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# ON THE STABILIZING PROPERTIES OF ENERGY-MOMENTUM INTEGRATORS AND MASS-ORTHOGONAL PROJECTIONS

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**Abstract.** *The modeling of multibody systems in natural coordinates leads to systems of differential-algebraic equations (DAE). Penalty and augmented Lagrangian techniques have been widely used in order to solve this kind of systems. In both cases, penalty forces proportional to the violation of the constraints are included in the equations of motion.*

*Consideration of penalty forces proportional to the violation of the constraints at position level seems to be a convenient option. However, the solutions obtained through such option show unstable behavior due to the progressive and unbounded growth of the constraints energy, being this effect even more noticeable in the augmented Lagrangian formulations.*

*Several methods have been proposed in the literature in order to stabilize the mentioned solutions. In this paper, two of those methods are revised and their respective stabilizing properties analyzed: an energy-momentum integrator, and the trapezoidal rule along with projections of velocities and accelerations onto the constraints manifold. In both cases, natural coordinates are used for the modeling, and the equations of motion are stated through a penalty formulation, in the case of the energy-momentum integrator and an augmented Lagrangian formulation, in the case of the trapezoidal rule with projections.*

*The main difference between the two methods of stabilization compared in the paper consists of the way in which they control the constraints energy: the energy-momentum integrator is obtained under the condition of the exact conservation of the system energy; on the other hand, the mass-orthogonal projections directly act upon the velocities and accelerations provided by the integrator.*

# 1 INTRODUCTION

Several considerations are important if we try to carry out fast and precise simulations in multibody dynamics: the choice of modeling coordinates, the choice of dynamical formulation and the numerical integration scheme along with the numerical implementation. All these matters are very important in order to decide whether a specific method is good or not for a particular purpose.

Some of the most robust methods for real-time dynamics in multibody systems make use of natural or fully Cartesian coordinates in the modeling [1]. These coordinates are dependent by nature, and lead to systems of differential-algebraic equations of motion (DAE) [2] if the widely known method of Lagrange multipliers is applied.

Different formulations used to solve these equations of motion in natural coordinates were developed, like the stabilization technique of Baumgarte [3], penalty and augmented Lagrangian schemes [5], or velocity transformations [6, 7].

Formulations based on penalty and augmented Lagrangian methods have the advantages of being very simple, computationally inexpensive and very robust in the presence of singular configurations or redundant constraints [8].

Generally, it can be said that the choice of the dynamic formulation determines that of the numerical integrator. In this direction different authors proposed several options to successfully integrate the equations arising from constrained multibody systems, using integrators coming from the field of structural dynamics [1, 4, 9].

In [10, 9] it was proposed the use of augmented Lagrangian techniques with penalty only at position level along with the trapezoidal rule. In order to guarantee the correct satisfaction of constraints, different kinds of velocities and acceleration projections were proposed. More recently [11], proposed the use of augmented Lagrangian techniques with other integrators of the Generalized-$\alpha$ family along with projections, which provides very good behavior for real-time applications. The advantages of the projections are the simplicity and the variety of integrators which can be used with them, since the projections are responsible for maintaining the stability of the formulation.

On the other hand, other authors [12, 13, 14], developed a formulation based on an energy conserving penalty scheme, enforcing constraints at the position level, and applied it to the dynamics of multibody systems parametrized with natural coordinates. In this case, the use of penalty at position level has the advantage that permits to derive the constraint forces from a potential function: the constraint energy. The formulation includes the employ of an energy-momentum integrator as integration scheme [16, 17], so that the conservation of the total energy of the system is imposed by construction of the algorithm. Here, the stabilization of the penalty equations of motion arises in a natural manner from the integration scheme.

# 2 PENALTY AND AUGMENTED LAGRANGIAN FORMULATIONS

## 2.1 Description of the formulations

Let us consider a multibody system, compound by rigid bodies, with a configuration defined by a vector $\mathbf{q} \in \mathbb{R}^n$ of natural coordinates. The system will be also subjected to $m$ holonomic constraints $\mathbf{\Phi} \in \mathbb{R}^m$, involving the different points and vectors of the system.

Penalty formulations [5] are a simple manner to introduce the constraints in the equations of motion in the case of dependent coordinates modeling, avoiding to solve a system of $(n+m)$ equations with the coordinates and the Lagrange multipliers. We can derive a penalty formulation by adding three terms to the unconstrained Lagrangian [1].

A fictitious potential:

$$V_{\boldsymbol{\Phi}} = \frac{1}{2}\boldsymbol{\Phi}^{\mathrm{T}}\alpha\omega^2\boldsymbol{\Phi} \tag{1}$$

where $\alpha$ is a penalty factor representing the stiffness of the constraint.

A fictitious dissipative Rayleigh function:

$$G_{\boldsymbol{\Phi}} = -2\alpha\xi\omega\dot{\boldsymbol{\Phi}} \tag{2}$$

where $\xi$ is a factor equivalent to the damping coefficient of the constraint. Finally, a fictitious kinetic energy term:

$$T_{\boldsymbol{\Phi}} = \frac{1}{2}\dot{\boldsymbol{\Phi}}^{\mathrm{T}}\alpha\dot{\boldsymbol{\Phi}} \tag{3}$$

The equations of motion after including these terms are the following,

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}\right) = \mathbf{Q}\left(\mathbf{q},\dot{\mathbf{q}}\right) \tag{4}$$

where **M** is the mass matrix, and **Q** is the generalized applied forces vector of the system, which contains all the external forces.

Penalty formulations have, among others, the problem of choosing the penalty factor $\alpha$. This choice is very important, since large penalty factors will more accurately enforce the fulfillment of the constraint equations but may also lead to numerical problems.

An alternative to overcome the numerical problems associated with penalty formulations, are the augmented Lagrangian formulations [5], whose equations are,

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}\right) + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^{*} = \mathbf{Q}\left(\mathbf{q},\dot{\mathbf{q}}\right) \tag{5}$$

$$\boldsymbol{\lambda}_{i+1}^{*} = \boldsymbol{\lambda}_{i}^{*} + \alpha\left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}\right) \tag{6}$$

being $\boldsymbol{\lambda}^{*}$ a vector containing all the Lagrange multipliers associated to the constraints of the system.

In the limit, the iterative scheme for the Lagrange multipliers leads to the true Lagrange multipliers, so the formulation does not need so large penalty factors to guarantee the fulfillment of the constraint equations, improving its numerical behavior.

### 2.2 Problems reported with penalty and augmented Lagrangian formulations

Several authors have used this approach or some modification of it for many years. One possibility is to enforce the constraints only, applying penalty or augmented Lagrangian formulations given by the following expressions,

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi} = \mathbf{Q}\left(\mathbf{q},\dot{\mathbf{q}}\right); \quad \text{(Penalty)} \tag{7}$$

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^{*} = \mathbf{Q}\left(\mathbf{q},\dot{\mathbf{q}}\right); \quad \text{(Augmented Lagrangian)} \tag{8}$$

These approaches avoid the dissipative term in the equations and the consequence is a slightly unstable behavior with standard integrators, characterized by a progressive and unbounded growth of the constraints energy.

