CONSERVING PROPERTIES IN MULTIBODY DYNAMICS WITH THE PENALTY METHOD

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1 Abstract

Conservation of basic dynamical properties, such as total energy and momentum, are analysed in this work in the context of a multibody formulation for mechanisms composed by both rigid and deformable bodies.

The proposed method is based on the use of dependent variables (cartesian coordinates of selected points in the mechanism) and the enforcement of the constraints through the penalty method. This choice has the advantage of setting a simple overall structure that allows the efficient treatment of both rigid bodies (discrete model) and deformable bodies (continuum model discretised with the finite element method) in order to build a joint set of equations to be solved.

Within this context, several time-stepping algorithms are considered: trapezoidal rule, HHT, mid-point rule, as well as an alternative energy-momentum algorithm. This method is based on a formulation of elements and constraints that enforces, by its intrinsic construction, the total energy and momentum conservation, generalising the ideas in [3] for multibody systems with rigid and deformable bodies and contacts. Conservation properties and robustness, two key ideas in long-term realistic simulations, are evaluated.

Several applications are presented testing the stability and conservation capabilities of the various methods with different types of mechanical systems.

2 Introduction

A multibody system is a collection of bodies (in general, rigid and deformable) linked by several types of joints, with the possibility of including active elements (like springs, dashpots, etc.). Under some circunstances, these systems undergo motions where some essential dynamical properties are conserved, such as angular momentum and total energy.

Integration algorithms that conserve energy and momentum have been discussed in [1], [3]. One of the main benefits is the confidence gained on the results for long-term simulations of conservative systems. Additionally, even though energy conservation doesn't guarantee unconditional stability in the non-linear regime [6], it appears that it can be improved in certain cases [3], specifically those arising in non-linear dynamics of solids.

In the method proposed in this paper, the configuration of the system is determined by the cartesian coordinates of selected points (natural coordinates [2]), and the constraints are enforced through the penalty method, such that large penalty values lead to small constraint violations.

A key feature of multibody systems with deformable bodies is the presence of large and slow overall motions combined with small and high-frequency internal motions. With the enforcement of the constraints through penalty, the effect on the system is physically similar to introducing very stiff elements between the constrained D.o.f's. In fact, a penalty approach introduces high-frequency components in addition to the already existing ones due to the deformable bodies. Besides, using cartesian coordinates of points and penalty has two main advantages: it makes the definition of the system simpler, and it makes possible to reduce the problem to a set of Ordinary Differential Equations (ODE's) with the same number of equations as variables in the model. This is not the case of the lagrange multipliers method, which leads to a set of differential-algebraic equations with additional variables (lagrange multipliers).

Regarding its conservation properties, the use of a penalty approach has the advantage that the constraint forces originate from a potential function, the constraint energy. The basic idea is to formulate the constraints such that the total energy (including the constraint energy) is conserved by construction of the algorithm, such that the constraints actually *store* a portion of energy, which is interchanged with the rest of the system. Using large penalty factors (or alternative methods such as augmented lagrangian), the violation of the constraint may be maintained small (and its energy too). The result is that the energy is not exactly conserved (some authors describe this situation as energy preservation), but with very small deviations, and it's exactly conserved at any time the constraints are exactly enforced during the movement.

As presented in the next sections, the use of cartesian coordinates and the penalty method makes up a convenient framework for applying the ideas originated in [3], extending these results to the formulation of multibody systems. Contacts can be treated with a similar approach, conducing to similar results as in [5] and [8].

