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On the Convergence and Correctness of Impulse-Based Dynamic Simulation[1]

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Abstract

Impulse-based dynamic simulation using the iterative method results in relatively simple algorithms which are easy to implement. However, two important theoretical questions have so far still remained open: (1) In what situations does the iterative procedure converge or diverge, and how can divergence be avoided? (2) Does the impulse-based simulation converge towards the exact solution of the dynamics problem as the step size is reduced? We will completely answer both questions in this paper. First we simplify the argumentation in that we prove that for every multibody system there is a dynamically and kinematically equivalent point mass system. Hence, our results on point mass systems also apply to multibody simulations. Next we show how to replace the iterative procedures by solving systems of linear equations. We prove that the matrices of these equation systems are non-singular if redundant constraints are removed from the point mass system in question. We prove further that the solution generated by the impulse-based procedure converges towards the exact solution of the dynamics problem as the step size is reduced towards zero. The proof is based on a detailed comparison of the impulse-based integration expression and the Taylor series solution. It is well known that the latter converges to the exact solution of the dynamics problem if a Lipschitz condition is satisfied.

Comparison with the standard numerics on the basis of Lagrange multipliers shows significant advantages for the impulse-based method because the latter is completely free of drift problems, and stabilizations in the sense of Baumgarte are unnecessary. Because of the existence of methods of higher order, we can finally conclude that the impulse-based method is superior to the method with Lagrange multipliers.

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Kurzfassung

Die impulsbasierte Dynamiksimulation mit der iterativen Methode führt zu vergleichsweise sehr einfachen Algorithmen, die leicht zu implementieren sind. Zwei von der Theorie her wesentliche Fragen waren bisher jedoch noch offen: (1) In welchen Situationen konvergiert bzw. divergiert das iterative Verfahren und wie kann man die Divergenz vermeiden? (2) Konvergiert das impulsbasierte Simulationsverfahren mit sinkender Zeitschrittweite gegen die exakte Lösung des Dynamik-Problems? Beide Fragen können wir in dieser Arbeit vollständig beantworten. Zunächst vereinfachen wir die Beweisführung, indem wir nachweisen, dass es zu jedem Mehrkörpersystem ein dynamisch und kinematisch völlig äquivalentes Massenpunktsystem gibt. Daher gelten unsere Ergebnisse über Massenpunktsysteme auch für Mehrkörper-Simulationen. Als nächstes zeigen wir, wie man die iterativen Verfahren durch das Lösen linearer Gleichungssysteme ersetzen kann. Wir zeigen, dass die Matrizen dieser Gleichungssysteme nichtsingulär sind, wenn redundante Zwangsbedingungen aus den betreffenden Dynamik-Systemen entfernt werden. Sodann beweisen wir, dass die vom Impulsverfahren erzeugte Lösung mit gegen null sinkender Zeitschrittweite gegen die exakte Lösung des Dynamik-Problems konvergiert. Der Beweis beruht auf einem detaillierten Vergleich der Integrationsausdrücke des impulsbasierten Verfahrens und der Lösung mit Taylorentwicklung. Es ist bekannt, dass letztere gegen die exakte Lösung des Dynamikproblems konvergiert, wenn eine Lipschitzbedingung erfüllt ist.

Ein Vergleich mit der Standard-Numerik auf der Basis von Lagrange-Multiplikatoren ergibt deutliche Vorteile für die impulsbasierte Methode, weil sie völlig frei von Drift-Problemen ist und Korrekturterme im Sinne von Baumgarte überflüssig sind. Wegen der Existenz der impulsbasierten Verfahren höherer Ordnung kann man also abschließend folgern, dass das Impulsverfahren dem Verfahren mit Lagrange-Multiplikatoren überlegen ist.

1. Introduction

In this work, we study theoretical questions concerning the impulse-based dynamic simulation of multibody systems. The impulse-based dynamic simulation of point mass systems was introduced in the report [Schmitt, Thüring 2000], whereas this method was extended to multibody systems in [Schmitt 2003] as well as [Finkenzeller et al. 2003]. Derived from the results achieved experimentally, it could be demonstrated that the impulse-based dynamic simulation method is competitive with the other methods known from the literature. The most important advantages are the comparatively simple program structure, the real-time capability even for complex models (e.g., six-legged walking machines), and the input specification and internal simulation in Cartesian coordinates as preferably used in computer graphics and also in almost all engineering applications. It is therefore unnecessary to introduce reduced or generalized coordinates related to the degrees of freedom, and no systems of differential-algebraic equations need be solved, which is particularly desirable for applications in virtual reality and computer animation.

A further advantage of the impulse-based method is the comparatively simple handling of collision and Coulomb friction. This is probably the most remarkable advantage of the impulse-based method. For multibody systems with several frictional body contacts, it is unnecessary to solve a linear or non-linear complementarity problem (see for example [Pfeiffer, Glocker 1996]) because the contact points are correctly handled by the iterative procedure for determination of the correction impulses [Schmitt 2003]. However, this procedure requires exact algorithms for collision detection and resolution as do all other simulation methods too.

The advantages of the impulse-based method are therefore quite clear. However, a number of theoretical questions remained unanswered, and we wish to deal with these here. These concern the termination of the iterative procedure which determines the correction impulses, and the fundamental question as to whether the impulse-based simulation converges towards the exact solution of the dynamics problem as the step size h is reduced.

Our argumentation when clarifying these questions is that we first of all prove that for each multibody system a kinematically and dynamically equivalent point mass system exists, and that this point mass system can be constructed using a simple method. It is then justifiable to carry out the theoretical studies on point mass systems, which results in significantly simpler formulae.

We next analyze the velocity correction procedure for point mass systems, and derive a system of linear equations (SLE) with which the impulses required for the velocity correction can be determined non-iteratively. The iterative procedure for velocity correction is very similar to the Gauß-Seidel method, and can diverge in cases in which the SLE has a solution.

These derivations also provide interesting statements on the structure of point mass systems: Our point mass systems can be converted into a dynamically and kinematically equivalent system by removing superfluous or redundant constraints, and for these reduced systems the velocity correction is always possible.

We then show that even the iterative procedure for integration time steps can be solved using a sequence of SLEs, where we apply Newton's method when searching a solution for systems of non-linear equations. The matrices of these equations are very similar to those for the velocity correction.

After this we study a method with which the solution for a time step is derived as a truncated Taylor series. This method is a version of the frequently used method with Lagrange multipliers. In the limiting case $h \to 0$ it provides the mathematically correct solution of the dynamics problem.

We finally show that in the limiting case $h \to 0$ the solution of the Taylor method coincides with that of the impulse-based procedure. It is also the case that the impulse-based procedure has the truncation error of order $O(h^3)$, which has already been repeatedly confirmed experimentally.

Before we occupy ourselves in detail with the impulse-based dynamic simulation method, a few important facts on impulses will be provided as an introduction. Impulses result from integration of forces $F(t) \in \mathbb{R}^3$:

$$I := \int_{t_1}^{t_2} F(t)dt\,.$$

Whereas a force $F(t)$ continuously accelerates a point mass $P(t)$ with mass m according to $m \cdot \ddot{P}(t) = F(t)$, impulses cannot have a continuous effect on a point mass but only at discrete times. The impulse I then provides the point mass with an instantaneous increment in velocity with the direction and magnitude $(1/m) \cdot I$. The impulse-based dynamic simulation method utilizes impulses in order to achieve equivalent dynamic effects as when applying continuous forces. The discrete nature of impulses results in significant simplification of the dynamic simulation method because it is possible to largely avoid the solution of differential equations. Discrete application of impulses is certainly comparable with the discretization of numeric methods for solving systems of differential equations.

