On the Stabilizing Properties of Energy-Momentum Integrators and Coordinate Projections for Constrained Mechanical Systems

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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 formulations 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 [11], which are dependent by nature. Different formulations used to solve the equations of motion with dependent coordinates have been developed, such as the widely known method of Lagrange multipliers, the penalty and augmented Lagrangian schemes [4], or velocity transformations [23, 27]. Some of them set a system of differential-algebraic equations (DAE) [8], others set system of ordinary differential equations (ODE).

Generally, it can be said that the dynamic formulation determines the choice 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 [9, 11]. 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 [3].

In [5, 9] the authors 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

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projections were proposed. More recently, in [10] the use of augmented Lagrangian techniques with other integrators of the generalized-α family along with projections was proposed, 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, 17, 18] developed a formulation based on an energy conserving penalty formulation, enforcing constraints at the position level, and applied it to the dynamics of multibody systems parametrized with Cartesian coordinates. In this case, the use of penalty at position level has the advantage of permitting to derive the constraint forces from a potential function: the constraint energy. The formulation includes the employment of an energy-momentum method as integration scheme [19, 25], so that the conservation of the total energy of the system is imposed by construction of the algorithm. Here, the stabilization of the equations of motion arises in a natural manner from the integration scheme.

The outline of this work is as follows. First, and overview of the most common formulations employed for the representation of the dynamics of constrained mechanical systems are presented. Next, the numerical difficulties that pose the different formulations are discussed. These issues prepare the context for the presentation of two proposed methods in the next sections, one of them based on the use of a standard ODE integrator with projections, the other on a conservative scheme. The following section analyzes with more detail their behaviour in terms of the discrete energy balance, and draws some interpretations about their stabilization features. Finally, a representative numerical example is presented, illustrating the most relevant issues introduced in the previous sections.

2 Dynamics of Constrained Mechanical Systems

In this section, we consider the formulation and the numerical solution of the dynamics of a constrained mechanical system; for instance, a set of rigid and deformable bodies linked by joints (represented by a vector of r holonomic constraints $\mathbf{0} = \mathbf{\Phi}(\mathbf{q}, t) \in \mathbb{R}^r$), being $\mathbf{q} \in \mathbb{R}^n$ a set of Cartesian coordinates.

In this work we focus on the different methods to impose constraints, which lead to different formulations for the equations of motion. Several strategies can be used to solve these equations, each of them posing special numerical difficulties that will be addressed with more detail in the following sections.

The three basic formulations considered here are based on Lagrange multipliers, penalty and augmented Lagrangian respectively. Following, a brief review of these three formulations is presented, along with a short description of the methods most commonly used to solve them.

2.1 Lagrange multiplier method

This method leads to an index-3 DAE system, given by:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{Q}, \qquad \boldsymbol{\Phi} = \mathbf{0}, \tag{1}$$

$\mathbf{M}$ being the mass matrix, $\boldsymbol{\lambda} \in \mathbb{R}^r$ the vector of Lagrange multipliers, $\mathbf{Q}(\mathbf{q}, \dot{\mathbf{q}}, t)$ the applied force vector, and denoting by $\boldsymbol{\Phi}_{\mathbf{q}} \stackrel{\text{def}}{=} \partial\boldsymbol{\Phi}/\partial\mathbf{q}$.

There are several methods that can be employed to solve the equation system (1):

1. Direct solution with a DAE solver. Backward Differentiation Formula (BDF), Implicit Runge–Kutta (IRK) and collocation methods are examples of numerical integration algorithms that are very efficient on the direct solution of these type of systems [8].
2. Index reduction (index-2). Differentiation of the constraint equation reduces the index by one, resulting in the following index-2 DAE system:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{Q}, \qquad \dot{\boldsymbol{\Phi}} = \mathbf{0}, \tag{2}$$

   which, again, can be solved directly by a suitable DAE solver.
3. Index reduction (index-1). Two differentiations of the constraint equation reduces the index by two, resulting in the following index-1 DAE system:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{Q}, \qquad \ddot{\boldsymbol{\Phi}} = \mathbf{0}. \tag{3}$$

   If desired, a further index reduction may be performed, eliminating the Lagrange multiplier vector $\boldsymbol{\lambda}$ and obtaining a standard ODE system. This can be done taking into account the differential system in (3) and the expression for the second derivative of the constraint $\ddot{\boldsymbol{\Phi}} = \boldsymbol{\Phi}_{\mathbf{q}}\ddot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_t$, with $\boldsymbol{\Phi}_t \stackrel{\text{def}}{=} \partial\boldsymbol{\Phi}/\partial t$; after some algebraic manipulations an ODE system results, given by:

$$\mathbf{M}\ddot{\mathbf{q}} = \mathbf{Q} - \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\big(\boldsymbol{\Phi}_{\mathbf{q}}\mathbf{M}^{-1}\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\big)^{-1}\big(\boldsymbol{\Phi}_{\mathbf{q}}\mathbf{M}^{-1}\mathbf{Q} + \dot{\boldsymbol{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_t\big), \tag{4}$$

   which can be solved with any ODE solver.

2.2 Penalty method

This method leads to an ODE system given by:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}(\boldsymbol{\alpha}\boldsymbol{\Phi}) = \mathbf{Q}, \tag{5}$$

$\boldsymbol{\alpha}$ being the penalty matrix, which is often defined with a single penalty parameter α, such that $\boldsymbol{\alpha} = \alpha\mathbf{1}$, $\mathbf{1}$ being the unit matrix.

This formulation can be interpreted as the perturbed DAE problem given by (1), verifying $\boldsymbol{\Phi} \to \mathbf{0}$ as $\alpha \to \infty$, and can be solved by a suitable ODE integrator.