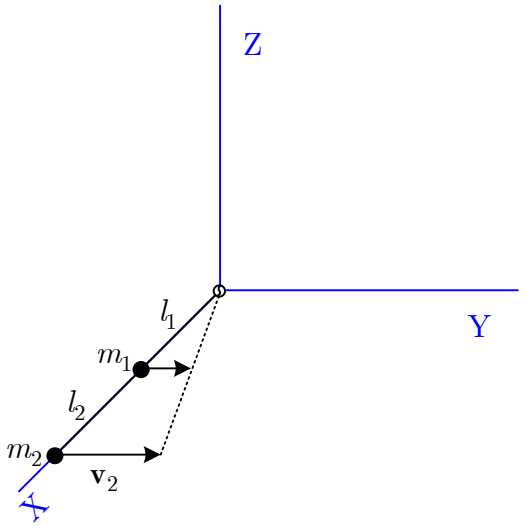


Figure 1: Spherical compound pendulum

In order to illustrate these difficulties, we will consider a spherical compound pendulum [14] (see Figure 1) with two particles with masses $m_1 = m_2 = 1\,\text{kg}$, placed in the center and end of a massless rod of total length $l_1 + l_2$ with $l_1 = l_2 = 1\,\text{m}$. The system is released from the position showed in the figure with initial velocity $\mathbf{v}_2 = 1\ \text{m/s}$.

The system is modeled in natural coordinates with five constraints. The fact that the system has two degrees of freedom and it is modeled with six coordinates (the absolute Cartesian coordinates of both particles), means that one of the constraints is redundant. The constraint equations are,

$$\left(\mathbf{r}_1 - \mathbf{r}_0\right)^{\mathrm{T}} \left(\mathbf{r}_1 - \mathbf{r}_0\right) - l_1^2 \tag{9}$$

$$\left(\mathbf{r}_2 - \mathbf{r}_1\right)^{\mathrm{T}} \left(\mathbf{r}_2 - \mathbf{r}_1\right) - l_2^2 \tag{10}$$

$$\left(\mathbf{r}_1 - \mathbf{r}_0\right) \times \left(\mathbf{r}_2 - \mathbf{r}_0\right) = \mathbf{0} \tag{11}$$

The constraint (9) imposes the constant distance between the origin and the point 1, while the constraint (10) imposes the constant distance between the points 1 and 2. The constraints (11) impose the alignment of the origin and both points. Only two out of the three constraints in (11) are independent.

The simulation is carried out for 20 seconds based on the formulation (7), and integrated with the trapezoidal rule with 0.02 s. of time step. The penalty factor chosen is $10^7$.

Figures 2, 3 and 4 show the behavior of the energy, and the norm of the constraints at position $\|\boldsymbol{\Phi}\|$, velocity $\|\dot{\boldsymbol{\Phi}}\|$, and acceleration level $\|\ddot{\boldsymbol{\Phi}}\|$ along time.

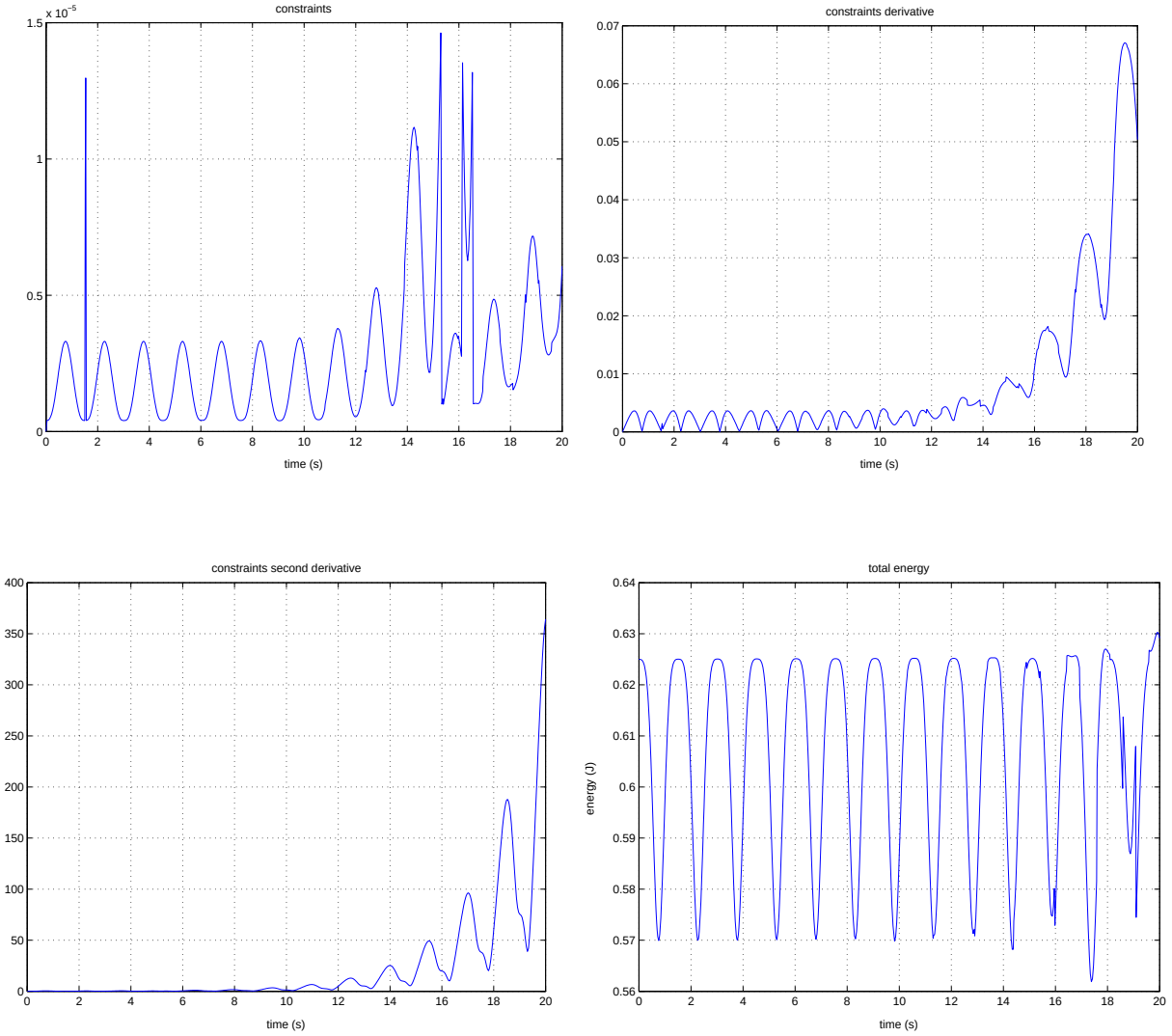


Figure 2: Constraints and energy behavior (Penalty with trapezoidal rule $h = 0.02$ s).