2. Iterative dynamic simulation of point mass systems (PMS)

A point mass system (PMS) consists of n points

$$P_i(t) \in \mathbb{R}^3 \qquad (i = 1,2,...,n)$$

with masses $m_i > 0$. We use $\dot{P}_i(t) := \frac{d}{dt} P_i(t)$ to identify the velocity of $P_i(t)$. The coordinate system used is an inertial system with gravity $g := (0, -g_0, 0)$. Some of the point masses can be fixed in space, i.e., they are permanently immovable, therefore $\dot{P}_i(t) = 0$ for all t, even if forces act on them. In the formulae further below, point masses fixed in space can be treated such that their mass term $(1/m)$ vanishes. The gravity acting on the point masses P_i is defined as

$$g_i := \begin{cases} (0,0,0), & \textit{if } P_i \textit{ is fixed in space} \\ g & \textit{otherwise.} \end{cases}$$

This definition will lead to simpler formulae in the following.

Between the point masses, m constraints ("joints") are defined:

$$C_k := (i_k, j_k, d_k) \qquad (k = 1,...,m).$$

Each such constraint specifies that the distance between the point masses $P_{i_k}(t)$ and $P_{j_k}(t)$ must always have the constant value d_k, which is equivalent to

(2.1) $$(P_{j_k}(t) - P_{i_k}(t))^2 - d_k^2 = 0 \qquad (k = 1,...,m).$$

Since the time parameter does not explicitly exist in our constraints, these are therefore scleronomic holonomic constraints.

In this paper, we are only interested in <u>*energy preserving point mass systems*</u> where, in addition to gravity and constraint forces, no other forces and no other types of joints (spring damper connections and drives, for example) are taken into consideration. Our systems can therefore be multiple-suspension constructions with rigid bodies, rotary axes between these, and open or closed kinematic chains with a simple or complicated coupling. The sum of the potential and kinetic energie is constant in time for our systems. This simplified type of PMSs is completely adequate for the investigations of this paper.

***Definition**: A PMS is in a <u>D-consistent</u> dynamic state if all constraint equations (2.1) are satisfied (D-consistent = consistent with respect to distance).*

The PMS is in a <u>V-consistent dynamic</u> state (V = velocity) if

(2.2) $$(P_{j_k}(t) - P_{i_k}(t))(\dot{P}_{j_k}(t) - \dot{P}_{i_k}(t)) = 0 \qquad (k = 1,...,m).$$

The dynamic state is called <u>consistent</u> if both conditions are satisfied.

If the point masses involved have a positive distance from one another, which we permanently assume, equation (2.2) means that the relative velocity between the point masses vanishes as must be the case with constant distances, since

$$\frac{d}{dt}((P_{j_k}(t) - P_{i_k}(t))^2 - d_k^2) = 0 = 2(P_{j_k}(t) - P_{i_k}(t))(\dot{P}_{j_k}(t) - \dot{P}_{i_k}(t)).$$

Constraints with $d_k = 0$ are superfluous because the masses located so closely together can be melted into one single point mass.

When solving practical problems such as the dynamic simulation of multibody systems, specific D-consistent point positions $P_l(t_0)$ are usually predefined or known. However, the question can also be asked whether D-consistent point positions can be calculated starting from the constraints alone. The problem can of course be solved, but only with possibly considerable computing efforts, for it belongs to the class of NP-complete problems:

***Theorem**: The decision problem whether point coordinates $P_l \in \mathbb{R}^3, \quad l = 1,...,n,$ can be found for a given set of constraints $C_k := (i_k, j_k, d_k), \quad k = 1,...,m,$ so that $(P_{j_k}(t) - P_{i_k}(t))^2 - d_k^2 = 0,$ $k = 1,...,m$, is satisfied, belongs to the class of NP-complete problems.*

Sketch of proof: Limiting ourselves to one-dimensional problems is possible. The problem of finding n coordinate values $x_1, x_2, ..., x_n \in \mathbb{R}$ so that *n* predefined constraints $d_i = |x_i - x_{i+1}|$ are satisfied for $i = 1,...,n-1$ and $d_n = |x_n - x_1|$ is equivalent to solving the partition problem [Garey, Johnson 1979]. For if $\overline{x}_1, \overline{x}_2, ..., \overline{x}_n$ is a solution, then $d_i = |\overline{x}_i - \overline{x}_{i+1}|$ must also apply and, because of the closed path, also

$$(\overline{x}_1 - \overline{x}_n) + \sum_{i=1}^{n-1} (\overline{x}_{i+1} - \overline{x}_i) = 0 .$$

The total of the positive values $\overline{x}_i - \overline{x}_{i+1} > 0$ must therefore be exactly as large as the absolute value of the total of the negative values.

The literature provides various references to the fact supported by the above theorem that it may be difficult to find consistent initial values for differential-algebraic systems.

In the following, we shall frequently use the notation

$$\begin{aligned} &A_k(t) := P_{j_k}(t) - P_{i_k}(t) && (k = 1,...,m), \\ &\dot{A}_k(t) := A_k^{(1)}(t) := \dot{P}_{j_k}(t) - \dot{P}_{i_k}(t) && (k = 1,...,m). \end{aligned} \tag{2.3}$$

We shall also use higher derivatives:

$$\frac{d^i}{dt^i} A_k(t) = A_k^{(i)}(t) := \frac{d^i}{dt^i} P_{j_k}(t) - \frac{d^i}{dt^i} P_{i_k}(t) \qquad (k = 1,...,m). \tag{2.4}$$

The dynamic simulation task (integration step)

The dynamic simulation task for a PMS is to calculate the dynamic motion of the system of point masses in the sense of Newton's second law

$$\ddot{P}_i(t) = g_i + (1/m_i) F_i(P_1(t),...,P_n(t)) \quad (i = 1,...,n)$$

starting at time t_0 in a consistent dynamic state and ending at time $t_1 > t_0$.

For us, the F_i are only constraint forces acting between the point masses. They retain the constant distances between constrained pairs of point masses and therefore do not generate or consume energy. (The above system of equations is still formally incomplete, we shall specify the complete representation with explicit incorporation of the constraint forces in Section 6.)

To start this short exposition on impulse-based dynamic simulation, we define the function *LA* = look-ahead by

(2.5) $$LA(P_r(t),h) := P_r(t) + \dot{P}_r(t)\cdot h + 0.5\cdot g_r \cdot h^2 .$$

It defines the location where the associated point mass will be found at time $t+h$ with a purely ballistic motion. (This equation is also applicable to point masses fixed in space, for $\dot{P}_r(t) = (0,0,0)$ and $g_r = (0,0,0)$ always apply to them.)