Formulation (5) penalizes the constraint at position level only ($\boldsymbol{\Phi}$), but it may include also the constraint at velocity and acceleration levels ($\dot{\boldsymbol{\Phi}}$ and $\ddot{\boldsymbol{\Phi}}$ respectively), taking the more general form:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha}\left(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}\right) = \mathbf{Q}, \tag{6}$$

where ω and ξ can be interpreted as the natural frequency and damping ratio of the penalized constraint [11].

2.3 Augmented Lagrangian method

It can be understood as a compromise between the Lagrange multiplier and the penalty method, and leads to and index-3 DAE system given by:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}(\boldsymbol{\alpha}\boldsymbol{\Phi}) = \mathbf{Q}, \qquad \boldsymbol{\Phi} = \mathbf{0}, \tag{7}$$

where $\boldsymbol{\lambda}^*$ represents the Lagrange multiplier vector. This formulation is commonly set, from an algorithmic point of view, by the Uzawa method, which introduces an iterative scheme for the multipliers. This algorithmic approach, in practice, transforms the DAE system into an ODE system, defining an update for the multipliers given by $\boldsymbol{\lambda}^*_{(k+1)} = \boldsymbol{\lambda}^*_{(k)} + \boldsymbol{\alpha}\boldsymbol{\Phi}$, verifying $\boldsymbol{\lambda}^* \to \boldsymbol{\lambda}$ as iteration in $\boldsymbol{\lambda}^*$ progresses, being $\boldsymbol{\lambda}$ the exact Lagrange multiplier vector.

Different strategies can be followed to solve the formulation (7). All of them assume the use of Uzawa's method, thus effectively leading to the application of an ODE solver. The basic difference among them is the index of the original DAE system to be solved.

1. Direct solution of the index-3 DAE system (7), applying Uzawa's method and a suitable ODE integrator.
2. Index reduction (index-2), introducing the first derivative of the constraint equation and obtaining:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\alpha}(2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}) = \mathbf{Q}\ , \qquad 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi} = \mathbf{0} \tag{8}$$

   to be solved applying Uzawa's method and a suitable ODE integrator.
3. Index reduction (index-1), introducing the second derivative of the constraint equation and obtaining:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\alpha}(\ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi}) = \mathbf{Q}\ , \quad \ddot{\boldsymbol{\Phi}} + 2\xi\omega\dot{\boldsymbol{\Phi}} + \omega^2\boldsymbol{\Phi} = \mathbf{0} \tag{9}$$

   to be solved applying Uzawa's method and a suitable ODE integrator.

All these formulations pose numerical difficulties, which are going to be explored with more detail in the following section, and they will motivate the search for improvements, particularly regarding stability issues.

3 Stability Problems of the Numerical Solution

As previously pointed out, the formulation of the dynamics of a constrained mechanical system pose numerical difficulties. These difficulties are, in general, different for each formulation and solution method, but they are typically related to stability properties of the numerical scheme, and they are going to be briefly exposed in the following paragraphs.

- Direct integration of DAEs of index higher than 1 (formulations (1), (2), (7) and (8)) is usually not recommended for stability reasons. Actually, there are index-2 and index-3 DAEs for which all of the multistep (including BDF) and Runge–Kutta methods are unstable, as pointed out in [8]. In the particular case of a constrained mechanical system described by the index-3 DAE given by (1),[1] or the augmented version (7), direct integration has been reported to show instability problems [9].
- The analytical differentiation of the constraint equations is an unstabilized index reduction (formulations (2), (3), (8) and (9)). Constraints on position, velocity or acceleration levels define invariant manifolds, where the exact solution lies. However, the numerical solution may depart from them, and indeed it usually does due to the referred unstable reduction.
  On the other hand, several numerical experiments by different authors suggest than the solution is more stable on the manifold than off it. This fact justifies the search for methods that enforce the solution to be on the constraint manifold, thus enhancing the stability of the resulting numerical scheme.
- ODE integrators may exhibit severe numerical instabilities for stiff systems, such as those resulting from a penalty formulation (5) or (6), where large penalty parameters are required in order to get a satisfactory constraint enforcement.
  Some integration schemes are better suited for these type of problems, such as implicit Runge–Kutta and BDF methods [20]. However, these methods usually introduce a significant amount of numerical damping, which can be unacceptable for long term simulations. In the context of Hamiltonian systems, energy-momentum methods [19] exhibit very good stability for stiff systems, while exactly conserving the total energy, and are actually a very adequate choice for robust long-term simulations.

These numerical problems motivate the interest in developing algorithms capable of providing stable and accurate solutions for reasonable time steps. Several methods have been proposed in the literature to alleviate these problems for the different formulations (e.g. [1, 2, 7, 8]). To collect and discuss all these different methods is not a simple task, because they are numerous and sometimes application-dependent, and it is out of the scope of this paper.

[1] This is a special DAE form, known in the literature as Hessenberg index-3 type.

Here we restrict ourselves to the analysis of two methods, both of them based on the augmented Lagrangian formulation (7), and discuss their stabilizing properties. The first proposed approach is a coordinate projection method, the second is a conservative formulation, and both will be outlined in the sections that follows.

4 Augmented Lagrangian with Projections

The point of departure of this approach is the index-3 DAE given by expression (7), repeated here for the sake of clarity:

$$\mathbf{M}\ddot{\mathbf{q}} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^{*} + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}(\boldsymbol{\alpha}\boldsymbol{\Phi}) = \mathbf{Q}, \qquad \boldsymbol{\Phi} = \mathbf{0}.$$

As stated in Section 2, a numerical solution can be obtained combining an ODE integrator with an update formula for the Lagrange multipliers, in a procedure referred to as the Uzawa method, or method of multipliers. Now, for non-linear problems, it is possible to define two main alternatives for the multipliers update scheme in a single time step:

- *Nested iteration*, setting two nested loops; an outer loop for the multiplier $\boldsymbol{\lambda}$, and an interior loop that solve the ODE for a fixed value of the multiplier. This is the most common implementation of this method, originally introduced in the context of constrained optimization [6] and applied in many engineering problems, as contact mechanics [21, 28].
- *Simultaneous iteration* sets only one loop, where the multiplier update is done simultaneously with the iterations required by the ODE solver. This implementation may exhibit stability problems in some applications, caused by the non-differentiability of the update [21], but nevertheless it has been successfully applied to multibody systems [4, 9].

