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Numerical problems in the dynamical simulation of wheel-rail systems

Wheel-rail systems can be modelled as mechanical multibody systems with holonomic constraints. The dynamical behaviour is described by a differential-algebraic system of index 3 in non–Hessenberg form ([10]). We discuss the efficient numerical solution of these model equations. A perturbation analysis suggests the integration of the model equations in the Gear–Gupta–Leimkuhler (GGL) formulation. The BDF code ODASSL ([6]) is adapted to the non–Hessenberg form of the differential-algebraic system. The theoretical results are illustrated by the dynamical simulation of a rigid wheelset.

1. Introduction

Multibody system (MBS) models have been successfully applied to simulate the dynamical behaviour of wheel-rail systems. Combined with a Hertzian one-point contact model for the geometrical description of the contact between wheels and rails the *descriptor form* of the model equations is given by ([10])

$$\begin{aligned} M(q)\ddot{q} &= f(q,s,\dot{q},\lambda,t) - G^T(q,s)\lambda \\ 0 &= h(q,s) \\ 0 &= g(q,s) \end{aligned} \tag{1}$$

with the position coordinates $q \in \mathbb{R}^{n_q}$, the Lagrangian multipliers $\lambda \in \mathbb{R}^{n_\lambda}$ and the symmetric, positive definite mass matrix $M(q)$. The coordinates $s \in \mathbb{R}^{n_s}$ define the position of the contact point on the wheel surface, they are completely given by the relative positions of wheels and rails and thus by the MBS coordinates q (the Jacobian h_s is non-singular). The holonomic constraints "$g(q,s) = 0$" guarantee that wheels and rails remain in contact, they are coupled to the dynamical equations via λ and $G(q,s) := [g_q - g_s h_s^{-1} h_q](q,s)$. Eqs. (1) form a differential-algebraic system of index 3. In contrast to the constrained mechanical systems with potential forces that are considered most often in the literature ([9, Section VI.5]) the vector f of applied forces contains friction forces between wheels and rails. These friction forces depend nonlinearly on the constraint forces $-G^T(q,s)\lambda$ and thus on λ.

Compared with traditional approaches that include a huge number of table look-ups the integration of the descriptor form (1) is much more efficient ([10]). It is successfully used whenever the motion of the wheel-rail system is smooth and the one-point contact model is applicable. Modifications and generalizations of the model equations (1) to wheel-rail systems with *wear profiles* that are characterized by a more complex contact geometry and by impacts in the system (that cause discontinuities in the solution) have recently been discussed in [3, 1].

In the present paper we focus on the efficient numerical integration of (1), the one-point contact model is supposed to be applicable. Following [10] the simulations are performed for wheels with *linearized* profiles, i. e. for conic wheels. In Section 2 we motivate why the GGL formulation ([8]) should be used to integrate (1). In the implementation of index reduced formulations of (1) the equations $h(q,s) = 0$ (i. e. the non–Hessenberg form of (1)) require special care. Appropriate modifications of the BDF code ODASSL ([6]) are discussed in Section 3.

2. Index reduction in the model equations

The differential-algebraic system (1) has index 3, i. e. severe problems have to be expected if standard methods (implicit Runge–Kutta, BDF) are applied to (1) directly: e. g. order reduction, trouble with stepsize and order control and the amplification of small errors during integration. That is why the index should be reduced before discretization. This is usually done substituting the constraint $g(q,s) = 0$ in (1) by one of its time derivatives $\dot{g} = 0$, $\ddot{g} = 0$ or coupling one or two of these time derivatives to (1). All these index reduced formulations are analytically equivalent to (1). In this section we compare some of these index reduced formulations w. r. t. reliability and efficiency and select a formulation that includes both $g = 0$ and $\dot{g} = 0$ but avoids the evaluation of $\ddot{g}$ during integration (GGL formulation).