With the iterative impulse-based method of dynamic simulation, a time step from t to $t+h$ is carried out as follows:

(2.6) Iterative integration step:

As long as a constraint $C_k = (i_k, j_k, d_k)$ *can be found satisfying*

$\left|\left|LA(P_{j_k}(t),h) - LA(P_{i_k}(t),h)\right| - d_k\right| > \delta_{\max}$, *proceed as follows:*

(1) The correction impulse has the magnitude and direction

$$I := \frac{\left|LA(P_{j_k}(t),h) - LA(P_{i_k}(t),h)\right| - d_k}{h\cdot((1/m_{j_k}) + (1/m_{i_k}))} \cdot \frac{A_k(t)}{\left|A_k(t)\right|}.$$

(2) Complementary application of the impulse I changes the velocities of the point masses involved at time t as follows:

$$\dot{P}_{i_k}(t) := \dot{P}_{i_k}(t) + (1/m_{i_k})\cdot I,$$
$$\dot{P}_{j_k}(t) := \dot{P}_{j_k}(t) - (1/m_{j_k})\cdot I.$$

(3) If such a constraint can no longer be found, update the dynamic state and advance the time to $t+h$ *by*

$$P_{i_k}(t+h) := LA(P_{i_k}(t),h), \quad P_{j_k}(t+h) := LA(P_{j_k}(t),h),$$
$$\dot{P}_{i_k}(t+h) := \dot{P}_{i_k}(t) + g_{i_k}\cdot h, \quad \dot{P}_{j_k}(t+h) := \dot{P}_{j_k}(t) + g_{j_k}\cdot h$$

and continue the simulation with this new dynamic state.

This is the simplest dynamic simulation algorithm known as far as the programming requirements are concerned. We apply correction impulses at the individual point masses, namely at time t, until all constraints are satisfied at the look-ahead time $t+h$, within tolerances smaller than $\delta_{\max}$.

Depending on the requirements, very small values such as $\delta_{\max} := 10^{-12}$ can be chosen.

Complementary application of the impulses conserves the linear momentum as well as the angular momentum of the PMS, but a requirement for this is that the system has no point masses fixed in space. (Note that gravity does change the linear momentum.)

We carry out the iterative velocity correction in a very similar manner, with the objective of converting a non-V-consistent PMS into a V-consistent one, merely through the application of complementary pairs of impulses. The point locations P_i are not modified in the process, only the $\dot{P}_i$.

(2.7) Iterative velocity correction:

As long as a joint $C_k = (i_k, j_k, d_k)$ *can be found with*

$D := A_k(t) \cdot \dot{A}_k(t) = (P_{j_k}(t) - P_{i_k}(t)) \cdot (\dot{P}_{j_k}(t) - \dot{P}_{i_k}(t))$ *and*

$|D| > v_{\max}$,

proceed as follows:

(1) The correction impulse has the magnitude and direction

$$I := \frac{D}{((1/m_{j_k}) + (1/m_{i_k}))} \cdot \frac{A_k(t)}{|A_k(t)|}.$$

(2) Correct the velocities of the point masses involved as follows:

$$\dot{P}_{i_k}(t) := \dot{P}_{i_k}(t) + (1/m_{i_k}) \cdot I,$$

$$\dot{P}_{j_k}(t) := \dot{P}_{j_k}(t) - (1/m_{j_k}) \cdot I.$$

In this case $v_{\max}$, analogous to $\delta_{\max}$, is a defined tolerance for differences in velocity. If high accuracy is desired for the simulation, these tolerance values must be selected very small. Since the mass term $(1/m_s)$ vanishes for point masses fixed in space, there are no changes in velocity of these points either.

Previously unclear for both iterative procedures were the conditions under which they terminate, and whether these iterative procedures – which usually work well – have room for improvement. We shall provide answers to these questions in the sequel.

3. The equivalence of point mass systems and multibody systems

We wish to show here that a dynamically and kinematically equivalent PMS can be constructed for each multibody system. We shall limit ourselves to energy conserving or conservative multibody systems, consisting of interconnected rigid bodies with simple joints such as point-to-point connections (ball joints, spherical joints) and rotary axes (hinges, revolute joints). Suspension points fixed in space are also permissible as with PMSs.

Given a multibody system we construct an equivalent PMS comprising a set of point masses for each rigid body. It must be guaranteed that the inertia tensors agree, and that a point mass is present at the position of each reference point located at a point-to-point connection of rigid bodies. This is because joints can only be connected to point masses.

We represent the given rigid body with mass m in its natural coordinate system with the origin at the center of mass and the principal inertia axes as the coordinate axes. Then the inertia tensor has the diagonal form

$$J = \begin{pmatrix} Y^2 + Z^2 & 0 & 0 \\ 0 & X^2 + Z^2 & 0 \\ 0 & 0 & X^2 + Y^2 \end{pmatrix}$$

where $X^2 := \int_m x^2 dm$ etc. and where we can assume $X^2 > 0, Y^2 > 0, Z^2 > 0$. (If one or two of the values vanish, the line of argument is analogous, yet simpler.)

May the rigid body have $q > 0$ joint or reference points at the coordinate positions

$$Q_i = (x_i, y_i, z_i) \quad (i = 1,...,q).$$

Let $0 < \tilde{m} < m$ be a sufficiently small mass. The PMS we are heading for is initially constructed from $8 \cdot q$ masses $\tilde{m}$ at the $8 \cdot q$ positions $(\pm x_i, \pm y_i, \pm z_i)$. The required reference points for joints, in particular, are then already present. The inertia terms of the point masses positioned in this manner are

$$\tilde{X}^2 = 8\tilde{m}\sum_{i=1}^{q} x_i^2, \quad \tilde{Y}^2 = 8\tilde{m}\sum_{i=1}^{q} y_i^2, \quad \tilde{Z}^2 = 8\tilde{m}\sum_{i=1}^{q} z_i^2$$

and the respective inertia tensor is in diagonal form. Select $\tilde{m} > 0$ such that the following inequalities are satisfied:

$$\tilde{X}^2 < X^2, \tilde{Y}^2 < Y^2, \tilde{Z}^2 < Z^2 \text{ and } 8 \cdot q \cdot \tilde{m} < m.$$

This is always possible. We must now add eight further point masses, each of mass $\hat{m} := (m - 8 \cdot q \cdot \tilde{m})/8$ and at the still unknown coordinates $(\pm\hat{x}, \pm\hat{y}, \pm\hat{z})$ in a manner such that the contribution to the inertia tensor is exactly the amounts which are still missing:

$$\hat{X}^2 := X^2 - \tilde{X}^2, \ \hat{Y}^2 := Y^2 - \tilde{Y}^2, \ \hat{Z}^2 := Z^2 - \tilde{Z}^2.$$

The coordinates $\hat{x}$, $\hat{y}$, $\hat{z}$ in question are given through solving the equations

$$\hat{X}^2 = 8\hat{m}\hat{x}^2, \ \hat{Y}^2 = 8\hat{m}\hat{y}^2, \ \hat{Z}^2 = 8\hat{m}\hat{z}^2.$$

We have thus positioned the point masses such that the total mass and inertia tensor exactly agree with those of the given rigid body in such a manner that point masses required for joint connections are also present. A rigid body is obtained from the point masses by introducing a sufficient number of constraints between these masses. We have therefore proven:

Theorem: *For each multibody system with point-to-point joints between the rigid bodies a dynamically and kinematically equivalent point mass system can be constructed.*

It is therefore sufficient for theoretical investigations – particularly with respect to the impulse method – to limit oneself to investigation of PMSs. However, for practical pusposes, one should avoid PMSs and simulate rigid body systems because significantly fewer constraints have to be processed in the latter case, permitting both faster and more accurate simulation.

4. Non-iterative velocity correction with a system of linear equations

We shall now again consider the velocity correction problem solved iteratively in (2.7), and wish to replace the iterative procedure by solution of an SLE. In the following, $t = 0$ is assumed, so that the time parameter is superfluous for the variables P_i and $\dot{P}_i$ of the considered PMS.