This augmented Lagrangian formulation leads to an exact fulfillment of the original position constraints ($\boldsymbol{\Phi} = \mathbf{0}$), but usually exhibits an unstable behaviour for moderate time step sizes, even with ODE integrators suited to stiff systems.

As mentioned in Section 3, based on previous results in the literature, the numerical solution of a constrained mechanical system seems to be more stable on the constraint manifold than off it. Based on this fact, the exact enforcement of the constraint not only at position level, but also at velocity and acceleration levels ($\dot{\boldsymbol{\Phi}} = \mathbf{0}$ and $\ddot{\boldsymbol{\Phi}} = \mathbf{0}$ respectively), which is not accomplished by the augmented Lagrangian formulation presented here, is foreseen to stabilize the numerical solution.

This enforcement can be accomplished by different methods; one of them is the so-called coordinate projection technique, which is the one selected in this work, and will be outlined in the next paragraphs.

In case of a *velocity projection*, the velocities computed with the ODE integrator ($\dot{\mathbf{q}}^{*}$) are projected onto the velocity constraint manifold to obtain new velocities ($\dot{\mathbf{q}}$), solving a constrained minimization problem given by:

$$\min_{\dot{\mathbf{q}}} \frac{1}{2}(\dot{\mathbf{q}} - \dot{\mathbf{q}}^*)^{\mathrm{T}}\mathbf{A}(\dot{\mathbf{q}} - \dot{\mathbf{q}}^*) \quad \text{such that} \quad \dot{\boldsymbol{\Phi}} = \mathbf{0}, \tag{10}$$

being $\mathbf{A}$ a definite positive matrix. This constrained minimization problem can be solved with different methods; one of the simplest is penalty, which leads to the solution for $\dot{\mathbf{q}}$ of a linear algebraic system given by:

$$\left(\mathbf{A} + \alpha \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\Phi}_{\mathbf{q}}\right)\dot{\mathbf{q}} = \mathbf{A}\dot{\mathbf{q}}^*, \tag{11}$$

being α a penalty parameter.

In case of a *acceleration projection*, the accelerations computed with the ODE integrator ($\ddot{\mathbf{q}}^*$) are projected onto the acceleration constraint manifold to obtain new accelerations ($\ddot{\mathbf{q}}$), solving a constrained minimization problem given by:

$$\min_{\ddot{\mathbf{q}}} \frac{1}{2}(\ddot{\mathbf{q}} - \ddot{\mathbf{q}}^*)^{\mathrm{T}}\mathbf{A}(\ddot{\mathbf{q}} - \ddot{\mathbf{q}}^*) \quad \text{such that} \quad \ddot{\boldsymbol{\Phi}} = \mathbf{0}, \tag{12}$$

$\mathbf{A}$ being a definite positive matrix.[2] Again, this constrained minimization problem can be solved with penalty, which leads to the solution for $\ddot{\mathbf{q}}$ of a linear algebraic system given by:

$$\left(\mathbf{A} + \alpha \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\Phi}_{\mathbf{q}}\right)\ddot{\mathbf{q}} = \mathbf{A}\ddot{\mathbf{q}}^* - \alpha \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \dot{\boldsymbol{\Phi}}_{\mathbf{q}} \dot{\mathbf{q}}. \tag{13}$$

5 Conserving Augmented Lagrangian Formulation

The point of departure of this approach is the algorithmic expression of the energy-momentum method [19, 24] applied to a conservative mechanical system given by (5), which enforces a set of holonomic constraints $\boldsymbol{\Phi}(\mathbf{q})$ with the penalty method [12, 17]:

$$\begin{aligned} &\mathbf{M}\left(\dot{\mathbf{q}}_{n+1} - \dot{\mathbf{q}}_n\right) + \Delta t \boldsymbol{\Phi}_{\mathbf{q}_{n+\beta}}^{\mathrm{T}} \boldsymbol{\alpha} \overline{\boldsymbol{\Phi}}_{n+\frac{1}{2}} = \mathbf{0}, \\ &\frac{1}{2}(\dot{\mathbf{q}}_{n+1} + \dot{\mathbf{q}}_n) = \frac{1}{\Delta t}(\mathbf{q}_{n+1} - \mathbf{q}_n), \end{aligned} \tag{14}$$

where it has been assumed, with no loss of generality for the following discussion, that will focus on the constraint forces, that the applied forces are null ($\mathbf{Q} = \mathbf{0}$), and denoting $\overline{(\cdot)}_{n+\frac{1}{2}} \overset{\text{def}}{=} [(\cdot)_n + (\cdot)_{n+1}]/2$ and $(\cdot)_{n+\beta}$ evaluation at $\mathbf{q}_{n+\beta} \overset{\text{def}}{=} \mathbf{q}_n + \beta(\mathbf{q}_{n+1} - \mathbf{q}_n)$.

The parameter $\beta \in [0, 1]$ has to be computed at each time step, imposing that the dot product between the gradient of the constraint and the increment in position verify:

[2] Not necessarily the same employed for the velocity projection.

$$\beta; \qquad \boldsymbol{\Phi}_{\mathbf{q}_{n+\beta}} (\mathbf{q}_{n+1} - \mathbf{q}_n) = \boldsymbol{\Phi}_{n+1} - \boldsymbol{\Phi}_n. \tag{15}$$

Note that when constraints are exactly fulfilled the gradient of the constraint (in other words, the constraint force) is orthogonal to the increment in position. As it will be shown later in Section 6, this condition leads to the exact algorithmic nullity of the work performed by the constraint forces, thus leading to exact conservation of total energy. If the constraint is at most quadratic, it is straightforward to see that $\beta = 1/2$. Besides, if the constraint is generally expressed in terms of an scalar variable (e.g. the distance between points), the constraint force term in (14) can be formulated in a closed form without any additional parameter [12].