3 Equations of motion

Let us call $\mathbf{q}$ and $\dot{\mathbf{q}}$ the vectors defined by the cartesian coordinates and velocities of selected points of the mechanism, such that both vectors define completely the configuration of the system at any time. In general, $\mathbf{q}$ contains a dependent set of variables, related through several constraint equations collected in a single constraint vector $\mathbf{\Phi}(\mathbf{q})$. With this choice of coordinates, the equations of motion, which may be deduced by the classical Lagrangian methods, are:

$$\mathbf{M}\ddot{\mathbf{q}} = \mathbf{f}_{\Phi} + \mathbf{Q}, \tag{1}$$

where:

- $\mathbf{M}$ is the mass matrix

- $\mathbf{f}_\Phi = \mathbf{f}_\Phi(\mathbf{q})$ is the force vector due to the constraints. If these are enforced through a penalty approach, this term can be written as $\mathbf{f}_\Phi = -(\partial_\mathbf{q}\mathbf{\Phi})^T \boldsymbol{\alpha}\mathbf{\Phi}$, where $\boldsymbol{\alpha}$ is the penalty matrix and $\partial_\mathbf{q}(\cdot) \stackrel{def}{=} \partial(\cdot)/\partial\mathbf{q}$.
- $\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \dot{\mathbf{q}}, t)$ is the applied force vector, due to external or internal forces (imposed loads, internal forces of deformable bodies, springs, dashpots, etc).

The use of penalty for the enforcement of constraints appears to have two main advantages compared to the traditional Lagrange multipliers method. First, equation (1) is simply a set of ordinary differential equations, instead of an differential-algebraic system. Second, the dimension of the problem does not increase: the only unknown is the $\mathbf{q}$ vector.

4 Time integration

Equation (1) is, in general, a set of highly non-linear coupled differential equations, and additionally, numerically ill conditioned due to the large penalty parameters. These features characterise a so-called "stiff" system. Physically, very different frequency responses exist within the overall movement; low-frequency for the rigid-body motions and high-frequency for the deformable bodies and constraints enforced through penalty.

These facts justify the use of implicit methods, so that very small time steps dictated by the high-frequency response can be avoided. This is computationally more expensive per time-step, since iterations for convergence check must be carried out, but nevertheless necessary.

There are several implicit integration schemes suitable for this purpose, both multistep methods (Adams-Bashforth, Adams-Moulton, HHT) and single-step methods like the trapezoidal rule.

Special attention has been paid to the implicit midpoint rule, since this algorithm is symplectic when applied to an arbitrary Hamiltonian system [9]. Applied to the general equations of motion in the form (1), the method can be written as:

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

with $(\cdot)_{n+\frac{1}{2}} = \frac{1}{2}\left[(\cdot)_{n+1} + (\cdot)_n\right]$ and $\dot{\mathbf{q}}_{n+1} = \frac{2}{\Delta t}(\mathbf{q}_{n+1} - \mathbf{q}_n) - \dot{\mathbf{q}}_n$. Nevertheless, it can experience stability problems for stiff systems, as shown in [3].

5 Energy-momentum method

This method follows the idea developed in [3], enforcing energy conservation directly by design of the integration algorithm. It may be considered as a perturbation of the implicit midpoint rule (2).

The simplest model, considered in [3], is a particle of mass m subject to a central force from the origin of a fixed reference system, whose position is denoted by $\boldsymbol{r}$. $\boldsymbol{F}(\boldsymbol{r})$ derives from a potential function $V(r)$, and can be written as:

$$\boldsymbol{F}(\boldsymbol{r}) = F(r)\frac{\boldsymbol{r}}{r} = -\frac{\partial V(r)}{\partial \boldsymbol{r}} \tag{3}$$

In this case, it's possible to impose algorithmically the exact total momentum and energy conservation with the enforcement of the following balance equation between steps n and $n+1$:

$$m(\dot{\boldsymbol{r}}_{n+1} - \dot{\boldsymbol{r}}_n) + \Delta t\, \sigma \boldsymbol{r}_{n+\frac{1}{2}} = 0 \tag{4}$$

with

$$\sigma = \frac{1}{r_{n+\frac{1}{2}}} \frac{V(r_{n+1}) - V(r_n)}{r_{n+1} - r_n} \qquad \text{and} \qquad \dot{\boldsymbol{r}}_{n+1} = \frac{2}{\Delta t}(\boldsymbol{r}_{n+1} - \boldsymbol{r}_n) - \dot{\boldsymbol{r}}_n \tag{5}$$

A generalisation of the former method for the formulation of elements and constraints in a general multibody system is presented next.