The given PMS must be in a D-consistent, but not V-consistent, dynamic state. We wish to determine complementary pairs of impulses $I_k, -I_k$ for all constraints $k = 1,...,m$ so that, through

a single application of these impulses, the PMS is transferred into a V-consistent dynamic state which is therefore totally consistent.

For correct handling of the signs in each case, it is important that the impulse I_k always acts in direction A_k (see (2.3)). The velocities therefore change as follows:

$$\dot{P}_{i_k} + (1/m_{i_k}) \cdot I_k \qquad \text{and} \qquad \dot{P}_{j_k} - (1/m_{j_k}) \cdot I_k .$$

The impulse I_k therefore always acts with a positive sign on the starting point P_{i_k} and with a negative sign on the target point P_{j_k}.

We are searching for unknown impulse strengths x_k, so that

$$I_k := (P_{j_k} - P_{i_k}) \cdot x_k = A_k \cdot x_k \tag{4.1}$$

and that the simultaneous application of these impulses to the PMS results in V-consistency. Because the impulses are all used complementary and in the direction A_k of the constraints, neither rotary nor translatory influences result for the whole PMS.

We first wish to determine how the impulses $I_k = A_k \cdot x_k$ change the velocities of the individual point masses P_r. With $X = (x_1, x_2, ..., x_m)^T$ as the column vector of the unknowns, we can write

$$\Delta v_r(X) := (1/m_r)\left(\sum_{\substack{k=1...m \\ \wedge\, i_k = r}} A_k \cdot x_k - \sum_{\substack{k=1...m \\ \wedge\, j_k = r}} A_k \cdot x_k \right) =$$

$$= \quad (1/m_r)\left(\sum_{\substack{k=1...m \\ \wedge\, (i_k = r\ (+) \\ \quad \vee\ j_k = r\ (-))}} (\pm) A_k \cdot x_k \right) \tag{4.2}$$

In order to permit a compact notation for these and similar sums, we introduce

$$sig(k,r) := \begin{cases} +1, & if\ i_k = r, \\ -1, & if\ j_k = r, \\ 0, & if\ i_k \neq r \wedge j_k \neq r. \end{cases} \tag{4.3}$$

Since it can be generally assumed that $\forall (k = 1,...,m)(i_k \neq j_k)$, for constraints only exist between different point masses, this function is well-defined and now permits the notation

$$\Delta v_r(X) := \quad (1/m_r)\left(\sum_{k=1}^{m} sig(k,r) \cdot A_k \cdot x_k \right).$$

$\Delta v_r(X)$ is the total change of the velocity of the point mass P_r, if the impulses defined by X act on the PMS. We have to sum up the effects for all constraints in which P_r is involved, i.e., for all constraints $C_k := (i_k, j_k, d_k)$ for which $i_k = r$ (positive sign) or $j_k = r$ (negative sign).

The relative velocity $\dot{P}_{j_k} - \dot{P}_{i_k}$ on the constraint C_k is therefore changed by the value

$$\Delta w_k(X) := \Delta v_{j_k}(X) - \Delta v_{i_k}(X).$$

Expanded, this results for a specific joint $C_r = (i_r, j_r, d_r)$ in

$$\Delta w_r(X) := \Delta v_{j_r}(X) - \Delta v_{i_r}(X) =$$

$$(4.4) \qquad = (1/m_{j_r})\left(\sum_{k=1}^{m} sig(k, j_r) A_k \cdot x_k\right) - (1/m_{i_r})\left(\sum_{k=1}^{m} sig(k, i_r) A_k \cdot x_k\right).$$

With the introduced notation, we can now establish the required equations for the x_k in that we attempt to satisfy (2.2):

$$(4.5) \quad \forall k = 1,...,m: \quad (P_{j_k} - P_{i_k})(\dot{P}_{j_k} - \dot{P}_{i_k} + \Delta w_k(X)) = 0.$$

With the abbreviated notation (2.3) we obtain

$$A_k \cdot (\dot{A}_k + \Delta w_k(X)) = 0 \qquad (k = 1,...,m).$$

We can now transfer the terms without X to the right side, and obtain a system of linear equations

$$(4.6) \qquad A_k \cdot \Delta w_k(X) = -A_k \cdot \dot{A}_k \qquad (k = 1,...,m).$$

For a specific joint $C_r = (i_r, j_r, d_r)$ this results in the equation

$$(4.7) \qquad (1/m_{j_r})\left(\sum_{k=1}^{m} sig(k, j_r) A_r A_k \cdot x_k\right) - (1/m_{i_r})\left(\sum_{k=1}^{m} sig(k, i_r) A_r A_k \cdot x_k\right) = -A_r \cdot \dot{A}_r.$$

Since we are striving for an SLE of the form

$$(4.8) \qquad M \cdot X = M \cdot \begin{pmatrix} x_1 \\ x_2 \\ . \\ . \\ x_m \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ . \\ . \\ b_m \end{pmatrix} = B,$$

we must now extract the elements $M[r,s]$ of the matrix M. (4.7) represents the *r*-th row of the SLE. It therefore delivers all matrix elements $M[r,1...m]$. Because of

$$M[r,s] = (1/m_{j_r}) sig(s, j_r) A_r A_s - (1/m_{i_r}) sig(s, i_r) A_r A_s$$

the result for $r \neq s$ is

$$(4.9)\qquad M_h[r,s] := \begin{cases} -(1/m_{j_r})A_r A_s & \text{if } j_r = j_s \\ +(1/m_{j_r})A_r A_s & \text{if } j_r = i_s \\ +(1/m_{i_r})A_r A_s & \text{if } i_r = j_s \\ -(1/m_{i_r})A_r A_s & \text{if } i_r = i_s \\ 0 & \text{otherwise.} \end{cases}$$

The diagonal elements of the matrix are

$$M[r,r] = -(1/m_{j_r}) \cdot A_r^2 - (1/m_{i_r}) \cdot A_r^2 = -((1/m_{j_r}) + (1/m_{i_r}))d_r^2 .$$

On the right side of the SLE we have

$$b_r = -A_r \cdot \dot{A}_r = -(P_{j_r} - P_{i_r})(\dot{P}_{j_r} - \dot{P}_{i_r}) .$$

Such equation systems have a unique solution if $Rank(M) = m$. The calculated impulses $A_k x_k$ correct all differences in velocity which are possibly present. If $Rank(M) < m$ applies, correction of the velocity can only be carried out if the right side B can be represented as a linear combination of the column vectors of M. In such cases we can obtain a solution for the SLE by determining the pseudo-inverse (also called Moore-Penrose inverse). It is well known that full rank matrices are a requirement for certain dynamic simulation procedures [Eich-Soellner et al. 1998].

If $Rank(M) < m$ is observed, this indicates that some of the constraints are redundant and can be deleted without changing the kinematic or dynamic properties of the mechanical system. A cuboid with 8 vertex masses and perfect "rigidity" provided by 7*8/2=28 constraints has $Rank(M) = 18$. However, if redundant constraints are removed (18 connections remain), a full rank matrix is obtained for the reduced system.

This procedure can be generalized. One identifies those point sets in a PMS which constitute a rigid body. The connection structure between the associated points is then reestablished by starting with three pairwise connected points and adding one new point at a time, connected to three already existing points (with constraints) whose connection vectors are linearly independent. If two rigid bodies structured in this manner are connected together by a revolute joint, i.e., by two point-to-point connections, a further constraint must be removed without injuring the rigid body properties.