To simplify the notation in these theoretical investigations we solve the equations $h(q,s) = 0$ formally w. r. t. s and get a function $s = s(q)$ with $h(q,s(q)) \equiv 0$. With the notations $\tilde{f}(q,\dot{q},\lambda,t) := f(q,s(q),\dot{q},\lambda,t)$, $\tilde{g}(q) := g(q,s(q))$

and $\tilde{G}(q) := \tilde{g}_q(q) = G(q, s(q))$ Eqs. (1) can be rewritten as system in Hessenberg form. This system and some of the analytically equivalent formulations can be summarized as

$$\begin{aligned} \dot{q} &= u - w_q^T(q,u)\mu \\ M(q)\dot{u} &= \tilde{f}(q,u,\lambda,t) - \tilde{G}^T(q)\lambda - w_u^T(q,u)\mu \\ 0 &= v(q,u,\lambda,t) \\ 0 &= w(q,u) \end{aligned} \tag{2}$$

with the velocity vector $u := \dot{q}$ and various choices of functions v and w. Here $\mu \in \mathrm{I\!R}^{n_\mu}$ denote some auxiliary variables that vanish identically for the analytical solution but might differ from 0 for the numerical solution (if $n_\mu > 0$). This notation covers

- with $w \equiv 0$, $n_\mu = 0$ the original index-3 formulation ($\dot{q} = u$, $v := \tilde{g}(q)$) and the index-2 ($v := \frac{d}{dt}\tilde{g}(q(t)) = \tilde{g}_q(q)\dot{q} = \tilde{G}(q)u$) and index-1 formulation ($v := \frac{d^2}{dt^2}\tilde{g}(q(t))$) and
- with $n_\mu > 0$ some derivative projection methods: the GGL formulation with $w = \tilde{g}$, $v := \frac{d}{dt}\tilde{g}$, $n_\mu = n_\lambda$ ([8]) and the *stabilized index-1 formulation* with $w = (\,\tilde{g}^T\,,\ \frac{d}{dt}\tilde{g}^T\,)^T$, $v := \frac{d^2}{dt^2}\tilde{g}$, $n_\mu = 2n_\lambda$ ([7]).

Remark 1. *The substitution of the holonomic constraints $\tilde{g} = 0$ by one of its time derivatives reduces the index to 2 and 1, respectively, but results usually in a numerical solution that drifts away from the manifold $\{\, q : \tilde{g}(q) = 0 \,\}$. The errors in $\tilde{g}(q)$ grow during integration, the physical interpretation would be wheels that leave the rails ("the flying wheelset"). Within a MBS simulation package these numerical results are completely useless, a drift that exceeds the error bounds is inacceptable.*

In the following we therefore restrict our analysis to formulations of the model equations that contain the original constraints $\tilde{g} = 0$. Roughly summarized the time derivatives of the constraints are coupled to the system to reduce the index of the system, both GGL formulation and stabilized index-1 formulation are systems of index 2. More precisely, however, the standard codes for differential-algebraic systems of index 2 and 3 are very sensitive to errors in the differential components q and u but much less sensitive to errors in the algebraic components λ and μ. Within the framework of perturbation index theory (e. g. [9, pp. 478ff]) the influence of small perturbations on the solution can be studied separately for various solution components: On a finite time interval $[t_0, t_e]$ the analytical solution (q, u, λ) of Eqs. (2) is compared with functions $(\hat{q}, \hat{u}, \hat{\lambda})$ that cause small residuals $\theta_v(t)$, $\theta_w(t)$ in the algebraic part of (2):

$$\begin{aligned} \dot{\hat{q}} &= \hat{u} - w_q^T(\hat{q},\hat{u})\hat{\mu} \\ M(\hat{q})\dot{\hat{u}} &= \tilde{f}(\hat{q},\hat{u},\hat{\lambda},t) - \tilde{G}^T(\hat{q})\hat{\lambda} - w_u^T(\hat{q},\hat{u})\hat{\mu} \\ \theta_v(t) &= v(\hat{q},\hat{u},\hat{\lambda},t) \\ \theta_w(t) &= w(\hat{q},\hat{u}) \end{aligned} \tag{3}$$

