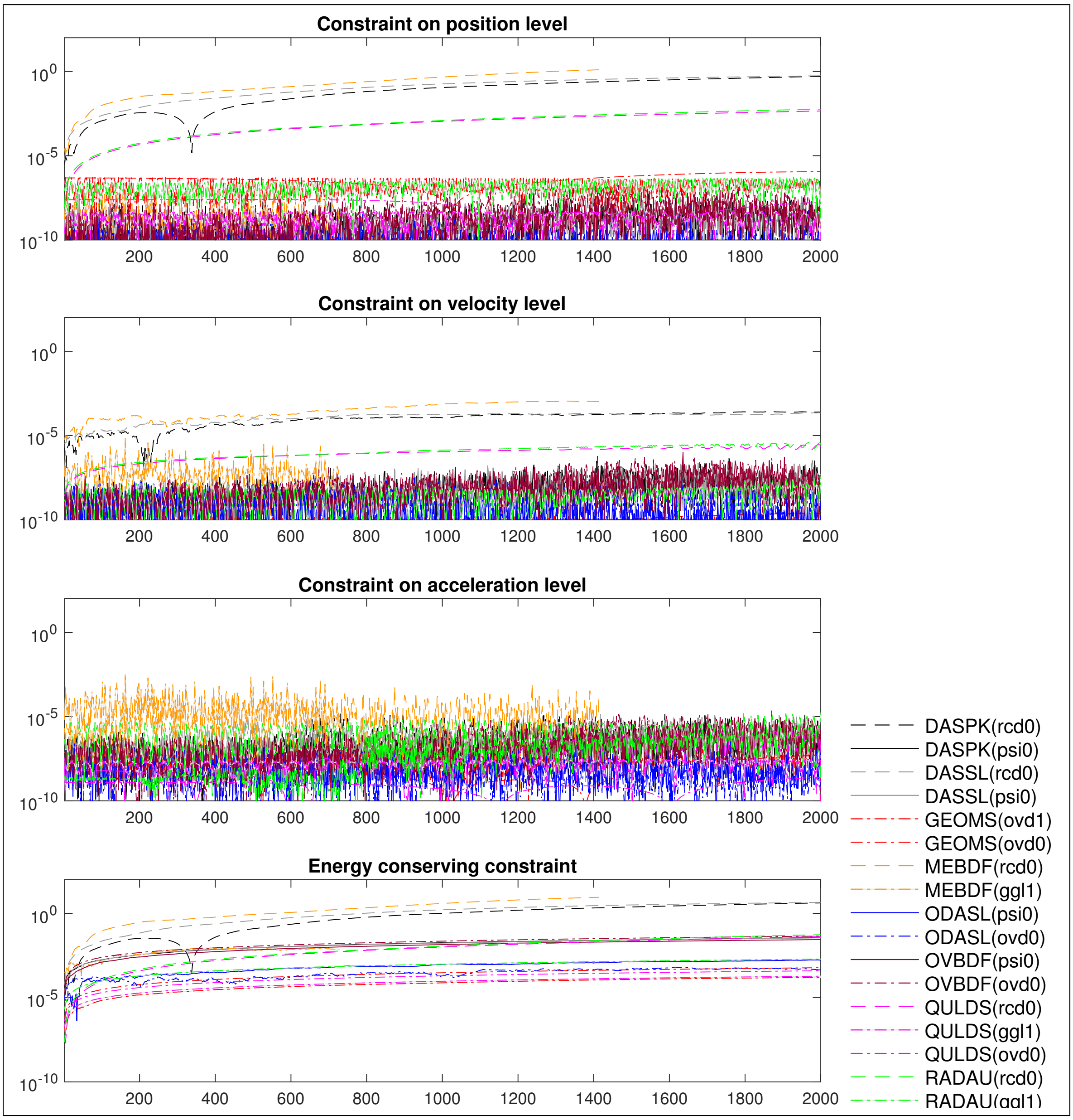

Figure 11: Scenario 02: Residuum of the constraints for a prescribed tolerance of RTOL=ATOL=10^{-7} (The residuum is plotted every 2s only.)