The problem can also be solved algebraically. If we have a redundant system with $Rank(M) = m_0 < m$, one determines a maximal subset of m_0 constraints, so that the matrix is regular for this reduced system. This method can always be carried out, and finally results in a maximum yet non-redundant connection structure with a regular matrix. This therefore proves:

Theorem: *For each D-consistent point mass system, a maximum subset of redundant and therefore superfluous constraints can be removed so that the dynamics and kinematics of the remaining system are equivalent to the initial system, and that the matrix M of the velocity correction is regular. The following therefore is true for all possible configurations of a non-redundant point mass system: $Rank(M) = m$ and $|\det(M)| > 0$. Arbitrary presettings of point velocities can be converted into a V-consistent state by correcting the velocity.*

PMSs can be imagined where the iterative correction of velocity does not converge even though $Rank(M) = m$ is true, since the iterative procedure of velocity correction solves the SLE with a variant of the Gauß-Seidel method, which does not guarantee convergence even if the SLE can be uniquely solved. It is therefore appropriate to solve the SLE for the velocity correction non-iteratively. This also has the advantage that the parameter $v_{\max}$ is of no use anymore. The matrices M are usually sparse and therefore permit faster solutions of the equation systems, see [Baraff 1996] for details.

5. Integration steps by Newton's method

To carry out an integration step, we usually assume that the PMS is in a consistent state (time $t = 0$) and has to be simulated in the forward direction for a time interval of length h. However, this condition is not always satisfied if higher order formulae [Schmitt et al. 2005] are used. In these cases we start with a purely ballistic forward motion with time intervals of length $h/2, h/3, h/4$ etc. The resulting dynamic state is neither D-consistent nor V-consistent. It is therefore necessary to examine the general case and not to assume that D-consistency or V-consistency exists. In the following, we do not deal with halve stepping as described above but always use full time steps of length *h* as it was done in (2.6).

Without the application of correction impulses the motion is ballistic (see also (2.5)):

(5.1) $$P_r(h) := P_r(0) + h \cdot \dot{P}_r(0) + 0.5 g_r h^2 = LA(P_r(0), h)$$

Using the abbreviation $A_k(h) := (P_{j_k}(h) - P_{i_k}(h))$ we introduce the constraint functions

$$f_k(X) := (A_k(h) + h \cdot \Delta w_k(X))^2 - d_k^2 \quad (k = 1, 2, ..., m).$$

We have to determine impulse strengths $X = (x_1, x_2, ..., x_m)^T$ which, when applied at time $t = 0$, satisfy the following equations

(5.2) $$f_k(X) = 0 \qquad (k = 1, ..., m)$$

at time $t = h$.

This is because f_k already includes the additional velocities caused by the still unknown impulses (terms $\Delta w_k(X)$) which should establish D-consistency again at time h.

In order to calculate an approximate solution X for the system (5.2) of quadratic equations, we apply a step of Newton's method with the start value $X_0 = (0, 0, ..., 0)^T$. With the $m \times m$ matrix (Jacobi matrix)

(5.3) $$M(X) := \begin{pmatrix} grad(f_1(X)) \\ grad(f_2(X)) \\ ..... \\ ..... \\ grad(f_m(X)) \end{pmatrix},$$

where the gradient is defined by

$$grad(f_k(X)) := \left(\frac{\partial}{\partial x_1} f_k(X), \frac{\partial}{\partial x_2} f_k(X), ..., \frac{\partial}{\partial x_m} f_k(X) \right),$$

and the vector $F(X)$ by $F(X) := (f_1(X), f_2(X), ..., f_m(X))^T$.

One computes an initial approximation X_1 by solving

(5.4) $$F(X_0) + M(X_0) \cdot X_1 = 0.$$

With the abbreviation $X_0 = 0$, we therefore have the SLE

(5.5) $$M(0) \cdot X_1 = -F(0).$$

The matrix $M(0)$ is constant, its elements are calculated as follows:

(5.6)
$$M[r,s] = \frac{\partial}{\partial x_s} f_r(X := 0) = 2(A_r(h) + h \cdot \Delta w_r(0)) h \frac{\partial}{\partial x_s} \Delta w_r(0) =$$
$$= 2hA_r(h) \frac{\partial}{\partial x_s} \Delta w_r(0),$$

since $\Delta w_r(0) = 0$. We transfer the factor $2h$ to the right side of the equation system, see (5.9).

A copy of (4.4) is

$$\Delta w_r(X) := \Delta v_{j_r}(X) - \Delta v_{i_r}(X) =$$
$$= (1/m_{j_r}) \left(\sum_{k=1}^{m} sig(k, j_r) A_k \cdot x_k \right) - (1/m_{i_r}) \left(\sum_{k=1}^{m} sig(k, i_r) A_k \cdot x_k \right).$$

From this the derivatives can be obtained:

(5.7)
$$\frac{\partial}{\partial x_s} \Delta w_r(X) = (1/m_{j_r}) \left(\sum_{k=s} sig(k, j_r) A_k \right) - (1/m_{i_r}) \left(\sum_{k=s} sig(k, i_r) A_k \right)$$
$$= (1/m_{j_r}) sig(s, j_r) A_s - (1/m_{i_r}) sig(s, i_r) A_s$$

We can now extract the individual matrix elements for $s \neq r$

(5.8)
$$M_h[r,s] := \begin{cases} -(1/m_{j_r}) A_r(h) A_s & if \ j_r = j_s \\ +(1/m_{j_r}) A_r(h) A_s & if \ j_r = i_s \\ +(1/m_{i_r}) A_r(h) A_s & if \ i_r = j_s \\ -(1/m_{i_r}) A_r(h) A_s & if \ i_r = i_s \\ 0 & otherwise. \end{cases}$$

and the diagonal elements

$$M_h[r,r] := -((1/m_{j_r}) + (1/m_{i_r})) A_r(h) A_r.$$

On the right side of the SLE, we have the elements

(5.9) $\quad b_r := -f_r(0)/2h = (d_r^2 - A_r(h)^2)/2h$.

This SLE is clearly also valid if the dynamic state at time $t = 0$ is neither D-consistent nor V-consistent, for we haven't made use of these properties anywhere.

If the vector of the impulse strengths $X = (x_1, x_2, ..., x_m)^T$ is computed and the impulses applied at time $t = 0$, we have the motion

(5.10) $$P_r(h) := P_r(0) + h \cdot \left(\dot{P}_r(0) + \frac{1}{m_r} \sum_{k=1}^{m} sig(k,r) A_r(0) \cdot x_k \right) + 0.5 g_r h^2 .$$

The equation system obtained for the impulses does not guarantee that the total correction is achieved in one step. Since Newton's method works iteratively, we must also carry out corrections here in several iterations. We have observed, however, that more than two or three steps are seldom required.

We execute the second and further steps of Newton's method such that we apply the impulses of the first solution X_1 to the appropriate point masses and thus achieve a new dynamic state. The A_k values remain unchanged in the process, the $\dot{A}_k$ values change. We can proceed exactly as above with this changed dynamic state in order to determine a further correction etc. Since each of the terms $A_r(h)$ is changed slightly, the SLE must be recomputed in each step. If, finally,

$$\left\| LA(P_{j_k}(t), h) - LA(P_{i_k}(t), h) \right| - d_k \Big| \le \delta_{\max}$$

is satisfied for all $k = 1, ..., m$ (see (2.6)), Newton's procedure is terminated.