Figure 2 shows that the position constraints are satisfied quite well, as we can expect, but velocities and accelerations show an unstable behavior and they don't satisfy the constraints. Moreover, this behavior is more and more noticeable as the time grows and the vibration of the constraints energy continues increasing, up to a point where the total energy of the system is significantly affected and begins to grow in an uncontrolled manner.

If we increase the time step a little bit up to 0.025 s. these effects are much more evident.

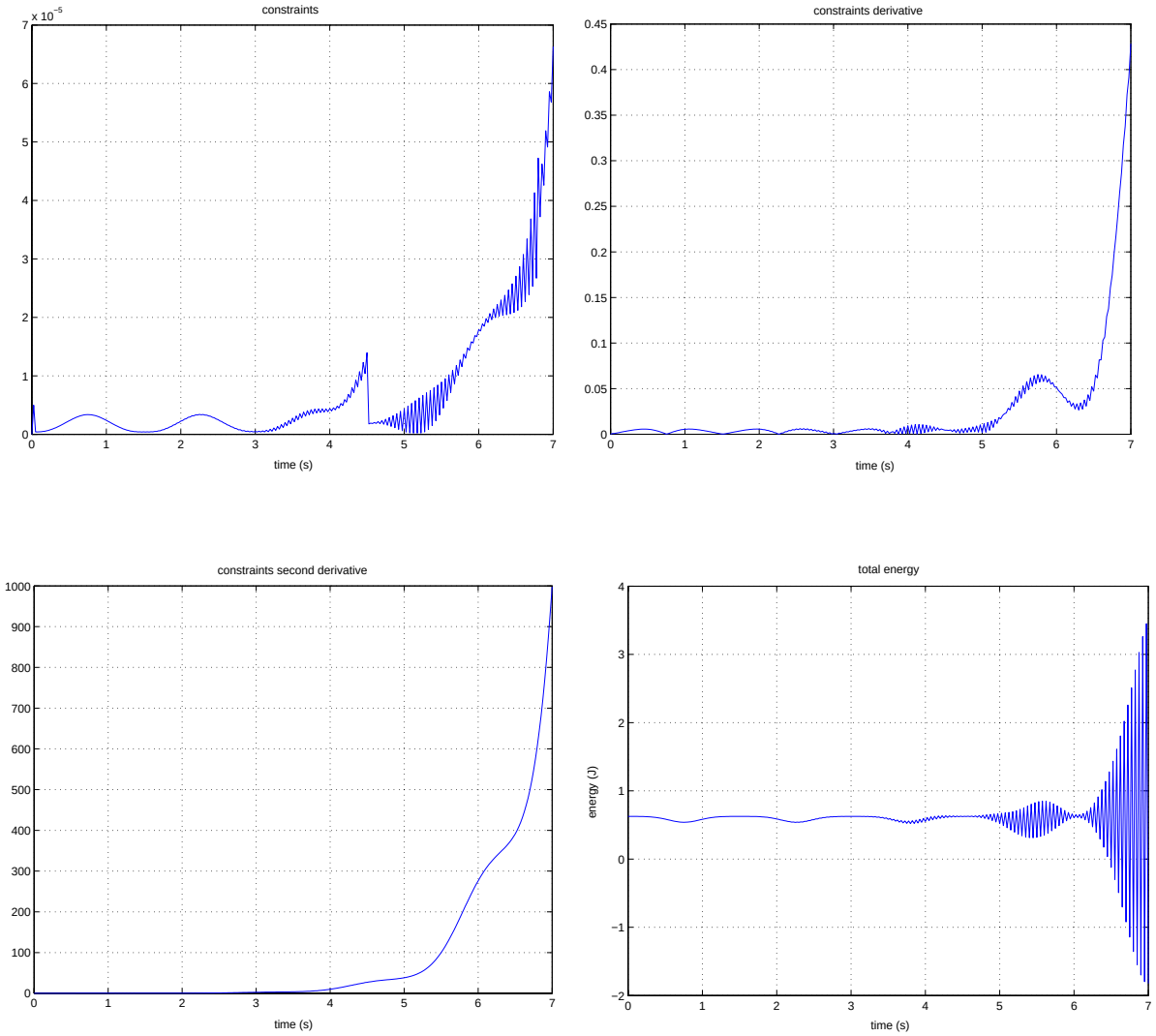


Figure 3: Constraints and energy behavior (Penalty with trapezoidal rule $h = 0.025$ s).

If we focus now on the augmented Lagrangian formulation given by (8), it can be said that it works more or less like the penalty formulation given by (7), and we can apply the same conclusions with the following remarks. Equations (8) does not need so large values of penalty factor as (7) to obtain a good solution and therefore the ill-conditioning problem of the matrices is avoided. Actually, the results are good as long as we put all the penalty terms in the scheme as shown in (5). However the augmented Lagrangian formulation performs worse than the penalty formulation (7), if we only use the penalty term in positions as in (8), as shown in Figure 4.