In order to obtain a conservative augmented Lagrangian formulation, it is convenient to read (14) as a second order approximation of an integral balance of linear momentum between n and $n + 1$:

$$\int_{t_n}^{t_{n+1}} \mathbf{M}\ddot{\mathbf{q}} \, \mathrm{d}t + \int_{t_n}^{t_{n+1}} \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \boldsymbol{\Phi} \, \mathrm{d}t = \mathbf{0}. \tag{16}$$

Equations (14) and (16) reveal that the term $\boldsymbol{\alpha}\boldsymbol{\Phi}$ is evaluated as $\boldsymbol{\alpha}\overline{\boldsymbol{\Phi}}_{n+\frac{1}{2}}$ in order to calculate this integral, that leads to the conserving formulation.

On the other hand, it is also possible to understand the augmented Lagrangian method (7) as an extended penalty method, where the penalized constraint $\boldsymbol{\alpha}\boldsymbol{\Phi}$ is corrected at each time step by a set $\boldsymbol{\lambda}^*$ of Lagrange multipliers, which are updated with a scheme given by $\boldsymbol{\lambda}^{*(k+1)} = \boldsymbol{\lambda}^{*(k)} + \boldsymbol{\alpha}\boldsymbol{\Phi}$ with a nested or simultaneous iteration strategy, as discussed in Section 4.

Taking into account these considerations, it is possible to define a conserving algorithm that incorporates the augmented term:

$$\mathbf{M}(\dot{\mathbf{q}}_{n+1} - \dot{\mathbf{q}}_n) + \Delta t \left[\boldsymbol{\Phi}_{\mathbf{q}_{n+\beta}}^{\mathrm{T}} \boldsymbol{\alpha} \overline{\boldsymbol{\Phi}}_{n+\frac{1}{2}} + \boldsymbol{\Phi}_{\mathbf{q}_{n+\beta}}^{\mathrm{T}} \boldsymbol{\lambda}^* \right] = \mathbf{0} \tag{17}$$

$$\frac{1}{2}(\dot{\mathbf{q}}_{n+1} + \dot{\mathbf{q}}_n) = \frac{1}{\Delta t}(\mathbf{q}_{n+1} - \mathbf{q}_n)$$

and accordingly sets an update scheme for the set of multipliers, given by:

$$\boldsymbol{\lambda}_{n+1}^{*(k+1)} = \boldsymbol{\lambda}_{n+1}^{*(k)} + \boldsymbol{\alpha}\overline{\boldsymbol{\Phi}}_{n+\frac{1}{2}}. \tag{18}$$

The proposed algorithm given by (17) and (18) achieve exact conservation of total energy (see [15] for more details) and exact fulfillment of the position constraints, as the augmented Lagrange multipliers set $\boldsymbol{\lambda}_{n+1}^*$ converge to the true Lagrange multipliers set $\boldsymbol{\lambda}_{n+1}$ when its iteration progresses.

Finally, note that the coordinate projection technique described in Section 4 can be applied here too in order to enforce the constraints at the velocity and/or acceleration levels at each time step, but then the energy is no longer conserved. The energy can grow or diminish depending on the way the projection is carried out, which is one of the main topics discussed in the following section.

6 Energetic Considerations

For ODE systems arising from the dynamics of mechanical systems, the stability properties of the numerical methods used to solve them are typically related to the concept of energy. Actually, in the linear case, exact algorithmic energy conservation and unconditional stability are directly related, as it happens, for instance, with the trapezoidal rule, which has both features [16]. However, this direct relationship does not hold for the non-linear case [22], which is the case of the equations resulting from practical multibody systems. Nevertheless, exact conservation of energy (or unconditional energy dissipation) has revealed extremely useful in the design of robust integration schemes, with excellent stability in the non linear case (see [26] and references therein).

With these arguments in mind, it is interesting to analyze how the two proposed methodologies behave in terms of discrete energy balance. As it will be shown next, it comes out that both methods actually controls the energy (thus providing a justification for their stabilization properties) but they do it differently; the projection method provides a means for conserving or dissipating energy, and the conservative approach exactly conserves it.

In order to study both cases from a common point of departure, let us consider a constrained mechanical system, parametrized with a set of coordinates $\mathbf{q} \in \mathbb{R}^n$, subjected to a set of r holonomic constraints $\boldsymbol{\Phi}(\mathbf{q}) \in \mathbb{R}^r$ and with no applied forces. The dynamics of this system is represented by the differential equation:

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{Q}_{\boldsymbol{\Phi}}(\mathbf{q}) = \mathbf{0}, \tag{19}$$

$\mathbf{Q}_{\boldsymbol{\Phi}}$ being the constraint force vector, which in the case of the augmented Lagrangian method is given by $\mathbf{Q}_{\boldsymbol{\Phi}} = \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\boldsymbol{\lambda}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}(\boldsymbol{\alpha}\boldsymbol{\Phi})$. Note that the dynamical system represented by (19) is conservative (the total mechanical energy remains constant), since the work performed by holonomic constraints which do not depend explicitly on time is null. This fact does not pose any practical limitation for our purposes and helps the understanding of the developments presented in the rest of the section.

Using an ODE integrator to calculate the solution from t_n to t_{n+1}, combined with the proper Lagrange multiplier update scheme, a solution $\mathbf{q}_{n+1}$ that exactly satisfies the position constraint can be obtained. Consequently, the constraint force at t_{n+1} takes the value $\mathbf{Q}_{\boldsymbol{\Phi}_{n+1}} = \boldsymbol{\Phi}_{\mathbf{q}_{n+1}}^{\mathrm{T}}\boldsymbol{\lambda}_{n+1}$, being $\boldsymbol{\lambda}_{n+1}$ the vector of exact Lagrange multipliers.