Following our considerations on the velocity correction, we can now state:

Theorem: *Each PMS with a regular matrix M for the velocity correction permits h-integration steps for a sufficiently small time interval h using Newton's method. This particularly applies to all point mass systems with non-redundant constraints.*

Proof: Since $A_k(h) = (P_{j_k}(h) - P_{i_k}(h)) = A_k + O(h)$ and $M_h[r,s] \approx \pm(1/m_{j_r}) A_r(h) A_s$ it is clear that we have

$$\lim_{h \to 0} M_h = M ,$$

where M is the corresponding matrix for the velocity correction which is not dependent on h.

If we have $\det(M) \neq 0$, which we can generally presuppose, it is also the case that for sufficiently small h $\det(M_h) \neq 0$ because of the continuity of M_h with respect to h. For sufficiently small values h we therefore have non-singular matrices when using Newton's method, not only with the first approximation step but also with all approximation steps which may subsequently follow.

The above stated theorem makes clear that in critical situations we have to shorten the step size *h* in order to establish convergence. It is always possible to find such h's if the constraints of the system are non-redundant.

6. Integration steps with Taylor expansion

In a consistent dynamic state at time $t_0 = 0$, the $P_l(t_0), \dot{P}_l(t_0) \quad (l = 1,...,n)$ are known and compatible with one another. The trajectory of the point masses starting at time $t_0 = 0$ can be approximated by the short Taylor series:

(6.1) $$P_l(t) = P_l(0) + \dot{P}_l(0) \cdot t + O(t^2).$$

Using Newton's second law as well as the conditions defined by the constraints, we try to extend this Taylor series in that we also determine the values for $\ddot{P}_l(0), \dddot{P}_l(0), \ddddot{P}_l(0)$ etc.

Newton's equations for a point mass system read

$$\ddot{P}_l(t) = g_l + (1/m_l)\sum_{k=1}^{m} sig(k,l)(P_{j_k}(t) - P_{i_k}(t))(\lambda_{0k} + \lambda_{1k}t + \lambda_{2k}t^2 + ...)$$

for all $l = 1,...,n$.

With the exception of g_l, there are only constraint forces in our PMS, and these must act exactly in the direction of the constraint vectors

$$A_k(t) := (P_{j_k}(t) - P_{i_k}(t)) \qquad (k = 1,...,m).$$

Their relative strengths are defined by the scalar weighting functions

(6.2) $$q_k(t) := \lambda_{0k} + \lambda_{1k}t + \lambda_{2k}t^2 + ...$$

which are generally time-dependent as well. Since the constraint forces only act in the direction of the constraint vectors and the point masses involved do not change their distance, these forces are workless which is in agreement with the principle of virtual work. With the abbreviated notation we obtain

(6.3) $$\ddot{P}_l(t) = g_l + (1/m_l)\sum_{k=1}^{m} sig(k,l)A_k(t)q_k(t).$$

We now attempt to determine the values $\ddot{P}_l(0)$ which are still unknown. For this we enlarge (6.1) for $l = 1,...,n$

(6.4) $$P_l(t) = P_l(0) + \dot{P}_l(0) \cdot t + (1/2) \cdot \ddot{P}_l(0) \cdot t^2 + O(t^3)$$

and wish to satisfy the constraints up to terms of order t^2. Using the notation from (2.3) and (2.4), we have to examine the following equation for every constraint $C_r = (i_r, j_r, d_r)$

$$(A_r(0) + A_r^{(1)}(0) \cdot t + (1/2) \cdot A_r^{(2)}(0) \cdot t^2)^2 - d_r^2 = 0,$$

or in abbreviated notation

(6.5) $$(A_{0r} + A_{1r} \cdot t + (1/2) \cdot A_{2r} \cdot t^2)^2 - d_r^2 = 0.$$

These equations $(r = 1...m)$ should be satisfied up to terms of order t^2. If the multiplication is carried out and the resulting terms sorted according to powers of *t*, the following conditions are obtained:

(6.6) For t^0: $(A_{0r})^2 - d_r^2 \stackrel{!}{=} 0$ is always satisfied because the dynamic state is D-consistent at time $t = 0$.

(6.7) For t^1: $2A_{0r} \cdot A_{1r} \stackrel{!}{=} 0$ is always satisfied because the dynamic state is V-consistent at time $t = 0$.

(6.8) For t^2: $A_{0r}A_{2r} + A_{1r}{}^2 \stackrel{!}{=} 0$

This equation contains the desired second derivatives in the term A_{2r}. We must therefore solve the SLE

(6.9) $\forall r = 1,...,m$: $A_{0r}A_{2r} = -(A_{1r})^2$

For a certain joint r with $C_r = (i_r, j_r, d_r)$ we obtain by inserting (6.3)

$$A_{2r} = (P_{j_r}^{(2)} - P_{i_r}^{(2)}) =$$

$$= g_{j_r} + (1/m_{j_r}) \sum_{k=1}^{m} sig(k, j_r) A_k(0) q_k(0) - g_{i_r} - (1/m_{i_r}) \sum_{k=1}^{m} sig(k, i_r) A_k(0) q_k(0)$$

When we set $gterm_r := g_{j_r} - g_{i_r}$ and use the abbreviated notation, we have

$$A_{2r} = (1/m_{j_r}) \sum_{k=1}^{m} sig(k, j_r) A_{0k} \lambda_{0k} - (1/m_{i_r}) \sum_{k=1}^{m} sig(k, i_r) A_{0k} \lambda_{0k} + gterm_r .$$

In order to calculate the values $\ddot{P}_l(0)$ we have to determine the unknowns λ_{0k}. Based on (6.8) we obtain for $r = 1,...,m$ the equations

(6.10)
$$A_{0r} \left((1/m_{j_r}) \sum_{k=1}^{m} sig(k, j_r) A_{0k} \lambda_{0k} - (1/m_{i_r}) \sum_{k=1}^{m} sig(k, i_r) A_{0k} \lambda_{0k} \right)$$
$$= -(A_{1r})^2 - A_{0r} \cdot gterm_r .$$

The matrix M of the SLE

$$M \cdot \begin{pmatrix} \lambda_{01} \\ \lambda_{02} \\ . \\ . \\ \lambda_{0m} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ . \\ . \\ b_m \end{pmatrix}$$

is therefore filled as follows:

For $r \neq s$, we have

$$(6.11a)\qquad M[r,s]=\begin{cases} -(1/m_{j_r})A_{0r}A_{0s} & \text{if } j_r = j_s \\ +(1/m_{j_r})A_{0r}A_{0s} & \text{if } j_r = i_s \\ +(1/m_{i_r})A_{0r}A_{0s} & \text{if } i_r = j_s \\ -(1/m_{i_r})A_{0r}A_{0s} & \text{if } i_r = i_s \\ 0 & \text{otherwise.} \end{cases}$$

and the diagonal elements are

$$(6.11b)\qquad M[r,r]=-((1/m_{j_r})+(1/m_{i_r}))A_{0r}^2 .$$

On the right side of the SLE we have

$$(6.11c)\qquad b_r := -(A_{1r})^2 - A_{0r}\cdot gterm_r = -(\dot{P}_{j_r}-\dot{P}_{i_r})^2 - A_{0r}\cdot gterm_r .$$

It is again remarkable here that there is a great similarity with the matrices (5.8) and (4.9) obtained in the previous paragraphs. The matrix (6.11a) is identical to that from the velocity correction.