Constraints.- With the penalty method, and with the variables being the cartesian coordinates of the points, any constraint force can be handled by the former algorithm.

Let's consider first a simple model with a single particle of mass m whose position is defined by $\boldsymbol{r}$, with a motion constrained by the equation $\Phi(\boldsymbol{r}) = 0$, and with no additional forces. Assume further that the constraint is a function of the modulus of the distance between the two points ($\Phi(\boldsymbol{r}) = \Phi(r)$). In this case, it's possible to define a potential given by $V_\Phi(r) = \frac{1}{2}\alpha\Phi(r)^2$, which gives rise to a constraint force parallel to $\boldsymbol{r}$:

$$\boldsymbol{f}_\Phi = -(\partial_{\boldsymbol{r}}\Phi)\alpha\Phi = -\frac{\partial\Phi(r)}{\partial r}\alpha\Phi\frac{\boldsymbol{r}}{r} = -\frac{\partial V_\Phi(r)}{\partial r}\frac{\boldsymbol{r}}{r} \tag{6}$$

From here it's possible to apply directly the scheme defined by (3), (4), and (5), since the effect of the constraint is a central force.

If the constraint equation takes the more general form $\Phi(\boldsymbol{r}) = 0$, the constraint force that acts over the particle is not, in general, central:

$$\boldsymbol{f}_\Phi = -\frac{\partial V_\Phi}{\partial \boldsymbol{r}} \tag{7}$$

In this case, it can be shown that it's possible to enforce the total momentum and energy conservation by the following algorithmic balance equation

$$m(\dot{\boldsymbol{r}}_{n+1} - \dot{\boldsymbol{r}}_n) + \Delta t\sigma(\partial_{\boldsymbol{r}}\Phi)_{n+\frac{1}{2}} = 0 \tag{8}$$

where:

$$\sigma = \frac{V_{\Phi_{n+1}} - V_{\Phi_n}}{(\partial_{\boldsymbol{r}}\Phi)_{n+\frac{1}{2}} \cdot (\boldsymbol{r}_{n+1} - \boldsymbol{r}_n)} \tag{9}$$

This procedure can be generalised for constraints acting over different points of a multibody system. In this case, the same algorithm can be applied just denoting by $\boldsymbol{r}$ the relative distance of the points and appropiately building the constraint force vector and mass matrix associated with the involved nodes.

Rigid bodies.- Once the constraints have been formulated such that the total momentum and energy are exactly conserved, the formulation of rigid bodies is straightforward. A rigid body is defined by a number of points at constant relative distances. The constraint of constant distance between two points is expressed as a function of the distance:

$$\Phi(r) = r^2 - r_0^2 = 0$$

This constraint has the same effect as a central force $F(\boldsymbol{r}) = -2\alpha\Phi\boldsymbol{r}$, with a potential $V(r) = \frac{1}{2}\alpha(r^2 - r_0^2)^2$.

The energy-momentum formulation of a rigid body is then complete defining the coordinates of four points (in order to have a constant mass matrix), the mass matrix, and enforcing as many constant-distance constraints as necessary. Guidelines for the mass matrix construction can be found in [2].

Deformable bodies.- The deformable bodies are discretised in elements, and the cartesian coordinates of the nodes define the configuration of the body at any time. The force which acts over any node, in a general 3D case, includes the internal force of the continuum. In a hyperelastic material, this force is derived from an elastic potential function, such that it would be possible to extend the ideas presented with central forces between two particles. The case of trusses is specially simple, since the force acting between the two ends of an element is truly central and, for a hyperelastic material, there is an elastic potential that only depends on the current length of the element, given by:

$$V_{elas} = \frac{1}{2} E A_0 l_0 \varepsilon^2 \qquad \text{with} \qquad \varepsilon = \varepsilon(l) \tag{10}$$