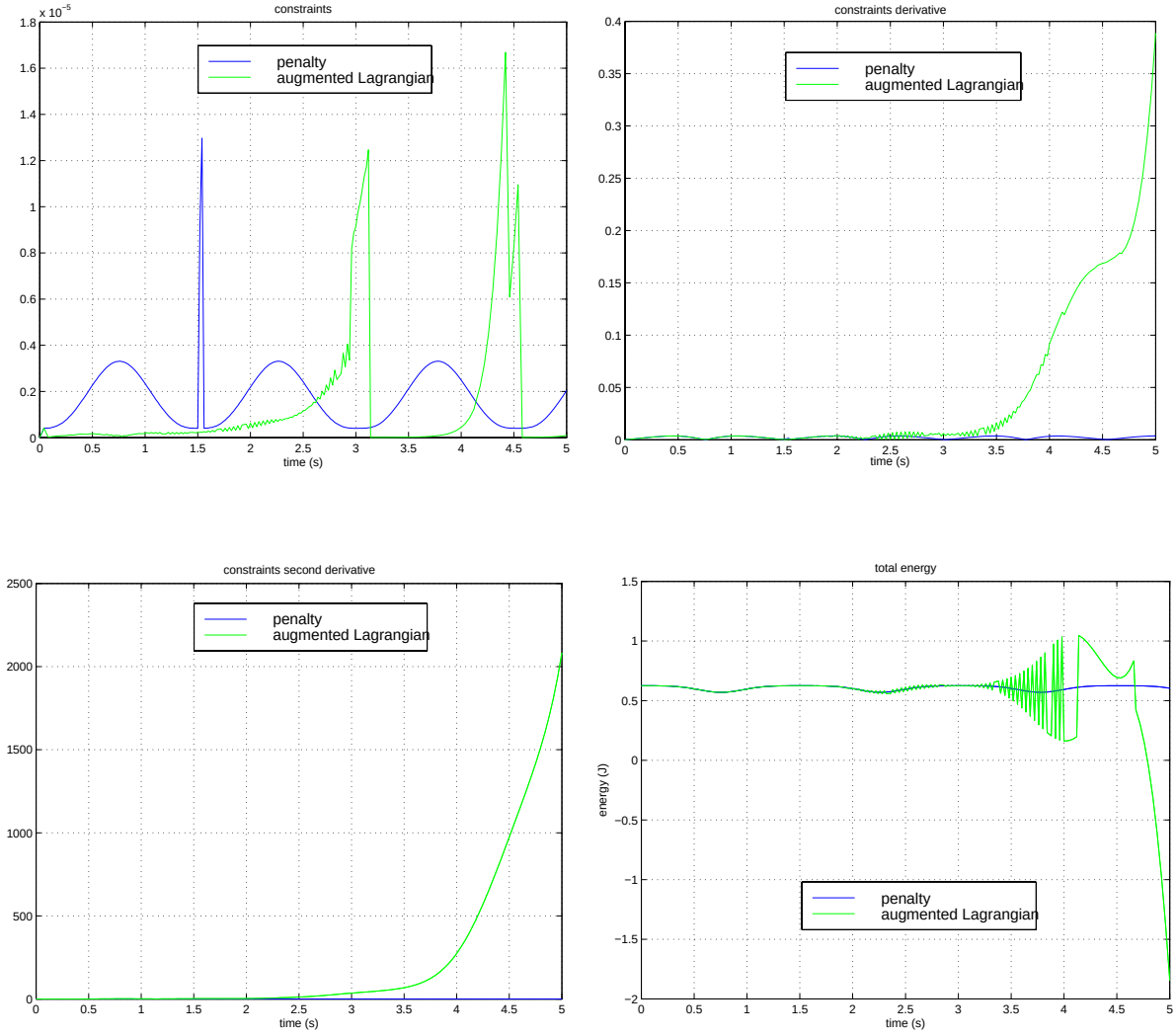


Figure 4: Penalty vs augmented Lagrangian

Figure 4 shows the instability introduced by the iteration of the Lagrange multipliers. It can be concluded that the resulting formulation shows bad properties and does not integrate the motion in cases in which the penalty scheme does.

In next sections, we are going to describe two methods that avoid this observed instability, while enforcing position constraints only.

## 3 THE PROPOSED DYNAMIC FORMULATIONS I: PENALTY WITH ENERGY MOMENTUM INTEGRATOR

This formulation was presented in [12,13,14,18] and exactly conserves the energy and the linear and angular momentum in conservative systems.

The formulation can be found explained in great detail in the cited references; nevertheless, we present here a brief introduction of the proposed methodology applied to the dynamics of multibody systems composed by rigid bodies.

The inclusion of the constraints through a potential (1) plays a key role in the formulation because it preserves the conservative character of the original equations. The form of the equations of motion is,

$$\mathbf{M}\ddot{\mathbf{q}} = \mathbf{Q}_{nc} - \nabla V = \mathbf{Q}_{nc} + \mathbf{Q}_{\Phi} + \mathbf{Q}_{c} \tag{12}$$

$$V = V_{\mathbf{\Phi}} + V_c \tag{13}$$

where $\mathbf{Q}_{nc}$ is the contribution of the non-conservative forces to the generalized forces vector, $V_{\mathbf{\Phi}}$ is the potential (1) of the constraints and $V_c$ is the potential of the remaining conservative forces of the problem (like springs, gravity loads, etc) and all the remaining terms have the same meaning explained before.

In the following subsections we are going to explain briefly how can $\mathbf{Q}_{nc}, \mathbf{Q}_{\mathbf{\Phi}}$ and $\mathbf{Q}_c$ be introduced in the energy-momentum formulation.

### 3.1 Formulation of the constraints

To illustrate the introduction of the constraint forces in the formulation, let us consider a multibody system with a configuration defined by a vector $\mathbf{q} \in \mathbb{R}^n$ of natural coordinates affected by a set of holonomic constraints $\mathbf{\Phi} \in \mathbb{R}^m$, each of them being at most quadratic. We want to pursue the conservation of the total energy between kinetic plus potential energy of the constraints by means of the integrator scheme.

The conservative formulation of the constraints can be rigorously obtained based on the discrete derivative concept introduzed by González [19], and the details can be found in [14, 18]. From a practical point of view, the method can be introduced departing from the implicit midpoint rule,

$$\begin{aligned} \mathbf{q}_{n+1} &= \mathbf{q}_n + h\dot{\mathbf{q}}_{n+1/2} \\ \dot{\mathbf{q}}_{n+1} &= \dot{\mathbf{q}}_n + h\ddot{\mathbf{q}}_{n+1/2} \end{aligned} \tag{14}$$

where $h = t_{n+1} - t_n$, the subscript $n$ represents magnitudes evaluated at the present time step, and the subscript $n+1$ represents magnitudes evaluated at the next time step. The subscript $n+1/2$ represents magnitudes evaluated at the midpoint, this is:

$$\begin{aligned} \mathbf{q}_{n+1/2} &= \frac{\mathbf{q}_{n+1} + \mathbf{q}_n}{2} \\ \dot{\mathbf{q}}_{n+1/2} &= \frac{\dot{\mathbf{q}}_{n+1} + \dot{\mathbf{q}}_n}{2} \end{aligned} \tag{15}$$

In this particular case of a system subjected only to the action of holonomic constraint forces, the equation of motion (12), stands at the midpoint,

$$\mathbf{M}\ddot{\mathbf{q}}_{n+1/2} = -\left(\nabla V_{\mathbf{\Phi}}\right)_{n+1/2} = -\left(\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \alpha \mathbf{\Phi}\right)_{n+1/2} \tag{16}$$

In the expression (16), the term $\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}$ provides the directions of the constraint forces. The idea is to replace the term $\alpha\mathbf{\Phi}$ in (16) by a generic term $\boldsymbol{\sigma}$, evaluated at some point of the interval, while keeping the term $\mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}}$ evaluated at the midpoint. The modified equation of motion, now holds,

$$\mathbf{M}\ddot{\mathbf{q}}_{n+1/2} = -\mathbf{\Phi}_{\mathbf{q}_{n+1/2}}^{\mathrm{T}} \boldsymbol{\sigma} \tag{17}$$

If we pose the balance between kinetic and potential energy at $n$ and $n+1$,

$$T_{n+1} - T_n = -\left(V_{n+1} - V_n\right) \tag{18}$$

$$\frac{1}{2}\left(\dot{\mathbf{q}}_{n+1}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1}-\dot{\mathbf{q}}_{n}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n}\right)=-\frac{1}{2}\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n}\right) \tag{19}$$

Using the second equation in (14) and with (17) the following relation is obtained,

$$T_{n+1}-T_{n}=-\left(\mathbf{q}_{n+1}^{\mathrm{T}}-\mathbf{q}_{n}^{\mathrm{T}}\right)\boldsymbol{\Phi}_{\mathbf{q}_{n+1/2}}^{\mathrm{T}}\boldsymbol{\sigma}=-\frac{1}{2}\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n}\right)=-\left(V_{n+1}-V_{n}\right) \tag{20}$$