After solving the SLE we can compute the accelerations $\ddot{P}_l(0)$ and therefore obtain the desired expanded Taylor series (6.4). Choosing a specific step size h we can carry out an h integration step:

$$(6.12)\qquad \begin{aligned} P_l(h) &= P_l(0)+\dot{P}_l(0)\cdot h+(1/2)\cdot\ddot{P}_l(0)\cdot h^2+O(h^3) \\ \dot{P}_l(h) &= \dot{P}_l(0)+\ddot{P}_l(0)\cdot h+O(h^2) \end{aligned}$$

From a practical viewpoint, this simulation method is uninteresting because it is not very accurate. The dynamic state after one integration step is only approximately D-consistent and V-consistent. However, the Taylor method has the great advantage that we have a specific truncation error of order $O(h^3)$. If a Lipschitz condition is fulfilled in an environment of the exact solution, it is guaranteed that the solution approximated by *h*-integration steps converges towards the exact solution if $h\to 0$.

It can be additionally stated for the Taylor method demonstrated here that, if the $\ddot{P}_l(0)$ are known, the derivatives $P_l^{(3)}(0)$, $P_l^{(4)}(0)$,... can also be calculated step-by-step using exactly the same course of action:

The approach (6.4) is continued analogously with

$$P_l(t)=P_l(0)+\dot{P}_l(0)\cdot t+(1/2)\cdot\ddot{P}_l(0)\cdot t^2+(1/6)\dddot{P}_l(0)\cdot t^3+O(t^4)$$

and the equation

$$(A_{0r}+A_{1r}\cdot t+(1/2)\cdot A_{2r}\cdot t^2+(1/6)\cdot A_{3r}\cdot t^3)^2-d_r^2=0$$

has now to be fulfilled up to terms of order t^3. For the term t^3 the resulting equation to be satisfied is

$$A_{1r}A_{2r}+(1/3)A_{0r}A_{3r}=0,$$

which leads to the SLE

$$A_{0r} A_{3r} = -3 A_{1r} A_{2r}$$

with which the λ_{1r} can finally be determined. In this manner, one could increase the order of the Taylor method as desired. However, such an increase in order is not relevant for our proof.

Some insight is obtained concerning the drift problem of the Taylor method. One observes permanently increasing constraint errors during the simulation which can no longer be corrected by the Taylor method and the essentially equivalent ubiquitous Lagrange multiplier method because a return to a consistent dynamic state cannot be enforced. The conditions (6.6) and (6.7) are simply ignored. Nevertheless, the solution converges towards the exact solution in the limiting case $h \to 0$. This generally known drift problem has been addressed in an important and frequently cited paper [Baumgarte 1972] and in numerous subsequent publications. In contrast to the Taylor and Lagrange multiplier method, the impulse procedure is completely free of drift problems if $\delta_{\max}$ (see (2.6)) is selected sufficiently small.

7. Remarks on our differential-algebraic equation system

We have to solve a system of differential-algebraic equations (DAE)

$$\begin{aligned} &\ddot{P}_r(t) = g_r + (1/m_r) \sum_{k=1}^{m} sig(k,r)(P_{j_k}(t) - P_{i_k}(t)) q_k(t) \qquad (r = 1,...,n) \\ &(P_{j_k}(t) - P_{i_k}(t))^2 - d_k^2 = 0 \qquad (k = 1,...,m) \end{aligned} \tag{7.1}$$

with consistent initial conditions. Using common abbreviations (see for example [Hairer, Wanner 1996]) this results in a system structure

$$\begin{aligned} &\ddot{P}(t) = f(P(t), q(t)), \\ &C(P(t)) = 0. \end{aligned}$$

Introducing $z_1(t) := P(t)$ and $z_2(t) := \dot{P}(t)$, this DAE of second order is converted into an equivalent system of first order

$$\dot{z}_1(t) = z_2(t) \tag{7.2}$$

$$\dot{z}_2(t) = f(z_1(t), q(t)) \tag{7.3}$$

$$C(z_1(t)) = 0 \quad . \tag{7.4}$$

with consistent initial conditions $z_1(0)$ and $z_2(0)$.

Since the $q_k(0) = \lambda_{0k}$ are not yet known, one cannot evaluate $f(z_1(0), q(0))$, and therefore the initial value problem cannot yet be solved numerically. The constraints C are now differentiated twice so that one obtains the equivalent conditions $\ddot{C}(z_1(t)) = 0$. If the corresponding expressions are written out in our notation, one obtains after canceling out constant factors

$$A_k(t) \cdot \ddot{A}_k(t) + \dot{A}_k^2(t) = 0 \quad (k = 1,...,m). \tag{7.5}$$

We set $t = 0$ and wish to determine λ_{0k} through substitution of $f(z_1(0), q(0)) = \ddot{P}(0)$ into this new constraint condition:

(7.6) $A_k(0)(f_{j_k}(z_1(0),q(0)) - f_{i_k}(z_1(0),q(0))) = -\dot{A}_k^2(0)$

In this expression, all terms are known with the exception of $\lambda_{0k} = q_k(0)$. This leads directly to (6.8) with the matrix M from the velocity correction. Such an equation system always has a unique solution if the constraints of the PMS are non-redundant. The terms $\lambda_{0k} = q_k(0)$ are available after solving the linear system. If consistent initial values $P(0), \dot{P}(0)$ and the λ_{0k} are known, the right sides of (7.2) and (7.3) can be evaluated. We are thus in a position to solve the DAE with methods known for the numeric solution of ordinary differential equations. For example, we can now use the simple Euler method in order to determine an approximate solution for $P(h), \dot{P}(h)$. Further integration steps can follow to compute $P(i \cdot h), \dot{P}(i \cdot h)\ (i = 2,3,...)$.

The described method agrees with the Lagrange multiplier method for dynamic simulations of multibody systems as repeatedly described in the literature and also frequently used. It is of course necessary to use integration codes of higher order such as Runge-Kutta and stability terms in the sense of Baumgarte or projection methods [Eich-Soellner, Führer1998], [Ascher et al. 1994] in order to achieve relatively accurate simulation results, for the conditions (6.6) and (6.7) are ignored.

It is well known (see [Stoer, Bulirsch 2002] and many others) that, under very weak prerequisites – namely the existence of a Lipschitz condition – the numerically calculated solution converges towards the exact solution of the DAE for $h \to 0$ provided the numeric procedure applied to solve the system of differential equations is at least of order $O(h)$, which already applies to the Euler method. We can thus state:

Theorem: *Point mass systems at least then possess uniquely determined solution trajectories for consistent initial conditions if the matrices for the velocity correction are nonsingular and if a Lipschitz condition is satisfied. Under these prerequisites, the solutions of the Taylor method then also converge towards the exact solution trajectories.*

8. Proof of correctness for the impulse-based dynamic simulation method

The proof of correctness should assure that the numeric solution of the impulse-based dynamic simulation converges towards the exact solution of the dynamics problem if $h \to 0$ and $\delta_{\max} \to 0$. We shall provide a proof for this in that we show that the solutions generated by the Taylor method and the impulse-based procedure converge towards the same functions for $h \to 0$. With the Taylor method, the following acceleration term results at the end of a time step h (see (6.12)):

(8.1) $$(1/2)\ddot{P}_r(0)h^2 = (1/2)h^2\left(g_r + \frac{1}{m_r}\sum_{k=1}^{m} sig(k,r)A_k(0)\cdot\lambda_{0k}\right).$$

With the impulse method, the corresponding term, i.e., the difference to $P_r(0) + h\dot{P}(0)$, is defined by the expression

(8.2) $$(1/2)g_r h^2 + h\frac{1}{m_r}\sum_{k=1}^{m} sig(k,r)A_k(0)\cdot x_k$$

(see (5.10)). Both terms clearly agree for $r = 1,...,n$ if

$$x_k = (h/2)\lambda_{0k}$$

for all $k = 1, 2, ..., m$.