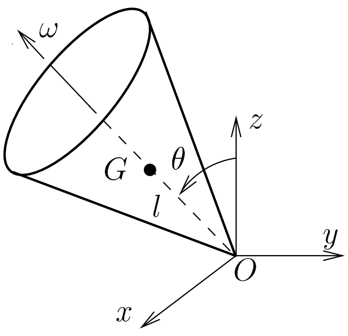
A_0, l_0 being the initial section and length, E the elastic modulus, and ε the measurement of the deformation. In the case of elastic-plastic materials, only the elastic deformation ε_e has to be considered.

Contacts.- It's possible to extend the ideas exposed for the formulation of the constraints to contacts with external rigid surfaces modeled with a penalty approach. Basically, a contact is a constraint that acts between two points (one of the body, and other from the rigid surface), for a limited time period (the time the geometrical interference lasts).

If penalty is used, the ideas exposed for constraints can be directly applied paying special attention to the detection of the contact. Physically, with this model, the energy of the contact is actually stored when the contact takes place and is restored as soon as it's released. The same basic idea was proposed in [5] and [8] for frictionless contacts.

6 Applications

Fast top.- The first application is a fast top studied previously in [1], with the following characteristics:



$$mg = 20 \text{ N} \qquad |\boldsymbol{OG}| = 1 \text{ m} \qquad \mathbf{I}_O = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{kgm}^2 \tag{11}$$

with the initial conditions

$$y_G = 0 \qquad \theta = 17.45^\circ \qquad \omega = 50 \text{ rad/s} \tag{12}$$

The body is defined with 4 points, hence a given configuration is defined by 12 parameters, the cartesian coordinates of the points. There are 9 constraint equations (6 enforcing constant relative distance among the body points, 3 more to fix a point), hence the body has three degrees of freedom. The penalty parameter (α) is $1 \cdot 10^8$. The theoretical period of the precession movement (rotation around the z axis) is 15.7 s, and the nutation period is 0.63 s.

In Fig.[1], a plot of the total energy (kinetic + gravitational potential) vs. time is shown for the HHT and energy-momentum formulations. The constraint energy is negligible compared with the other terms. The HHT curve corresponds to the maximum time step achieved ($\Delta t = 0.005$, around 15° incremental rotation angle), at the cost of introducing a rather high energy dissipation ($\alpha = -0.2$). The maximum step achieved with the trapezoidal and the mid-point rules is $\Delta t = 0.001$ s. The energy-momentum algorithm allows much larger time steps ($\Delta t = 0.017$, around 46° incremental rotation) with no dissipation. Fig.[2] shows the trajectory of the center of mass computed with the energy-momentum algorithm.

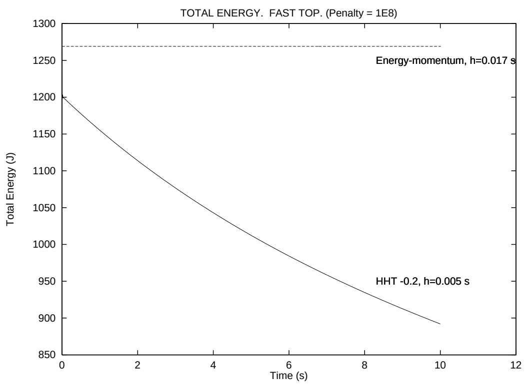


Figure 1: *Fast top. Total energy vs. time*

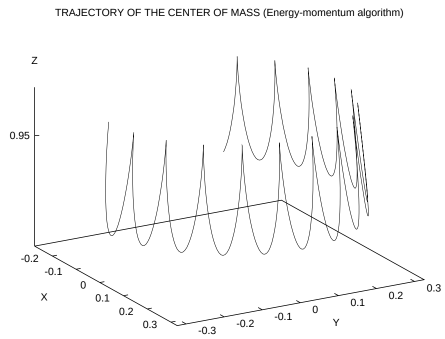
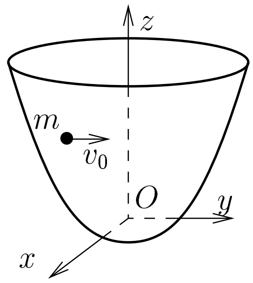