A velocity vector $\dot{\mathbf{q}}_{n+1}^*$ is also obtained but, in general, the velocity constraint $\dot{\boldsymbol{\Phi}}_{n+1}$ is not exactly satisfied. In order to move the solution back to the velocity manifold, let us assume that a velocity projection is performed at the end of each time step as explained in Section 4, obtaining a new velocity vector $\dot{\mathbf{q}}_{n+1}$.

The total energy balance ΔE between t_n and t_{n+1} is given by:

$$\Delta E = \frac{1}{2}\dot{\mathbf{q}}_{n+1}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1} - \frac{1}{2}\dot{\mathbf{q}}_{n}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n}. \tag{20}$$

Note that the total energy balance ΔE given by (20) equals the kinetic energy balance ΔT, which means that $\Delta V = 0$. This is due to the fact that there are not applied forces, the position constraints are exactly satisfied and the position $\mathbf{q}_{n+1}$ does not change under the projection.

Adding and subtracting a term $(1/2)\dot{\mathbf{q}}_{n+1}^{*\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1}^{*}$ to equation (20), the following relation is obtained:

$$\Delta E = \underbrace{\frac{1}{2}\dot{\mathbf{q}}_{n+1}^{*\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1}^{*} - \frac{1}{2}\dot{\mathbf{q}}_{n}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n}}_{\Delta E_i} + \underbrace{\frac{1}{2}\dot{\mathbf{q}}_{n+1}^{\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1} - \frac{1}{2}\dot{\mathbf{q}}_{n+1}^{*\mathrm{T}}\mathbf{M}\dot{\mathbf{q}}_{n+1}^{*}}_{\Delta E_p}, \tag{21}$$

where ΔE_i is the energy variation introduced by the ODE integrator, and ΔE_p the energy variation introduced by the velocity projection.

It is possible to calculate the energy variation introduced by any ODE integrator employing the following preliminary equation:

$$\Delta E_i = \frac{1}{2}(\dot{\mathbf{q}}_{n+1}^{*} + \dot{\mathbf{q}}_{n})^{\mathrm{T}}\mathbf{M}(\dot{\mathbf{q}}_{n+1}^{*} - \dot{\mathbf{q}}_{n}) \tag{22}$$

and using the algorithmic expressions of the method with the original system (19). For instance, for the *trapezoidal rule* the following relations hold:

$$\dot{\mathbf{q}}_{n+1}^{*} + \dot{\mathbf{q}}_{n} = \frac{2}{\Delta t}(\mathbf{q}_{n+1} - \mathbf{q}_{n}) \tag{23}$$

$$\dot{\mathbf{q}}_{n+1}^{*} - \dot{\mathbf{q}}_{n} = -\frac{\Delta t}{2}\mathbf{M}^{-1}\big(\mathbf{Q}_{\boldsymbol{\Phi}_n} + \mathbf{Q}_{\boldsymbol{\Phi}_{n+1}}\big) \tag{24}$$

which introduced in expression (22) gives:

$$\Delta E_i = -(\mathbf{q}_{n+1} - \mathbf{q}_{n})^{\mathrm{T}}\,\overline{\mathbf{Q}}_{\boldsymbol{\Phi}_{n+\frac{1}{2}}}, \tag{25}$$

where the notation $\overline{(\cdot)}_{n+\frac{1}{2}} \stackrel{\text{def}}{=} [(\cdot)_n + (\cdot)_{n+1}]/2$ introduced already in Section 5 has been employed again.

Other example is the *implicit midpoint rule*, that introduces an energy variation given by:

$$\Delta E_i = -(\mathbf{q}_{n+1} - \mathbf{q}_{n})^{\mathrm{T}}\,\mathbf{Q}_{\boldsymbol{\Phi}_{n+\frac{1}{2}}}, \tag{26}$$

where $(\cdot)_{n+\frac{1}{2}}$ denotes evaluation at the midpoint. Note that, in a general non linear case, $\overline{\mathbf{Q}}_{\boldsymbol{\Phi}_{n+\frac{1}{2}}} \neq \mathbf{Q}_{\boldsymbol{\Phi}_{n+\frac{1}{2}}}$ and $\Delta E_i \neq 0$ can be positive or negative. Note from (25) and (26) that both numerical schemes are the same and exactly conserve energy ($\Delta E_i = 0$) if the constraints are linear.

Finally, using relation (15), it can be shown that the energy variation of the *conserving method* is null, given by:

$$\Delta E_i = -(\mathbf{q}_{n+1} - \mathbf{q}_n)^{\mathrm{T}} \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}_{n+\beta}} \boldsymbol{\lambda}_{n+1} = 0. \tag{27}$$

Other expressions similar to (25), (26) and (27) can be obtained for other integrators, but this exhaustive description falls out of the scope of the work presented here. It is important to remark that the sign of the energy contribution ΔE_i may not be constant along the simulation, thus increasing or decreasing the total energy, which can in turn affect the numerical stability.

The second contribution to the energy variation is ΔE_p, associated with the velocity projection described in Section 4, and can be obtained solving a minimization problem with a definite positive matrix $\mathbf{A}$ with a penalty method. This leads to the solution for $\dot{\mathbf{q}}_{n+1}$ of the linear algebraic equation system (11), given by:

$$\dot{\mathbf{q}}_{n+1} = \mathbf{P}^{-1}\, \dot{\mathbf{q}}^*_{n+1} \quad \text{with} \quad \mathbf{P} = \left(\mathbf{1} + \alpha \mathbf{A}^{-1} \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}} \boldsymbol{\Phi}_{\mathbf{q}}\right). \tag{28}$$

Introducing the first expression in (28) in the following relation for ΔE_p:

$$\Delta E_p = \frac{1}{2}(\dot{\mathbf{q}}_{n+1} + \dot{\mathbf{q}}^*_{n+1})^{\mathrm{T}} \mathbf{M} (\dot{\mathbf{q}}_{n+1} - \dot{\mathbf{q}}^*_{n+1}), \tag{29}$$

the following expression is obtained for the energy variation introduced by the velocity projection:

$$\Delta E_p = \dot{\mathbf{q}}^{\mathrm{T}}_{n+1} \mathbf{D} \dot{\mathbf{q}}_{n+1} \quad \text{with} \quad \mathbf{D} = \frac{1}{2}(\mathbf{1} + \mathbf{P})^{\mathrm{T}} \mathbf{M} (\mathbf{1} - \mathbf{P}). \tag{30}$$

Therefore, the effect of projection upon the energy depends of the properties of matrix $\mathbf{D}$, which is the matrix associated to the quadratic form ΔE_p, and governs the damping behaviour of the projection. If this matrix is semidefinite negative, artificial energy growth is avoided in any case, and a significant improvement of the stability of the overall numerical scheme would be expected.