For simplicity we suppose the differential equations to be satisfied exactly since errors in the differential part are known to cause much less trouble than errors in the algebraic part. The following theorem summarizes the results of this perturbation analysis for index-3 formulation, GGL formulation and stabilized index-1 formulation. In the error estimates the velocity vector u is splitted into $u = S(q,u,\lambda)u + (I - S(q,u,\lambda))u$ with the matrix $S(q,u,\lambda) := I - [M^{-1}\Gamma(\tilde{G}M^{-1}\Gamma)^{-1}\tilde{G}](q,u,\lambda)$ that represents a projection of $\mathrm{I\!R}^{n_q}$ onto the tangential space of $\{\, q : \tilde{g}(q) = 0 \,\}$, $\Gamma(q,u,\lambda) := \tilde{f}_\lambda(q,u,\lambda) - \tilde{G}^T(q)$. For $m > 0$ we use the notations

$$\frac{1}{h^m}\theta := \theta + \sum_{i=1}^{m} \max_{t\in[t_0,t_e]} \|\frac{d^i}{dt^i}\theta_v(t)\| + \max_{t\in[t_0,t_e]} \|\frac{d^i}{dt^i}\theta_w(t)\| \ , \quad \theta := \max_{t\in[t_0,t_e]} \|\theta_v(t)\| + \max_{t\in[t_0,t_e]} \|\theta_w(t)\| \ .$$

Theorem 1. *There is a constant C_0 so that for all functions $\hat{q}$, $\hat{u}$, $\hat{\lambda}$ with (3) and $\theta_v, \theta_w \in \mathcal{C}^2[t_0, t_e]$ the estimates*

$$\|\hat{q}(t) - q(t)\| + \|[S(\hat{q},u,\lambda)\hat{u}](t) - [S(q,u,\lambda)u](t)\| \le$$

$$\le \begin{cases} C_0(\theta + (\frac{1}{h}\theta)^2 + \max\|\tilde{f}_{u\lambda}\| \cdot (\frac{1}{h}\theta)(\frac{1}{h^2}\theta) + \max\|\tilde{f}_{\lambda\lambda}\| \cdot (\frac{1}{h^2}\theta)^2) & \textit{(index-3)} \\ C_0(\theta + \theta \cdot \frac{1}{h}\theta + \max\|\tilde{f}_{\lambda\lambda}\| \cdot (\frac{1}{h}\theta)^2) & \textit{(GGL)} \\ C_0(\theta + \theta \cdot \frac{1}{h}\theta) & \textit{(stabilized index-1)} \end{cases} \tag{4}$$

$$\|\hat{\lambda}(t)-\lambda(t)\| \leq \begin{cases} C_0 \cdot \frac{1}{h^2}\theta & \textit{(index-3)} \\ C_0 \cdot \frac{1}{h}\theta & \textit{(GGL)} \\ C_0(\theta + \theta \cdot \frac{1}{h}\theta) & \textit{(stabilized index-1)} \end{cases}$$

are satisfied for all $t \in [t_0, t_e]$ *whenever the expressions at the right hand side of (4) are sufficiently small. Furthermore it holds* $[\tilde{G}(q)u](t) \equiv 0$ *and* $\|[\tilde{G}(\hat{q})\hat{u}](t)\| \leq \frac{1}{h}\theta$ *(index-3 formulation) and* $\|[\tilde{G}(\hat{q})\hat{u}](t)\| \leq \theta$ *(GGL and stabilized index-1 formulation). The notations* $\max\|\tilde{f}_{u\lambda}\|$, $\max\|\tilde{f}_{\lambda\lambda}\|$ *stand for* $\max\{\|\tilde{f}_{u\lambda}(q,u,\lambda)\| \,:\, (q,u,\lambda) \in \mathcal{U}\}$, ... *where* $\mathcal{U}$ *denotes a (small) compact neighbourhood of the analytical solution* $\{\,(q(t),u(t),\lambda(t)) \,:\, t \in [t_o,t_e]\,\}$ *of (1).*