numerical results obtained with the GGL-Formulation (ggl1) and the overdetermined formulation (ovd0) offer a good energy conservation.
Details in the efficiency are listed in Table 9 for all successful computations and illustrated in Figure 12 for a selection of the numerical results. For this scenario the numerical solutions from `QUALIDAES` with the overdetermined c-level 0 formulation (ovd0) (7) together with `ODASSL` with the projected s-index 0 formulation (psi0) (10) offer the best efficiency. The efficiency of `RADAU5` is also very good, while the most precise results are `GEOMS`(ovd1), `ODASSL`(psi0), and `QUALIDAES`(ggl1). The codes based on BDF methods are almost not able to solve this problem, except `ODASSL`.

	Tol	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}	10^{-11}	10^{-12}
DASPK(rcd0)	Tsim	1.7e-01	4.3e-01	8.5e-01	1.2e+00	1.6e+00	-	-	-
	ERR	2.9e+02	3.2e+02	4.2e+02	4.6e+02	3.9e+02	-	-	-
DASPK(psi0)	Tsim	7.8e-01	1.1e+00	1.6e+00	2.2e+00	-	-	-	-
	ERR	5.6e+02	5.3e+02	4.9e+02	1.9e+01	-	-	-	-
DASSL(rcd0)	Tsim	1.8e-01	5.0e-01	9.0e-01	1.3e+00	1.8e+00	-	-	-
	ERR	3.1e+02	3.2e+02	4.6e+02	4.5e+02	4.1e+02	-	-	-
DASSL(psi0)	Tsim	8.4e-01	1.2e+00	1.8e+00	2.4e+00	-	-	-	-
	ERR	5.6e+02	5.3e+02	4.8e+02	1.8e+01	-	-	-	-
GEOMS(ovd1)	Tsim	2.0e+00	2.9e+00	4.0e+00	6.3e+00	1.1e+01	1.8e+01	3.3e+01	5.6e+01
	ERR	1.2e+02	2.6e-01	7.1e-01	8.1e-02	1.9e-02	9.7e-04	2.3e-04	5.8e-05
GEOMS(ovd0)	Tsim	1.2e+00	1.6e+00	2.2e+00	3.0e+00	4.3e+00	6.2e+00	9.0e+00	1.3e+01
	ERR	2.3e+02	2.9e+01	2.8e+00	2.9e-01	4.2e-02	4.7e-03	5.8e-04	1.3e-04
MEBDF(rcd0)	Tsim	1.6e-01	2.9e-01	-	-	-	-	-	-
	ERR	2.8e+02	2.6e+02	-	-	-	-	-	-
ODASSL(rcd0)	Tsim	-	-	9.4e-01	1.1e+00	1.6e+00	2.9e+00	3.5e+00	5.5e+00
	ERR	-	-	7.4e+02	4.9e+02	3.5e+02	5.0e+00	1.3e+00	6.8e-02
ODASSL(psi0)	Tsim	6.4e-01	8.4e-01	1.1e+00	1.5e+00	2.1e+00	2.9e+00	4.0e+00	5.7e+00
	ERR	5.4e+02	4.2e+01	8.1e+00	1.5e-01	2.1e-01	1.4e-02	2.3e-03	4.4e-05
ODASSL(ovd0)	Tsim	9.2e-01	1.3e+00	1.7e+00	2.4e+00	3.2e+00	4.3e+00	6.0e+00	8.5e+00