In this work the modeling of the systems is made with natural coordinates, where the majority of the constraints are quadratic at most. In this case the following relation holds,

$$\boldsymbol{\Phi}_{\mathbf{q}_{n+1/2}}^{\mathrm{T}}\left(\mathbf{q}_{n+1}-\mathbf{q}_{n}\right)=\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n} \tag{21}$$

which introduced in (20) results,

$$T_{n+1}-T_{n}=-\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\right)\boldsymbol{\sigma}=-\frac{1}{2}\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n}\right)=-\left(V_{n+1}-V_{n}\right) \tag{22}$$

We can see that the equality (22) is true if we make $\boldsymbol{\sigma}=\alpha\bar{\boldsymbol{\Phi}}_{n+1/2}=1/2\,\alpha\left(\boldsymbol{\Phi}_{n+1}+\boldsymbol{\Phi}_{n}\right)$,

$$\begin{aligned}T_{n+1}-T_{n}&=-\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\right)\alpha\bar{\boldsymbol{\Phi}}_{n+1/2}=-\frac{1}{2}\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}+\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n}-\boldsymbol{\Phi}_{n}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}\right)=\\&-\frac{1}{2}\left(\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n+1}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1}\right)=-\left(V_{n+1}-V_{n}\right)\end{aligned} \tag{23}$$

In case we have constraints of order higher than two, the mean value theorem guarantees the existence of a position $\mathbf{q}_{n+\beta}=\mathbf{q}_{n}+\beta\left(\mathbf{q}_{n+1}-\mathbf{q}_{n}\right)$ where the following relation holds,

$$\boldsymbol{\Phi}_{\mathbf{q}_{n+\beta}}^{\mathrm{T}}\left(\mathbf{q}_{n+1}-\mathbf{q}_{n}\right)=\boldsymbol{\Phi}_{n+1}-\boldsymbol{\Phi}_{n} \tag{24}$$

and therefore the conservative properties of the algorithm are preserved.

### 3.2 Formulation of springs

Let us suppose that we have a multibody system with a spring, acting between two points $A$ and $B$. The expression of the force exerted by the spring over point A is,

$$\mathbf{f}_{A}^{s}=\mathrm{f}^{s}\left(s\right)\frac{\left(\mathbf{r}_{A}-\mathbf{r}_{B}\right)}{s} \tag{25}$$

Where $s=\left\|\mathbf{r}_{A}-\mathbf{r}_{B}\right\|$.

In this case we can proceed in a similar way like we did in the last subsection. The final expression for the energy-momentum formulation of the spring force over point A, leads to the following relation,

$$\mathbf{f}_{A}^{s}=-\frac{2\left(V_{n+1}^{s}-V_{n}^{s}\right)}{s_{n+1}^{2}-s_{n}^{2}}\left(\mathbf{r}_{A}-\mathbf{r}_{B}\right)_{n+1/2} \tag{26}$$

where $V_{n+1}^{s}$ and $V_{n}^{s}$, are the potential energy of the spring at $t_{n+1}$ and $t_{n}$ respectively. In the general case of a nonlinear spring, this potential can be defined as follows.

$$V^{s}\left(s\right)=-\int_{s_{0}}^{s}\mathrm{f}^{s}\left(\psi\right)d\psi \tag{27}$$

being $s_0$ the position of the spring in which the potential energy is zero, and $s$ the position in which we want to calculate the potential energy.

With this formulation, the contribution of the spring to the generalized forces vector is,

$$\mathbf{Q}_c^s = \begin{pmatrix} \mathbf{f}_A^s \\ \mathbf{f}_B^s \end{pmatrix} = -\frac{2\left(V_{n+1}^s - V_n^s\right)}{s_{n+1}^2 - s_n^2} \begin{pmatrix} \mathbf{r}_A - \mathbf{r}_B \\ \mathbf{r}_B - \mathbf{r}_A \end{pmatrix}_{n+1/2} \tag{28}$$

Despite of the convenience of natural coordinates, it can be very useful to have a relative coordinate, between the points on which the spring is acting. In this case, the force exerted by the spring is included as a scalar force to this relative coordinate, so the contribution of the spring to the generalized forces vector is,

$$Q_c^s = \mathrm{f}^s(s) \tag{29}$$

In the case of the energy-momentum formulation, the expression (29) is given by,

$$Q_c^s = -\frac{V_{n+1}^s - V_n^s}{s_{n+1} - s_n} \tag{30}$$

The formulae (28) or (30) guarantee that the spring will not remove or introduce artificial energy in the whole system.

### 3.3 Gravity forces

The gravity forces can be included as constants in the vector of conservative generalized forces, $\mathbf{Q}_c$, to the corresponding points of each body, without affecting to the conservative properties of the system.

### 3.4 Non-conservative forces

Non-conservative forces are calculated with the standard midpoint rule. So the contribution of general force, $\mathbf{f}_{nc}$ to the generalized forces vector $\mathbf{Q}_{nc}$, takes the form,

$$\mathbf{Q}_{nc} = \left(\mathbf{f}_{nc}\right)_{n+1/2} \tag{31}$$

### 3.5 Final form of the equations of motion

Summarizing the results of the previous sections, the conservative formulation of the discrete equations of motion have the following form,

$$\mathbf{M}\ddot{\mathbf{q}}_{n+1/2} + \boldsymbol{\Phi}_{\mathbf{q}_{n+1/2}}^{\mathrm{T}} \alpha \bar{\boldsymbol{\Phi}}_{n+1/2} - \mathbf{Q}_c - \left(\mathbf{Q}_{nc}\right)_{n+1/2} = \mathbf{0} \tag{32}$$

Taking into account the midpoint rule equations.

$$\begin{aligned} \dot{\mathbf{q}}_{n+1/2} &= \frac{\mathbf{q}_{n+1} - \mathbf{q}_n}{h} \\ \ddot{\mathbf{q}}_{n+1/2} &= \frac{2}{h^2}\left(\mathbf{q}_{n+1} - \mathbf{q}_n\right) - \frac{2}{h}\dot{\mathbf{q}}_n \end{aligned} \tag{33}$$

and using (33) in (32) we arrive at the following system of nonlinear equations in the time step $n+1$.

$$\mathbf{M}\left(\frac{2}{h^2}\left(\mathbf{q}_{n+1}-\mathbf{q}_n\right)-\frac{2}{h}\dot{\mathbf{q}}_n\right)+\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}_{n+1/2}}\alpha\bar{\boldsymbol{\Phi}}_{n+1/2}-\mathbf{Q}_c-\left(\mathbf{Q}_{nc}\right)_{n+1/2}=\mathbf{0} \tag{34}$$

The system (34) leads to the following approximate residual and tangent matrix,

$$\mathbf{f}\left(\mathbf{q}\right)=\frac{h^2}{2}\left(\mathbf{M}\ddot{\mathbf{q}}_{n+1/2}+\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}_{n+1/2}}\alpha\bar{\boldsymbol{\Phi}}_{n+1/2}-\mathbf{Q}_c-\left(\mathbf{Q}_{nc}\right)_{n+1/2}\right) \tag{35}$$

$$\frac{\partial\mathbf{f}\left(\mathbf{q}\right)}{\partial\mathbf{q}_{n+1}}\cong\mathbf{M}+\frac{h^2}{4}\left(\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}_{n+1/2}}\alpha\boldsymbol{\Phi}_{\mathbf{q}_{n+1}}+\mathbf{K}_{nc}+2\mathbf{K}_c\right)+\frac{h}{2}\mathbf{C}_{nc} \tag{36}$$