Proof. In the special case $\tilde{f} = \tilde{f}(q,u,t)$, i. e. $\tilde{f}_{u\lambda} \equiv 0$, $\tilde{f}_{\lambda\lambda} \equiv 0$, the estimates for the index-3 formulation are given in [2, Theorem 1]. The generalization to systems with friction forces (i. e. $\tilde{f}_\lambda \neq 0$) is proven applying Gronwall's Lemma to $y(t) := (\,(S(q,u,\lambda)(\hat{q}-q))^T,\,(S(\hat{q},u,\lambda)\hat{u} - S(q,u,\lambda)u - (\Phi(\hat{q}) - \Phi(q)))^T\,)^T$ with

$$\Phi(\xi) := [SM^{-1}f_u](q,u,\lambda)\xi + S_q(q,u,\lambda)(u,\xi) + S_q(q,u,\lambda)(\xi,u) + S_u(q,u,\lambda)(\xi,\dot{u}) + S_\lambda(q,u,\lambda)(\xi,\dot{\lambda})\ ,$$

it corresponds to a similar result for systems of index 2 in [5]. The estimates for GGL formulation and stabilized index-1 formulation are obtained applying [5, Theorem 1] to index-2 systems of the special structure (2).

Remark 2. *A more detailed perturbation analysis for analytical and numerical solution of (1) is given in [2]. Theorem 1 improves the error bounds of [2, Table 1 and Theorem 4] substantially if* $\max\|\tilde{f}_{u\lambda}\| \ll 1$, $\max\|\tilde{f}_{\lambda\lambda}\| \ll 1$, *i. e. for systems with small friction forces.*

Remark 3. *The error estimates for the analytical solution have discrete counterparts ([2, 5]): In this case let* θ *denote an upper bound for the errors in the algebraic part that arise if a numerical method is implemented on a computer (e. g. round-off errors, errors that are caused by stopping the iterative solution of nonlinear equations). If appropriate discretization methods are used then the amplification of these errors during integration is bounded by terms like the ones in Theorem 1 (in this case* h *denotes the stepsize of integration). Integrating the index-3 formulation there is e. g. besides the global discretization error an additional error term of size* $\mathcal{O}(\theta + \frac{1}{h^2}\theta^2 + \max\|\tilde{f}_{u\lambda}\| \cdot \frac{1}{h^3}\theta^2 + \max\|\tilde{f}_{\lambda\lambda}\| \cdot \frac{1}{h^4}\theta^2)$ *in* q *and* $S(q,u,\lambda)u$, *of size* $\mathcal{O}(\frac{1}{h}\theta)$ *in* $\tilde{G}(q)u$ *and of size* $\mathcal{O}(\frac{1}{h^2}\theta)$ *in* λ. *This additional error term is characteristic of higher index systems. Compared with the discretization error it is small if the stepsize* h *is large but it causes severe difficulties if the stepsize becomes small.*

If discretization methods are applied directly to the index-3 formulation (1) of the model equations then the largest additional error term has to be expected in the Lagrangian multipliers λ. Position coordinates q and the projection $S(q,u,\lambda)u$ of the velocity vector are the solution components that are most robust against perturbations during integration. Coupling the time derivative $\frac{d}{dt}\tilde{g}(q) = 0$ of the holonomic constraints to the system (GGL formulation) the index of the system is decreased and the additional error term is reduced (at least) by the factor h in all solution components — this is especially important in the critical case of small stepsizes. If the GGL formulation is discretized and $\theta \ll 1$, i. e. if the errors in the algebraic equations are kept small during integration (e. g. small stopping bounds for the iterative solution of nonlinear equations) then the additional error terms in q and u are negligible compared with the discretization error. In a large number of numerical tests we used successfully the BDF discretization of the GGL formulation to simulate the dynamical behaviour of wheel-rail systems (stepsize and order control are based on the errors in q and u), the amplification of errors has never caused problems in these computations. In contrast to these positive results the additional consideration of the second time derivative $\frac{d^2}{dt^2}\tilde{g}(q) = 0$ (stabilized index-1 formulation) does not pay in our case: the cpu-time increases approximately by 20% since the evaluation of $\frac{d^2}{dt^2}\tilde{g}(q)$ is time-consuming and the dimension of system (2) is increased by n_λ additional equations. On the other hand the resulting system is again of index 2 and the additional error terms are not much smaller than for the GGL formulation. The stabilized index-1 formulation could reduce the additional error in λ but compared with reality the errors in the constraint forces remain large because of large errors in physical parameters of the model equations.