Because $A_r \dot{A}_r = 0$ and $A_r{}^2 = d_r^2$, the right side (5.9) of the SLE (5.8) for the impulse method can be converted as follows

$$\begin{aligned} -f_r(0)/2h &= (d_r^2 - A_r(h)^2)/2h = \\ &= (1/2h)(d_r^2 - (A_r + \dot{A}_r h + (1/2)gterm_r h^2)^2) \\ &= (1/2h)(d_r^2 - A_r^2 - \dot{A}_r^2 h^2 - (1/4)gterm_r^2 h^4 \\ &= -2A_r \dot{A}_r h - A_r gterm_r h^2 - \dot{A}_r gterm_r h^3) \\ &= -(h/2)(\dot{A}_r{}^2 + A_r gterm_r) + O(h^2). \end{aligned}$$

Comparison with the right side of the Taylor system (6.11c) shows that, apart from the $O(h^2)$ term, only the factor $h/2$ is different.

The matrices M_h of (5.8) and M of (6.11a) of the two systems for determination of x_k and λ_{0k} respectively are very similar. With the Taylor method, the matrix M does not have terms with h. Because $A_r(h) = (P_{j_r}(h) - P_{i_r}(h)) = A_r + O(h)$ with the impulse method, it is always the case that $A_r(h)A_s = A_r A_s + O(h)$, and we have therefore $M_h = M + \tilde{M}(h)$. Here, $\tilde{M}(h)$ means that each matrix element is at least of order $O(h)$. The following relationships now result between the solutions of the two equation systems:

$M\lambda = b$	Solution is λ
$M\lambda' = (h/2)b$	Solution is $\lambda' = (h/2)\lambda$
$(M + \tilde{M}(h))\lambda'' = (h/2)b$	Solution is $\lambda'' = (h/2)\lambda + O(h^2)$

In order to verify the last line, we use Cramers rule to solve linear systems. We use $A \setminus b$ to identify the matrix A, where one column is substituted by the vector b. For specific components $\bar{\lambda}', \bar{\lambda}''$ of the respective vectors, we have

$$\bar{\lambda}' = \frac{N \cdot h}{D}$$

where $\det(M \setminus (h/2)b) = N \cdot h$ and $\det(M) = D$.

The solution for $\bar{\lambda}''$ is

$$\bar{\lambda}'' = \frac{\det((M + \tilde{M}(h)) \setminus (h/2)b)}{\det(M + h\bar{M})} = \frac{\det(M \setminus (h/2)b) + O(h^2)}{\det(M) + O(h)} = \frac{N \cdot h + O(h^2)}{D + O(h)}$$

The term $O(h^2)$ is part of the numerator because the numerator without the contribution of $\tilde{M}(h)$ already is of order $O(h)$. If an explicit division is now carried out, the result is

$$(N \cdot h + O(h^2)) : (D + O(h)) = \frac{N \cdot h}{D} + \frac{1}{D} \cdot O(h^2) = \lambda'' = \lambda' + O(h^2).$$

The following trial calculation confirms this result:

$$\left(\frac{Z\cdot h}{N}+\frac{1}{N}\cdot O(h^2)\right)\cdot\left(N+O(h)\right)=Z\cdot h+\frac{N}{N}O(h^2)+\frac{Z\cdot h}{N}O(h)+\frac{1}{N}\cdot O(h^3)$$
$$=Z\cdot h+O(h^2)$$

Specific components $\bar{x}$ of the solution of $(M+\tilde{M}(h))x=(2/h)b+O(h^2)$ are now calculated by

$$\bar{x}=\frac{\det((M+\tilde{M}(h))\setminus((h/2)b+O(h^2)))}{\det(M+\tilde{M}(h))}=\frac{\det(M\setminus(h/2)b)+O(h^2)}{\det(M)+O(h)}$$
$$=\frac{N\cdot h+O(h^2)}{D+O(h)}=\bar{\lambda}'+O(h^2)=(h/2)\bar{\lambda}+O(h^2)$$

If these values for x are used in (8.2), agreement with (8.1) exists up to terms of order $O(h^2)$, and the difference is of order $O(h^3)$ which is the order of the truncation error. This proves

Theorem: *(Correctness of the impulse method)*

If only one step of Newton's method is carried out at a time step when implementing the impulse method, the solutions of the impulse and Taylor method converge towards the same solution trajectories for $h\to 0$. Since the Taylor method converges towards the correct solution under the Lipschitz prerequisite for $h\to 0$, the impulse method therefore also converges towards the exact solution of the dynamics problem. Since the impulse method can also be extended to the dynamic simulation of multibody systems in the known manner, the above statements also apply to the impulse-based multibody simulation.

The impulse method normally uses more than one Newton step because it is free of drift effects, i.e., it has to compute a closer approximation than the Taylor method. However, in the case of very small values h, only one step is required to match the constraints accurately because of the usually quadratic convergence of Newton's method.

Extension of the theorem from PMSs to multibody systems is the result of the equivalence construction of Section 3. It also clearly results from the above proof that both the presented Taylor method and the impulse-based method have a truncation error of order $O(h^3)$.

9. Concluding discussion

Because we were able to show that a kinematically and dynamically equivalent point mass system can be constructed for each multibody system, we could focus ourselves on point mass systems, thus greatly simplifying our derivations. We could show that the iterative procedures of impulse determination can be substituted by solving linear systems. Because regular matrices result for PMSs with non-redundant constraints, these equations can always be solved. For specifically designed PMSs the iterative procedures converge very slowly because of the similarity with the Gauß-Seidel method. It is therefore recommendable to favor noniterative methods to solve the linear systems.

Through detailed comparison of the impulse method with a Taylor method of second order, we were able to prove that the impulse method converges towards the exact solution of the dynamics problem. This behavior could already be repeatedly observed in numeric simulations.

The argumentation provides further insight into the impulse-based simulation method. The reason for the occasionally significant drift problems with the Taylor method and the essentially identical Lagrange multiplier method was made clear. These methods do not maintain consistent dynamic states, for which reason Baumgarte stabilization and similar procedures have to be applied in order to reduce the drift tendency. Considering this, it is clear why generalized or reduced coordinate formulations are popular especially in the area of engineering dynamics since the drift problem can be eliminated with these formalisms. With closed kinematic chains and complex mechanisms, however, Lagrange multipliers cannot always be avoided, so that one often has to select a combination of the two methods.

On the other hand, the impulse method is shown to be completely free of drifts because the corresponding simulation parameter $\delta_{\max}$ can be chosen as small as desired and combined with the velocity correction, consistent dynamic states are maintained in the course of simulation.

We can finally sum up that the impulse method in the non-iterative form is superior to the widely used method with Lagrange multipliers since it is free of drift problems and is very powerful when impact, collision and friction have to be covered in addition. The existence of impulse methods of higher order [Schmitt et al. 2005] and thus also of higher accuracy, supports the above statement.

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