	ERR	5.5e+02	2.8e+02	3.1e+00	3.7e+00	1.9e-01	1.4e-03	1.9e-03	1.4e-03
OVDBDF(rcd0)	Tsim	2.0e-01	5.4e-01	1.0e+00	1.3e+00	1.7e+00	-	-	-
	ERR	2.8e+02	3.5e+02	5.7e+02	5.3e+02	4.3e+02	-	-	-
OVDBDF(psi0)	Tsim	8.4e-01	1.2e+00	1.7e+00	2.4e+00	-	-	-	-
	ERR	5.5e+02	5.2e+02	3.9e+02	1.2e+01	-	-	-	-
OVDBDF(ovd0)	Tsim	4.7e-01	6.7e-01	1.0e+00	1.5e+00	1.9e+00	2.5e+00	3.5e+00	4.5e+00
	ERR	5.7e+02	5.3e+02	5.1e+02	3.7e+01	2.4e+00	1.5e-01	2.1e-02	1.2e-03
QUALIDAES(rcd1)	Tsim	9.2e-01	1.5e+00	3.3e+00	5.4e+00	-	-	-	-
	ERR	8.6e+01	5.7e+00	5.5e-01	4.1e-02	-	-	-	-
QUALIDAES(rcd0)	Tsim	5.1e-01	7.2e-01	1.0e+00	1.5e+00	2.2e+00	3.2e+00	4.2e+00	5.7e+00
	ERR	4.2e+02	4.1e+02	1.5e+02	8.8e+00	9.2e-01	1.8e-01	2.2e-02	3.9e-03
QUALIDAES(psi1)	Tsim	1.5e+00	2.1e+00	3.1e+00	4.8e+00	7.7e+00	1.2e+01	2.0e+01	3.2e+01
	ERR	3.3e+01	2.8e+00	6.0e-02	2.2e-02	1.2e-02	1.5e-03	2.7e-04	6.1e-05
QUALIDAES(psi0)	Tsim	6.8e-01	9.6e-01	1.3e+00	1.9e+00	2.6e+00	3.8e+00	5.5e+00	7.9e+00
	ERR	5.0e+02	1.1e+02	6.4e+00	9.8e-01	1.2e-01	2.2e-02	3.2e-03	5.6e-04
QUALIDAES(ggl1)	Tsim	1.2e+00	2.0e+00	3.3e+00	5.5e+00	9.1e+00	1.5e+01	2.4e+01	3.9e+01
	ERR	1.4e+02	1.1e+01	8.6e-01	7.7e-02	6.6e-03	5.4e-04	1.7e-05	2.7e-05
QUALIDAES(ovd1)	Tsim	1.0e+00	1.5e+00	2.3e+00	3.8e+00	6.5e+00	9.6e+00	1.6e+01	2.6e+01
	ERR	2.0e+02	6.0e+00	3.2e-01	2.0e-02	1.6e-02	1.2e-03	2.0e-04	6.9e-05
QUALIDAES(ovd0)	Tsim	6.1e-01	8.4e-01	1.2e+00	1.7e+00	2.4e+00	3.5e+00	5.1e+00	7.5e+00
	ERR	2.1e+02	1.4e+01	1.8e+00	2.9e-01	3.8e-02	5.3e-03	6.5e-04	1.1e-04
RADAU5(ori2)	Tsim	1.2e+00	1.6e+00	2.4e+00	3.7e+00	5.9e+00	9.4e+00	-	-
	ERR	4.5e+02	3.6e+02	1.6e+01	9.6e-01	8.3e-02	5.1e-03	-	-
RADAU5(rcd1)	Tsim	4.3e-01	5.8e-01	8.0e-01	1.1e+00	1.6e+00	2.4e+00	3.5e+00	5.1e+00
	ERR	4.6e+02	2.1e+01	3.8e+00	2.7e-01	7.1e-02	1.5e-02	3.5e-03	5.5e-04
RADAU5(rcd0)	Tsim	4.4e-01	6.1e-01	8.7e-01	1.2e+00	1.8e+00	2.6e+00	3.7e+00	5.3e+00
	ERR	5.7e+02	4.3e+02	2.0e+02	1.9e+01	8.8e-01	1.1e-01	8.0e-03	2.3e-03
RADAU5(ggl1)	Tsim	5.8e-01	7.5e-01	1.0e+00	1.5e+00	2.2e+00	3.2e+00	4.7e+00	6.9e+00
	ERR	4.7e+02	7.9e+01	9.2e+00	1.1e+00	1.5e-01	2.3e-02	3.4e-03	5.2e-04