A detailed analysis of the quadratic form (30) can be performed [13], providing a practical assessment about the adequate selection of the projection matrix $\mathbf{A}$, such that artificial energy growth is unconditionally avoided. One preliminary and interesting result of this analysis is that the selection $\mathbf{A} = \mathbf{M}$ introduces unconditional dissipation to any incompatible velocity field (which is a velocity field that falls out of the velocity manifold $\dot{\boldsymbol{\Phi}} = \mathbf{0}$). This property, and the impact that it has over the stability of the resulting numerical algorithm will be observed in the numerical experiment performed in the next section, and perfectly agrees with results previously reported by other authors [5].

7 Numerical Simulation

To better understand the behavior of the formulations presented in Sections 4 and 5, let us present a simple but representative example that poses the essential numerical difficulties typically associated to the constrained dynamics of more complex mechanical systems.

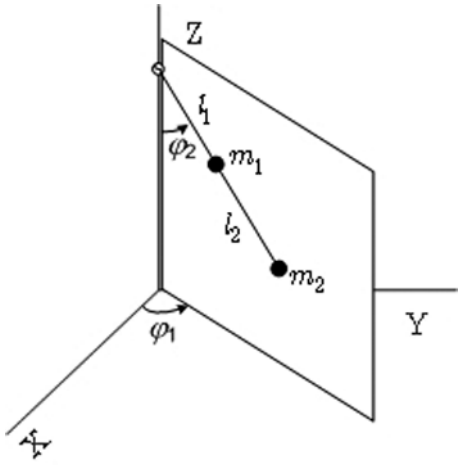

Fig. 1. Numerical simulation: an spherical compound pendulum.

Let us consider a spherical compound pendulum [14], shown in Figure 1 with two particles with masses $m_1 = m_2 = 1$ kg, placed at distances $l_1 = 1$ m and $l_2 = 1$ m on a rigid massless rod of total length $l_1 + l_2$. The system is released from the position $\varphi_1 = 0$, $\varphi_2 = \pi/2$ rad with initial velocities $\dot{\varphi}_1 = 0.5$ and $\dot{\varphi}_2 = 0$ rad/s. The system has two degrees of freedom and it is modeled with six coordinates ($\mathbf{q} \in \mathbb{R}^6$), which are the absolute Cartesian coordinates of both particles. There are five constraint equations; two of them express that distances l_1 and l_2 are constant, and the other three express the alignment of the two segments connecting the particles through a cross product. Note that one of these three equations is redundant, which means that the system has 2 degrees of freedom.

We will use this example to illustrate the main issues discussed in the previous sections; namely:

- the effect of different implementations of the augmented Lagrangian scheme (nested and simultaneous simulation);
- the numerical difficulties associated to the augmented Lagrangian approach when used with a standard ODE integrator, without stabilization;
- the comparison in terms of stability between the conservative integration scheme and the use of a standard ODE integrator with projections;
- the evaluation of a conservative scheme with projections, that will allow to take a deeper look to the energy balance of the projection technique and its effect over stability.

In all the following cases the simulation is carried out for 20 seconds and integrated with 0.025 s of time step. The penalty factor is set to 10^7.

7.1 Augmented Lagrangian schemes: Nested and simultaneous iteration

As explained in Section 4, there are two different possibilities for implementing the augmented Lagrangian schemes in a non linear case:

- *Nested iteration*, with an outer iteration for the Lagrange multipliers and an inner Newton–Raphson iteration.
- *Simultaneous iteration*: with an unique iteration loop for Newton–Raphson, which includes the update of the Lagrange multipliers.

It is observed that the first scheme, in general, leads to a slower convergence and needs more number of iterations. Moreover, small differences in the fulfillment of the constraints are obtained depending on the tolerances imposed to the outer iteration of the first scheme. But this differences have no significance on the response of the solution, or the conservation of energy. If we pay attention to the stability of the methods, it is neither observed a better performance of the nested iteration implementation, since the maximum time steps achieved are similar.

Finally, note that in the nested iteration we have an additional uncertain parameter to take into account: the outer iteration tolerance, which should be supplied by the user and directly determines the accuracy of the constraint fulfillment.

7.2 Stability problems of the index-3 augmented Lagrangian scheme with a standard integrator

To illustrate the problems exhibited by the augmented Lagrangian formulation (7) if no stabilization method is used, the example of the compound pendulum is solved using the trapezoidal rule without projections.

Figure 2 shows the behavior of the energy, and the quadratic norm of the constraints at position $||\mathbf{\Phi}||$, velocity $||\dot{\mathbf{\Phi}}||$, and acceleration $||\ddot{\mathbf{\Phi}}||$ levels along time.

Note that the instability is characterized by the unbounded growth of the violation of the constraint equations at velocity and acceleration levels, together with the unbounded growth of the vibrating energy associated to the constraints. Other integration schemes, such as implicit Runge–Kutta or BDF, better suited for stiff ODE systems than the trapezoidal rule, exhibit qualitatively the same behaviour with slightly larger time steps.