Where.

$$\begin{aligned}\mathbf{K}_{nc}&=-\frac{\partial\mathbf{Q}_{nc}}{\partial\mathbf{q}_{n+1/2}}\\ \mathbf{C}_{nc}&=-\frac{\partial\mathbf{Q}_{nc}}{\partial\dot{\mathbf{q}}_{n+1/2}}\\ \mathbf{K}_c&=-\frac{\partial\mathbf{Q}_c}{\partial\mathbf{q}_{n+1}}\end{aligned} \tag{37}$$

Several terms has been neglected in the calculation of the tangent matrix (36), in particular the derivatives of the jacobian matrix $\boldsymbol{\Phi}_{\mathbf{q}}$. This term, due to the linear and quadratic character of the constraints, typically give a very sparse third order tensor which contribution can be neglected in most cases, as explained in [1].

## 4 THE PROPOSED DYNAMIC FORMULATIONS II: INDEX-3 AUGMENTED LAGRANGIAN WITH PROJECTIONS AND TRAPEZOIDAL RULE

This formulation was presented in [9,15]; and it is based on the an augmented Lagrangian formulation with penalty forces proportional only to the violation of the constraints at position level.

The idea of this formulation is to take to zero, not the term $\left(\ddot{\boldsymbol{\Phi}}+2\xi\omega\dot{\boldsymbol{\Phi}}+\omega^2\boldsymbol{\Phi}\right)$, but each one of the terms $\boldsymbol{\Phi}$, $\dot{\boldsymbol{\Phi}}$ and $\ddot{\boldsymbol{\Phi}}$ separately. It can be seen that this idea improves the precision and stability of the integration.

### 4.1 Final form of the equations of motion

Let's suppose a multibody system which configuration can be defined by a vector $\mathbf{q}\in\mathbb{R}^n$ of natural coordinates, subjected to the action of a set of holonomic constraints $\boldsymbol{\Phi}\in\mathbb{R}^m$. The nullity of the first term, $\boldsymbol{\Phi}$, is directly imposed through the following motion equations,

$$\mathbf{M}\ddot{\mathbf{q}}+\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\lambda}^*+\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\alpha\boldsymbol{\Phi}=\mathbf{Q}\left(\mathbf{q},\dot{\mathbf{q}}\right) \tag{38}$$

$$\boldsymbol{\lambda}^*_{i+1}=\boldsymbol{\lambda}^*_i+\alpha\boldsymbol{\Phi} \tag{39}$$

where $\boldsymbol{\lambda}^*$ is a vector which contains the $m$ Lagrange multipliers and all the remaining terms are known.

The selected integrator is the single step trapezoidal rule, given by,

$$\begin{aligned}
\dot{\mathbf{q}}_{n+1} &= \frac{2}{h}\mathbf{q}_{n+1} + \hat{\dot{\mathbf{q}}}_n \quad ; \qquad \hat{\dot{\mathbf{q}}}_n = -\left(\frac{2}{h}\mathbf{q}_n + \dot{\mathbf{q}}_n\right) \\
\ddot{\mathbf{q}}_{n+1} &= \frac{4}{h^2}\mathbf{q}_{n+1} + \hat{\ddot{\mathbf{q}}}_n \quad ; \qquad \hat{\ddot{\mathbf{q}}}_n = -\left(\frac{4}{h^2}\mathbf{q}_n + \frac{4}{h}\dot{\mathbf{q}}_n + \ddot{\mathbf{q}}_n\right)
\end{aligned} \tag{40}$$

Combining the equations (40) and (38) at the step $n+1$, we arrive at the following system of nonlinear equations.

$$\frac{4}{h^2}\mathbf{M}\mathbf{q}_{n+1} + \boldsymbol{\Phi}_{\mathbf{q}_{n+1}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}_{n+1}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{n+1} - \mathbf{Q}\left(\mathbf{q}_{n+1}, \dot{\mathbf{q}}_{n+1}\right) + \mathbf{M}\hat{\ddot{\mathbf{q}}}_n = \mathbf{0} \tag{41}$$

Which leads to the following residual and tangent matrix.

$$\mathrm{f}\left(\mathbf{q}\right) = \frac{h^2}{4}\left(\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi} - \mathbf{Q}\right)_{n+1} \tag{42}$$

$$\frac{\partial \mathrm{f}\left(\mathbf{q}\right)}{\partial \mathbf{q}_{n+1}} \cong \mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\left(\boldsymbol{\Phi}_{\mathbf{q}_{n+1}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}_{n+1}} + \mathbf{K}\right) \tag{43}$$

where,

$$\begin{aligned}
\mathbf{K} &= -\frac{\partial \mathbf{Q}_{n+1}}{\partial \mathbf{q}_{n+1}} \\
\mathbf{C} &= -\frac{\partial \mathbf{Q}_{n+1}}{\partial \dot{\mathbf{q}}_{n+1}}
\end{aligned} \tag{44}$$

The equations of motion (38) impose the dynamic equilibrium and the constraint equations at position level. Theoretically, the enforcement of the constraints at position level guarantees the fulfillment of their derivatives under the adequate initial conditions. However, velocities and accelerations are calculated by means of the integrator equations (40), so they are not the exact derivatives of the positions. Moreover, the numerical errors lead to the non fulfillment of the constraint equations at velocity and acceleration level. Due to this fact, and as we commented before, this formulation is unstable.

In next sub-sections we are going to see the way to fulfill the constraints at velocity and acceleration levels, by means of projections in velocities and accelerations onto the manifolds of $\dot{\boldsymbol{\Phi}} = \mathbf{0}$ and $\ddot{\boldsymbol{\Phi}} = \mathbf{0}$. This projections stabilize also the unstable character of the formulation.

### 4.2 Projection of velocities

These projections were introduced in [9, 20]. They use the previous factorization of the tangent matrix (43) to project, saving computational time. The idea is to solve the following problem of minimization.

$$\begin{aligned}
&\min V = \frac{1}{2}\left(\dot{\mathbf{q}} - \dot{\mathbf{q}}^*\right)^{\mathrm{T}}\mathbf{P}\left(\dot{\mathbf{q}} - \dot{\mathbf{q}}^*\right) \\
&\text{s.t.} \qquad \frac{h^2}{4}\dot{\boldsymbol{\Phi}}\left(\mathbf{q}, \dot{\mathbf{q}}, t\right) = \mathbf{0}
\end{aligned} \tag{45}$$

where,

$$\mathbf{P} = \mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\mathbf{K} \tag{46}$$

If we use an penalty scheme, analogous to the one seen before, we can arrive at the following linear system of equations,

$$\left(\mathbf{P} + \frac{h^2}{4}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}}\right)\dot{\mathbf{q}} = \mathbf{P}\dot{\mathbf{q}}^{*} - \frac{h^2}{4}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{t} \tag{47}$$