Figure 2: *Fast top. Trajectory of the center of mass*



Heavy particle on a surface.- This example shows the capability of the energy-momentum algorithm in handling constraints that depend on the relative distance vector ($\boldsymbol{r}$) through a general expression $\Phi(\boldsymbol{r}) = 0$ rather than only on the modulus ($\Phi(r) = 0$), as in the constraints involved in the rigid body model.
A particle with mass m is released from the surface of a paraboloid with equation $x^2 + y^2 - z = 0$ from the point $\boldsymbol{r}_0 = (1., 0., 1.)$ with an initial velocity $\boldsymbol{v}_0 = (0., 0.5, 0.)$ m/s, being the gravity acceleration $g = 9$ m/s^2. The penalty value is set to $\alpha = 1 \cdot 10^7$, and the movement is analysed up to 1 min. with $\Delta t = 0.1$ s.

Fig.[3] and Fig.[4] show the trajectory of the particle computed with the energy-momentum algorithm. Fig.[5] shows that all the algorithms except the energy-momentum one present severe instabilities in early stages of the movement for the total energy. Fig.[6] depicts the three components of the total momentum calculated with the energy-momentum algorithm, showing that the vertical component of the momentum is exactly conserved. The plots presented for the energy-momentum algorithm have been obtained with $\Delta t = 0.1$ s. The time-step can be increased without loss of long-term stability up to a value of $\Delta t = 4$ s., with exact conservation of total energy and momentum, but with some loss of accuracy.

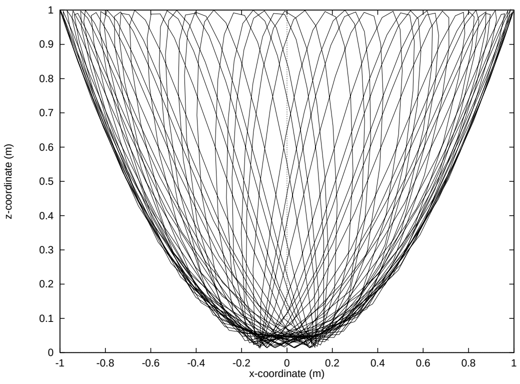


Figure 3: *Particle on paraboloid. Trajectory: xz projection. Energy-momentum algorithm, $\Delta t = 0.1$ s.*

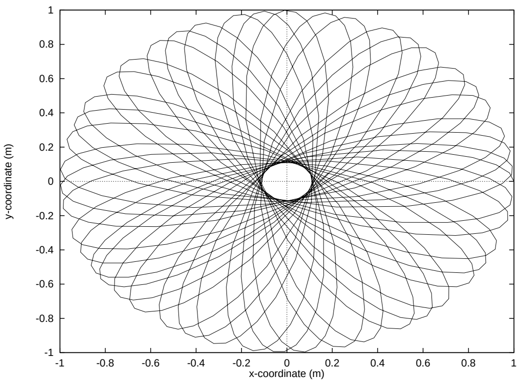
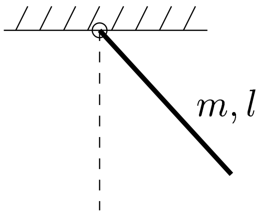


Figure 4: *Particle on paraboloid. Trajectory: xy projection. Energy-momentum algorithm, $\Delta t = 0.1$ s.*

Elastic-plastic truss.- A pendulum is made with a single deformable element (truss type) made of an elastic-plastic material with the following characteristics:



$m = 78.5$ kg	$l = 1$ m	$\rho = 7850$ kg/m^3
$E = 2 \cdot 10^5$ Pa	$\sigma_Y = 1.5 \cdot 10^5$ Pa	$H = 1 \cdot 10^5$Pa

where σ_Y is chosen such that plastic deformation will occur. Initially, the element is at rest on a horizontal position.