Summarizing the results of theoretical investigations and practical computations we selected the GGL formulation of the model equations (1) for the dynamical simulation of wheel-rail systems.

3. Implementation of index reduced formulations for systems in non–Hessenberg form

MBS formalisms generate the model equations (1) and — on request — also the time derivatives $\dot{g}$, $\ddot{g}$ of the holonomic constraints automatically. In this context [6] developed the concept of *overdetermined* differential-algebraic systems: $\dot{g}$ or $\dot{g}$ and $\ddot{g}$ are added to system (1) and this overdetermined system is discretized by BDF. So we get in each time step an overdetermined system of nonlinear equations that has in general no (classical) solution, i. e. there is no vector such that the residual in this system of nonlinear equations vanishes. To make the method well-defined a *generalized* solution is introduced by the condition that this residual belongs to range$\,(\,g_q\,,\,0\,,\,g_s\,,\,0\,,\,0\,)^T$ if $\dot{g}=0$ was added and to range $\begin{pmatrix} g_q & 0 & g_s & 0 & 0 & 0 \\ \dot{g}_q & \dot{g}_u & \dot{g}_s & 0 & 0 & 0 \end{pmatrix}^T$ if both $\dot{g}=0$ and $\ddot{g}=0$ were added to (1). This strategy is straightforwardly implemented in a BDF code (ODASSL) since all the Jacobians g_q, $\dot{g}_q$, ... are readily available during the corrector iteration ([6]). For systems in Hessenberg form this approach is equivalent to GGL formulation and stabilized index-1 formulation, respectively ([7]). The code ODASSL is successfully applied for the dynamical simulation of constrained mechanical systems.

For wheel-rail systems with model equations (1), however, the standard form of ODASSL fails since the numerical solution satisfies $h(q_n, s_n) \in \mathrm{range}\, g_s^T$ or $h(q_n, s_n) \in \mathrm{range}\,(\,g_s^T\,,\,\dot{g}_s^T\,)$ but *not* $h(q_n, s_n) = 0$. Thus errors are introduced into the contact point coordinates s, the numerical solution is incorrect ([4]). Fig. 1 shows simulation results for a rigid wheelset in stabilized index-1 formulation where the integration even totally breaks down. Fig. 1 shows also results for the *correct* generalization of the index reduced formulations to system (1): we start with Eqs. (2) and rewrite them in terms of q, s, u and λ with $h(q,s) = 0$. The generalized solution of the system of nonlinear equations is now defined by the condition that the residual belongs to range$\,(\,g_q - g_s h_s^{-1} h_q\,,\,0\,,\,0\,,\,0\,,\,0\,)^T$ and range $\begin{pmatrix} g_q - g_s h_s^{-1} h_q & 0 & 0 & 0 & 0 & 0 \\ \dot{g}_q - \dot{g}_s h_s^{-1} h_q & \dot{g}_u & 0 & 0 & 0 & 0 \end{pmatrix}^T$, respectively. This strategy is implemented by a modification of the corrector iteration in ODASSL and needs (compared with original ODASSL) no additional numerical effort ([4]).

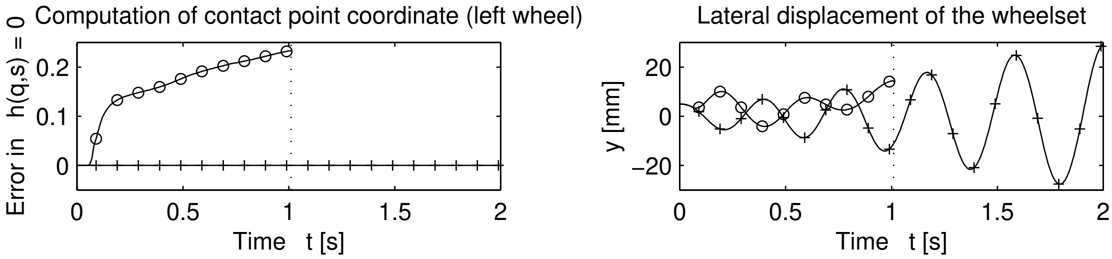

Figure 1: Dynamical simulation of a rigid wheelset, standard ("∘") and modified ("+") corrector.

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