Replacing the weight matrix $\mathbf{P}$, we have,

$$\left(\mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\left(\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{\mathbf{q}} + \mathbf{K}\right)\right)\dot{\mathbf{q}} = \left(\mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\mathbf{K}\right)\dot{\mathbf{q}}^{*} - \frac{h^2}{4}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{t} \tag{48}$$

and taking into account the equation (43) we have the final form,

$$\left(\frac{\partial \mathrm{f}(\mathbf{q})}{\partial \mathbf{q}}\right)\dot{\mathbf{q}} = \left(\mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\mathbf{K}\right)\dot{\mathbf{q}}^{*} - \frac{h^2}{4}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\boldsymbol{\Phi}_{t} \tag{49}$$

### 4.3 Projection of accelerations

Now the minimization problem is the following,

$$\begin{aligned} &\min V = \frac{1}{2}\left(\ddot{\mathbf{q}} - \ddot{\mathbf{q}}^{*}\right)^{\mathrm{T}}\mathbf{P}\left(\ddot{\mathbf{q}} - \ddot{\mathbf{q}}^{*}\right) \\ &\text{s.t.} \qquad \frac{h^2}{4}\ddot{\boldsymbol{\Phi}}\left(\mathbf{q}, \dot{\mathbf{q}}, t\right) = \mathbf{0} \end{aligned} \tag{50}$$

Where $\mathbf{P}$ is the matrix(46).
The final equations for the projections of accelerations,

$$\left(\frac{\partial \mathrm{f}(\mathbf{q})}{\partial \mathbf{q}}\right)\ddot{\mathbf{q}} = \left(\mathbf{M} + \frac{h}{2}\mathbf{C} + \frac{h^2}{4}\mathbf{K}\right)\ddot{\mathbf{q}}^{*} - \frac{h^2}{4}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\alpha\left(\dot{\boldsymbol{\Phi}}_{\dot{\mathbf{q}}}\dot{\mathbf{q}} + \boldsymbol{\Phi}_{t}\right) \tag{51}$$

## 5 NUMERICAL SIMULATION

In section 2, the example of the spherical compound pendulum (Figure 1) was presented, and the problems found with penalty and augmented Lagrangian formulations were reported. The results solving the same example with the formulations of the sections 3 and 4 are going to be presented now, to better understand the behavior of the proposed formulations.

### 5.1 Penalty and energy-momentum integrator

The formulation proposed in section 3 stabilizes the behavior of the equations (7), as shown in Figure 5. This stabilization is made by means of the control of the energy in the system.

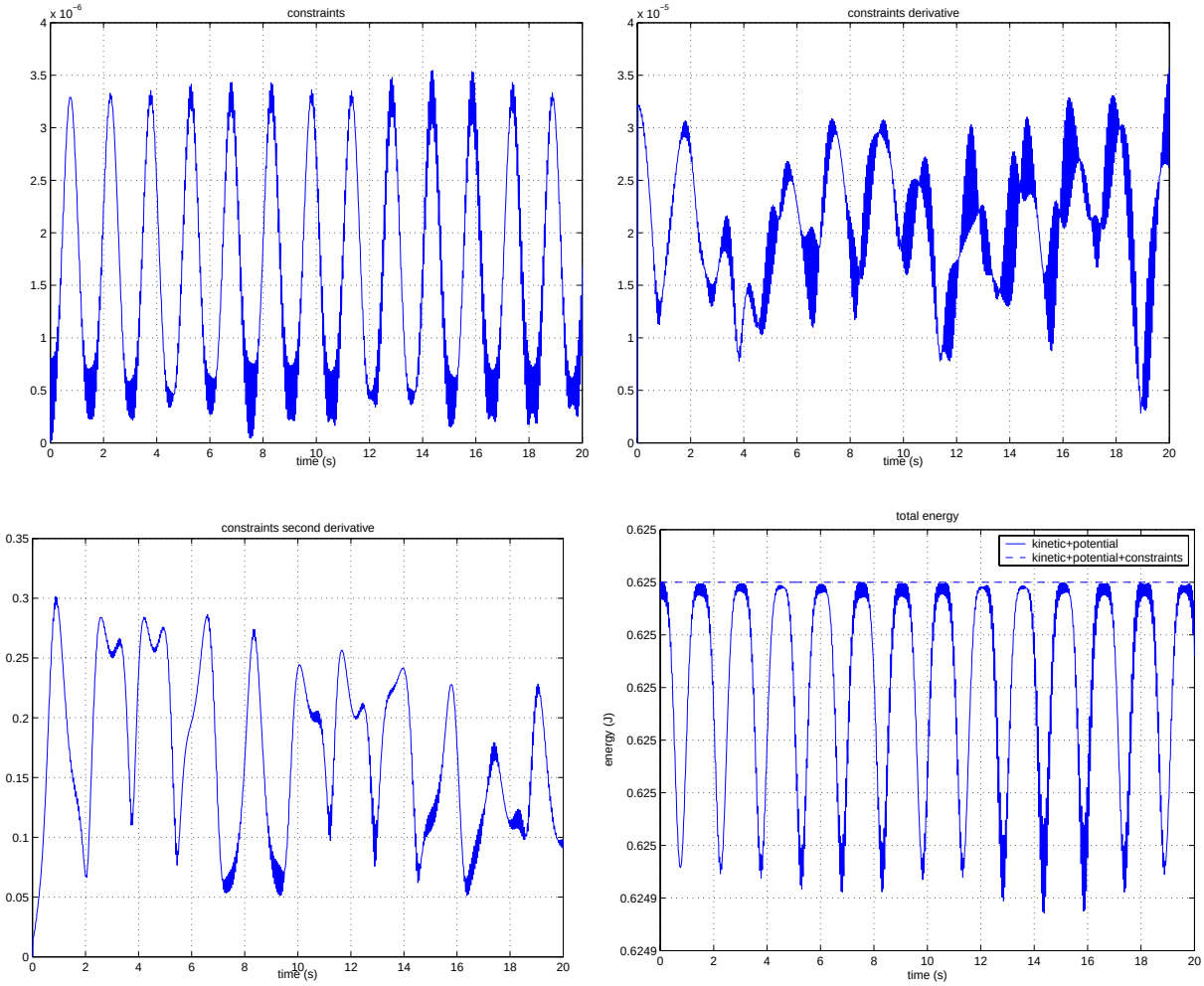


Figure 5: Constraints and energy behavior ( $h = 0.025$ s)

As we could expect nor the constraints at position neither at velocity level are zero. Nevertheless, the constraints at position level are near to zero because of the penalty term present in the motion equations. The constraints at velocity level are also near to zero because of the conservation of energy imposed by the energy-momentum integrator. On the other hand, the constraints at acceleration level are not imposed by the motion equations neither by the integrator so their fulfillment is quite poor.

If we look at the energy, as we could expect, the sum of kinetic and potential energy shows an oscillation due to the vibration of the constraints energy, because the satisfaction of the constraints is not exact and they take and release energy from the system along the simulation. If we look at the sum of kinetic, potential and constraints energy, we can see that conservation imposed by the energy-momentum integration is exact, which leads to a very robust formulation.