7.3 Augmented Lagrangian stabilized formulations: Coordinate projection vs. conservative formulation

We analyze here two methods, both based on the augmented Lagrange formulation and presented in Sections 4 and 5. These two methods are designed to overcome the stability problems, explained in Section 3 and illustrated in Section 7.2, associated to the numerical solution of the DAE representing the system's dynamics.

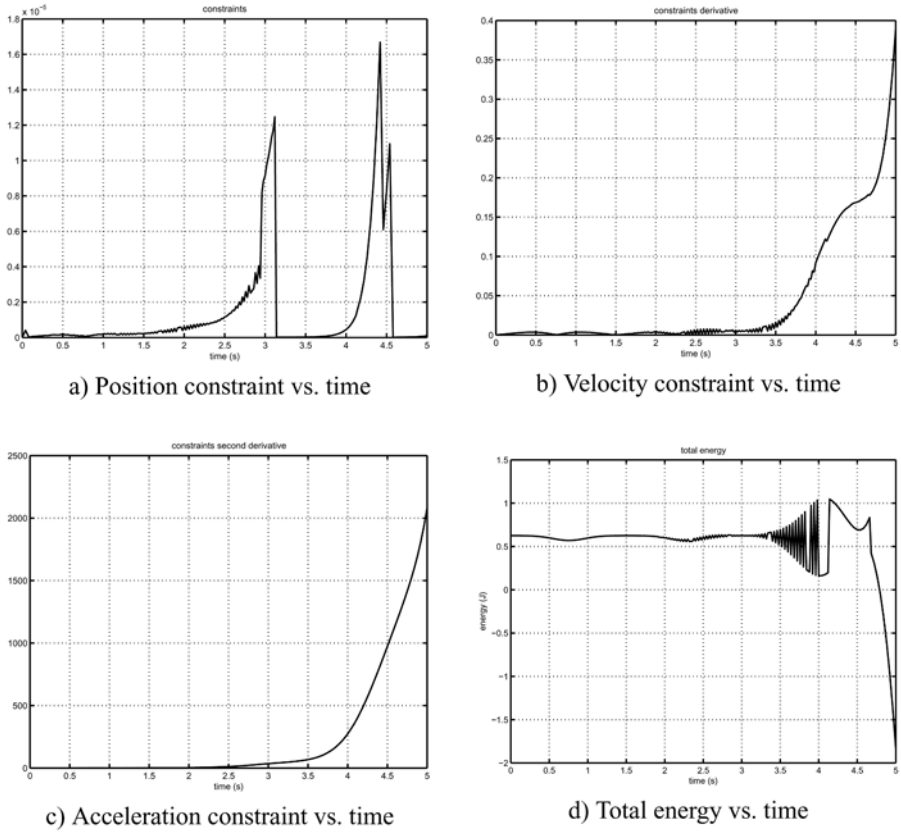

Fig. 2. Index-3 augmented Lagrangian with trapezoidal rule, without projections.

Figure 3 shows that the scheme with coordinate projections better fulfills the constraint equations at velocity and position levels than expected, while the conservative scheme achieves the exact conservation of the total energy. Nevertheless, the important remark to be made is that both schemes provide an adequate stabilization to the equations, while enforcing accurately the constraints at position level. Note from Figure 3 that a stable simulation is carried out up to 20 s, while Figure 2 shows severe instabilities after the first 3.5 s for the same time step.

If we try to achieve the highest possible time step for a stable simulation during 20 s, we find similar situations for both schemes. In the case of trapezoidal rule with coordinate projection, we can achieve a maximum time step of 0.25 s, while in the case of the conservative formulation we achieve a maximum time step of 0.20 s.

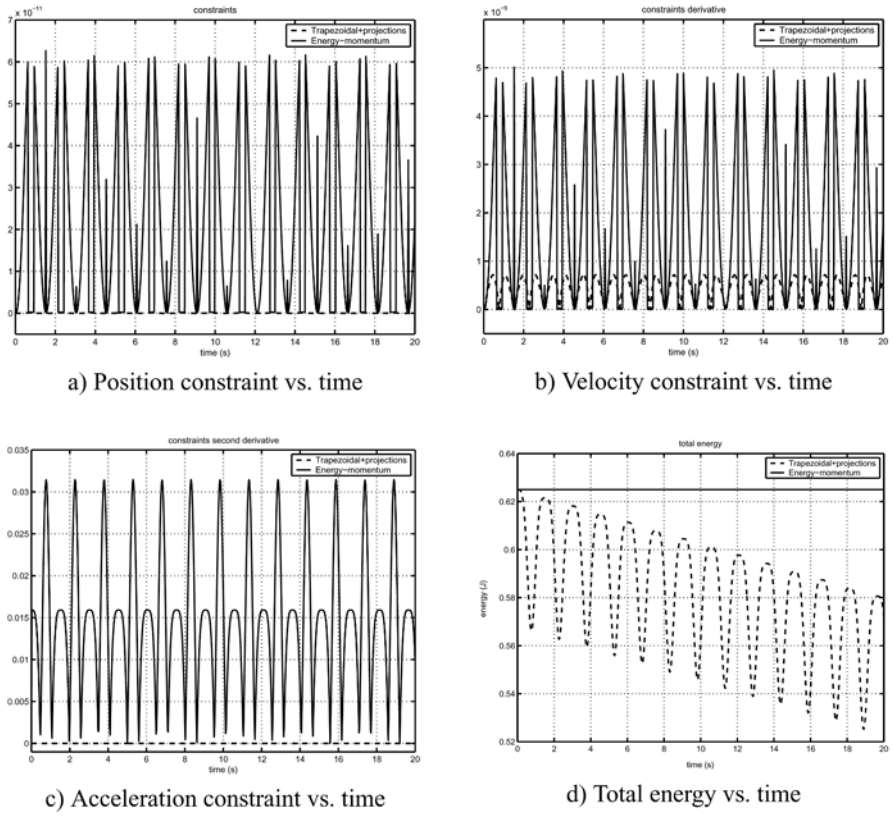

Fig. 3. Comparison between trapezoidal rule with projections and the energy conserving scheme.