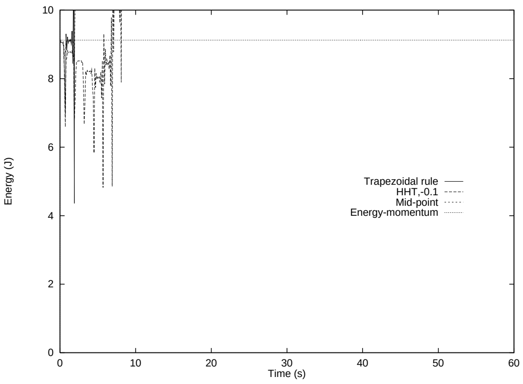


Figure 5: *Particle on paraboloid. Total energy vs. time with different integration schemes (constraint energy not included).* $\Delta t = 0.1$ *s.*

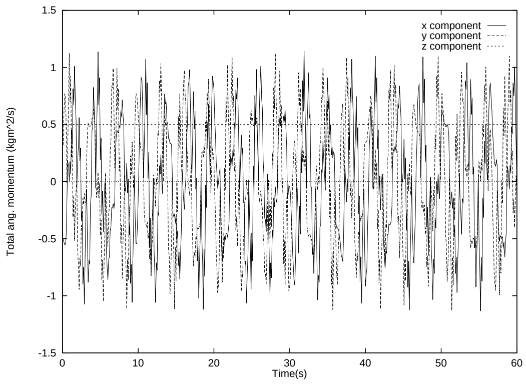


Figure 6: *Particle on paraboloid. Total angular momentum vs. time, energy-momentum algorithm.* $\Delta t = 0.1$ *s.*

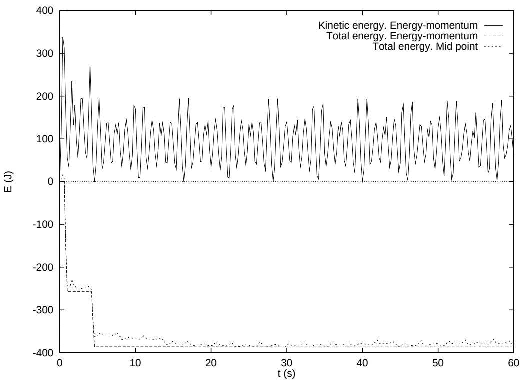


Figure 7: *Elastic-plastic compound pendulum. Energy vs. time*

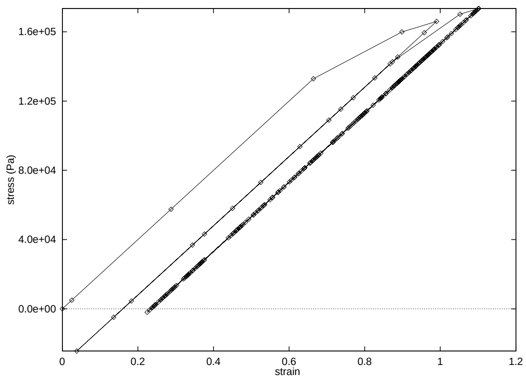


Figure 8: *Elastic-plastic compound pendulum. Strain - stress*

Fig.[7] shows the evolution of the energy with the symplectic midpoint rule and the energy-momentum algorithm, for a time step $\Delta t = 0.2$ s. The total energy curve is the result of kinetic + gravitational potential + elastic energy, and it shows two steps where permanent deformation occurs. Fig.[8] shows the evolution on the strain-stress diagram, where it can be verified that the deformation goes twice into the plastic regime.

Contact against a rigid surface.- A body is thrown against a rigid wall under the gravity effect. The upper side of the body is a rigid semisphere, and the lower side is a space truss of elastic bars. Fig.[10] shows some snapshots of the movement, and Fig.[9] shows the evolution of both kinetic energy and total energy with the energy-momentum algorithm.