## 5.2 Index-3 augmented Lagrangian with projections and trapezoidal rule

The formulation proposed in section 4, clearly stabilizes the behavior of the augmented Lagrangian equations.

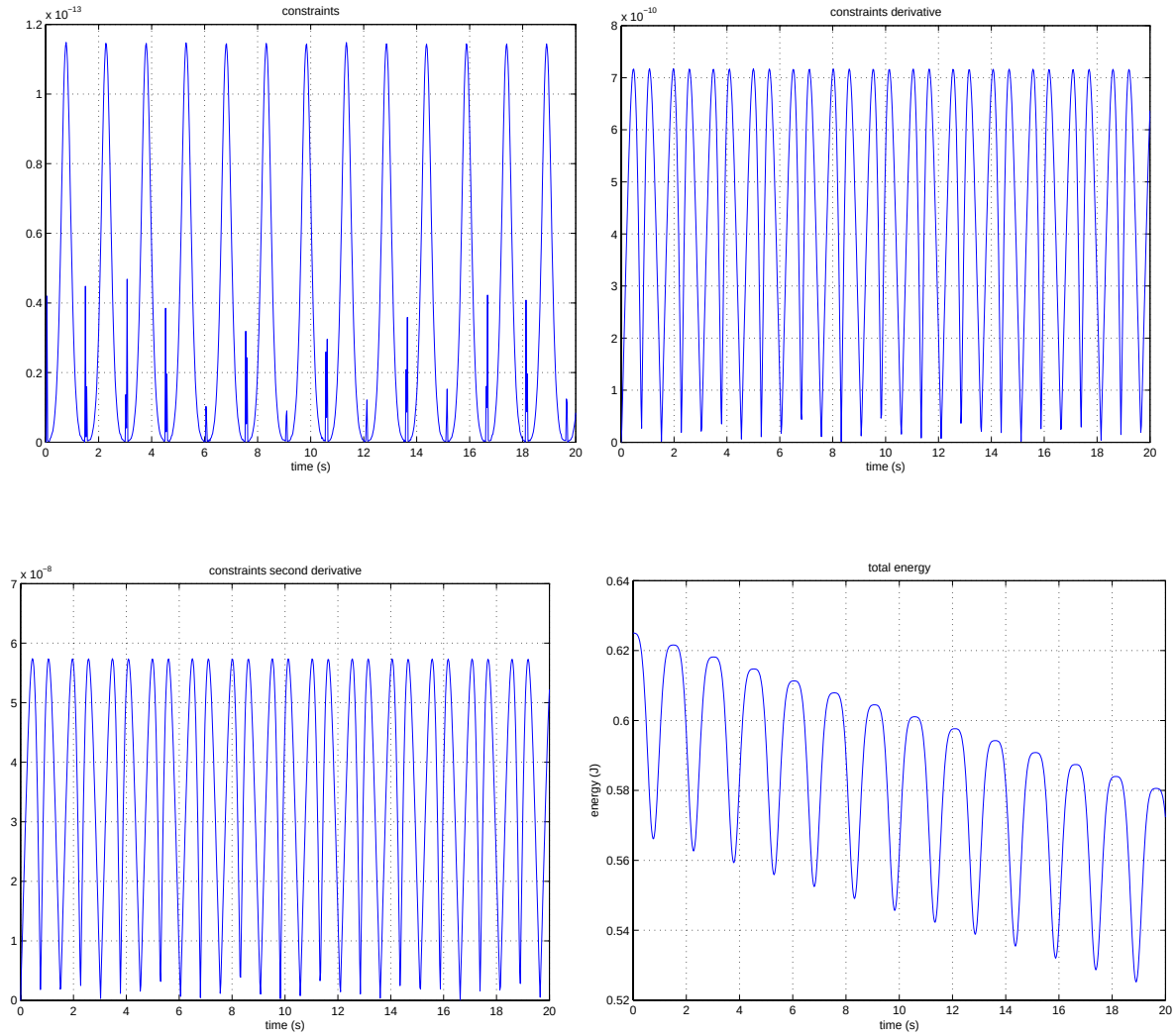


Figure 6: Constraints and energy behavior ( $h = 0.025$ s)

As shown in Figure 6, the satisfaction of the constraint equations is very good at position, velocity and acceleration levels.

In this case the energy taken by the constraints is negligible, but the sum of kinetic and potential energy is not conserved, mainly because the augmented Lagrangian formulation along with the trapezoidal rule introduces instabilities in the constraints which are damped out by the projections.

In any case, the energy variations resulting from this approach is not very significant in global terms, as shown in Figure 7.

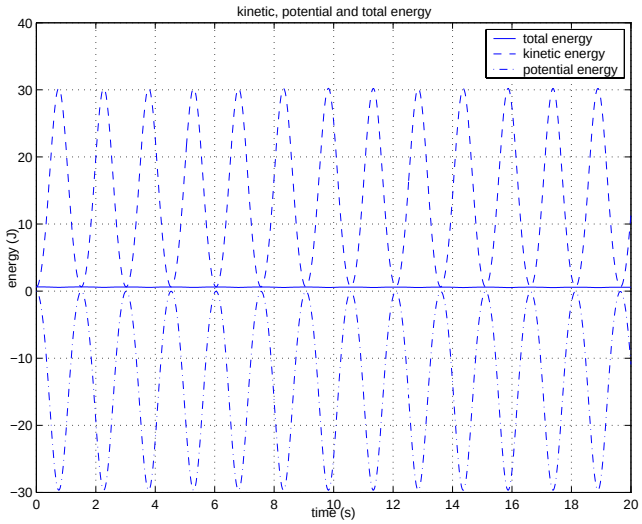


Figure 7: Kinetic, potential and total energy ( $h = 0.025$ s)

## 6 CONCLUSIONS

- Two solutions to integrate the equations of constrained multibody systems have been presented: one based on a specialized integrator which exactly conserves the energy and the other based in projections of velocities and accelerations onto the constraints manifolds.
- The conserving penalty formulation shows a very good behavior, specially with long term simulations in conservative systems, in which the conservation of the energy is one of the key points in the solution. Nevertheless the fulfillment of the constraint equations is not exact, in particular at acceleration, and may motivate future modifications of this methodology, based, for instance, on the augmented lagrangian formulation. Other disadvantage is that this method leads to non-symmetric tangent matrices.
- The augmented Lagrangian formulation with projections shows a very robust behaviour along with an acceptable precision. The formulation is not as adequate for long term simulations with conservative systems as the previous one, but it is a good candidate for hard real time simulations, because it is very simple and does not require the use of specialized integrators to achieve stability [20]. The tangent matrix resulting from the method is symmetric with integrators of the Newmark family, which is very convenient. Moreover, the factorization of the tangent matrix can be used to make the projections. With the present integrator the main drawback is the dissipative character of the algorithm. Improvements can be achieved by changing the integrator, since the scheme is valid with other integrators, including the energy-momentum integrator. Nevertheless, it can be interesting to explore futher the relation between the projections and the energy dissipation.

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