7.4 A conservative scheme with projections

As pointed out at the end of Section 5, the conserving augmented Lagrangian formulation and the projection technique are not incompatible at all. When combined, the resulting scheme has two important features:

- It introduces two stabilization effects; the energy-momentum integrator stabilizes the equations keeping the energy on the system bounded, while the projection stabilize the equations maintaining the solution onto the constraints manifold, at velocity and acceleration levels. As a result, a more stable algorithm is obtained.
- It allows to appreciate clearly the effect of the projections over the energy balance, represented by the contribution ΔE_p in expression (21), since the other contribution ΔE_i is null for the conserving scheme.

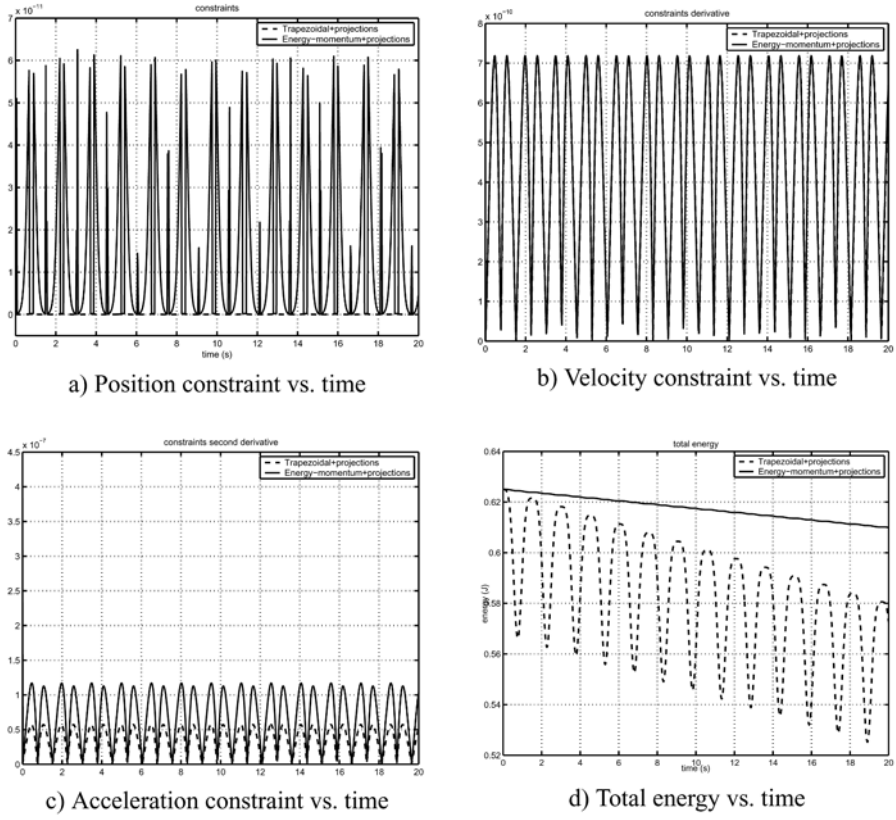

Fig. 4. Effect of projections over the trapezoidal rule and the conserving scheme.

Figure 4 shows a comparison between the results obtained applying coordinate projections on both the trapezoidal rule and the conserving scheme, using as a projection matrix the system mass matrix **M**.

Note that energy decreases in both cases, but it does it monotonically only with the conservative method. This result agrees with the theoretical results discussed in Section 6, since the energy dissipation observed in the conserving case entirely comes from the projection phase, which unconditionally dissipates energy when the mass matrix is used to perform the projection. For the trapezoidal rule, the decrease of energy is not monotonic because the contribution of the integration scheme ΔE_i, which takes positive and negative values along the simulation.

8 Conclusions

The main conclusions that can be drawn from the results presented in this work are:

- Several formulations may be used to represent the dynamics of constrained mechanical systems. These formulations differs on the method employed to enforce constraints, commonly based on the Lagrange multiplier, penalty and augmented Lagrangian methods. All these formulations pose numerical difficulties, mainly related to stability; some of these difficulties come from an unstable index reduction of the original index-3 DAE, and some arise from the intrinsic characteristics of the solution method.
- Two methods that alleviate these stability problems have been presented; the use of a standard ODE integrator (such as the trapezoidal rule) with projections, and a conservative integrator. Both exhibit excellent stability characteristics, both comply with the constraints at position level, and are very adequate to carry out robust long term simulations.
- The stability properties of the conserving method can be understood as an effect of the control over the energy. This idea comes as a natural extrapolation of the situation observed in linear conservative systems, where energy conservation implies unconditional stability. This property no longer holds in the nonlinear regime, but nevertheless provides a valid intuitive justification for the observed improvement in the stability performance of conservative schemes.
- The stability properties of the projection (combined with a standard integrator such as the trapezoidal rule or with the conservative scheme) can be understood in two different manners.
  The first is related with its effect over the energy; it has been justified that under some assumptions (mainly based on the selection of the projection matrix) no growth of energy, even unconditional dissipation, can be guaranteed for the projection, justifying its stabilization effect.
  The second interpretation is based on the observation, supported by different studies at the literature, that the numerical solution is more stable on the constraint manifold than off it. Thus, exact fulfillment of the constraints at all levels (position, velocity, acceleration) is expected to improve the overall stability of the algorithm, which is indeed observed at the numerical simulation presented at this work.
- The combination of the conservative scheme with the coordinate projection technique results is a very stable algorithm, very adequate for long term simulations. Besides, provides an optimal framework for a deeper study of the energy control provided by projections, that is naturally related to their stabilization effect, and may lead to obtain practical assessments on the projection matrix selection.
- The two alternative implementations of the Uzawa method for the augmented Lagrangian formulation (nested and simultaneous iteration) lead to similar results

with moderate time steps, with no significant impact on the overall algorithm's stability.

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