Tsim - Simulation time in seconds, ERR - error w.r.t. reference solution, '-' numerical integration was not successful

Table 9: Scenario 02: Efficiency

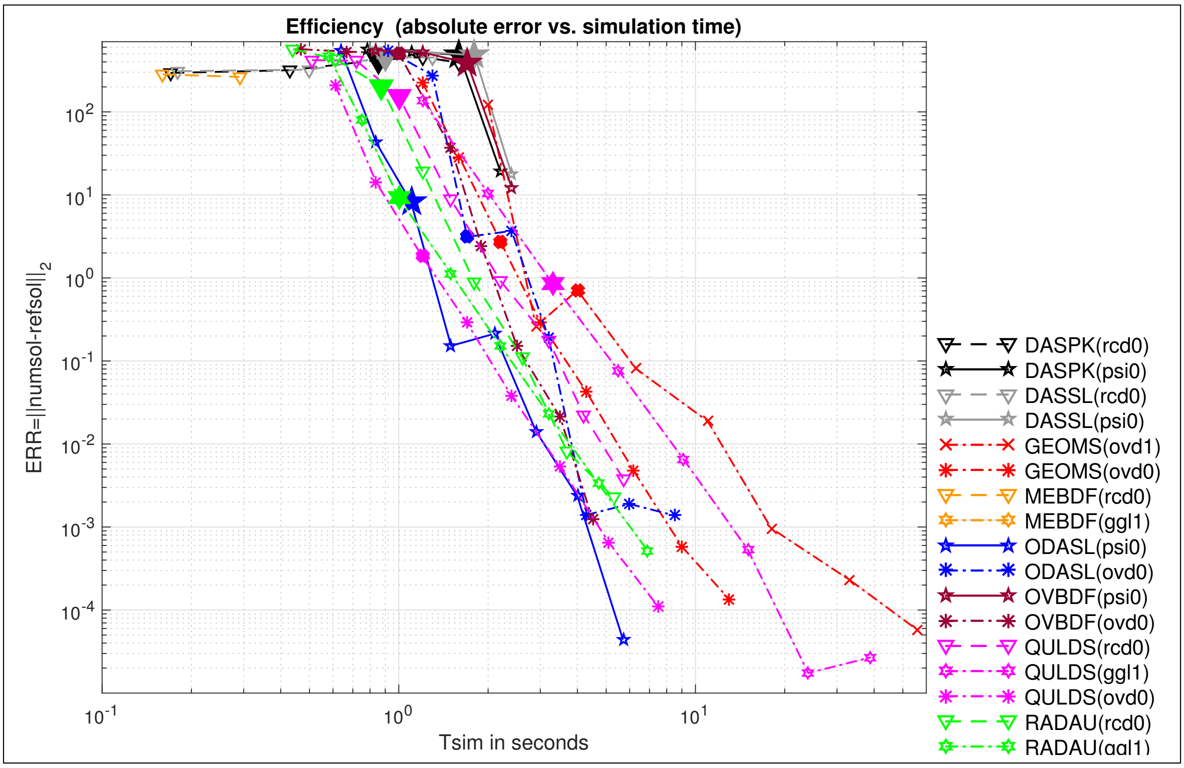

Figure 12: Scenario 02: Efficiency

3 Summary

On the example of *The Simple Pendulum*, we considered the applicability, efficiency, accuracy, and robustness of different numerical solvers for differential-algebraic equations in combination with several formulations, i.e., regularized formulations or also index reduced formulations, for the model equations.

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References

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