In this application, the contact has been modelled with the energy-momentum algorithm too, causing slight oscillations on the energy as shown in Fig.[9] at around $t = 0.3$ s. The total energy curve (including the constraint energy, not shown in the figure) is perfectly flat.

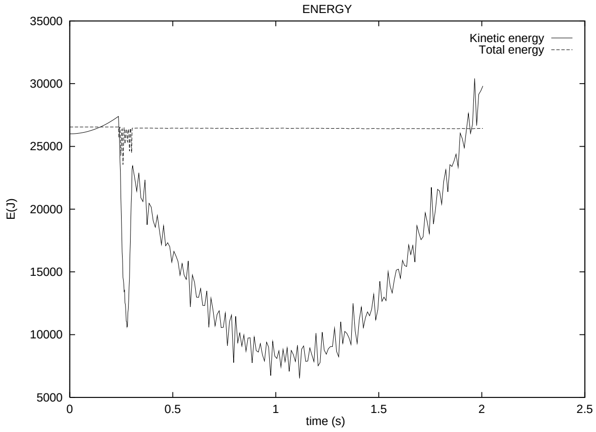
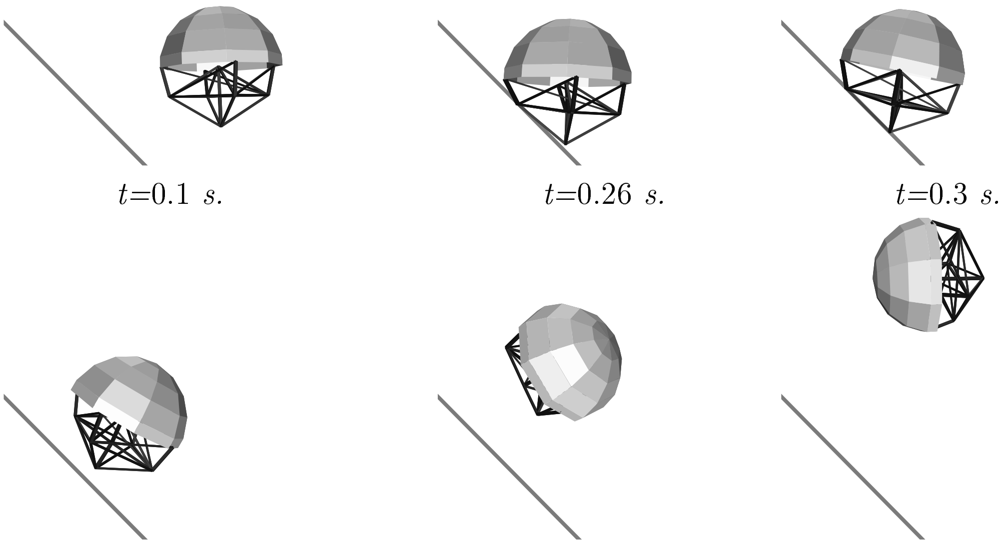


Figure 9: *Energy vs. time (contact energy not included)*



t=0.1 s. t=0.26 s. t=0.3 s.

t=0.35 s. t=0.5 s. t=1.0 s.

Figure 10: Contact with a rigid surface.

7 Conclusions

A method based on the enforcement of the constraints through penalty that conserves total energy (including the penalty potential) has been presented.

The time-stepping scheme is defined such that exact total energy conservation is algorithmically enforced at each time step, as proposed in [3]. These results have been applied to the formulation of general multibody systems composed of both rigid and deformable bodies.

The method has shown good performance in terms of energy conservation and stability, compared with other schemes like the trapezoidal rule, HHT and symplectic mid-point rule.

Further work has to be done generalising these results to more complex deformable elements (structural elements as beams, shells, and solid 3D elements) and more complex constraints. Additionally, the implementation of the augmented lagrangian method for the constraint enforcement will reduce the constraints energy and make penalty values less application-dependent, allowing more automated calculations.

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