Primal and mixed forms of Hamilton's principle for constrained rigid body systems: numerical studies

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Abstract. Constraint equations arise in the dynamics of mechanical systems whenever there is the need to restrict kinematically possible motions of the system. In practical applications, constraint equations can be used to simulate complex, connected systems. If the simulation must be carried out numerically, it is useful to look for a formulation that leads straightforwardly to a numerical approximation.

In this paper, we extend the methodology of our previous work to incorporate the dynamics of holonomically and nonholonomically constrained systems. The constraint equations are cast in a variational form, which may be included easily, in the time finite element framework. The development of the weak constraint equations and their associated "tangent" operators is presented. We also show that this approach to constraint equations may be employed to develop time finite elements using a quaternion parameterization of finite rotation. Familiarity with the notation and methodology of our previously presented work is assumed.

1 Introduction

Very often the vectorial and variational theories of mechanics are considered to be completely equivalent. Many times, variational principles are used only as an alternative approach for obtaining differential equations of motion.

Here, we assert that variational methods provide more robust formulations, which not only afford a general, unified approach, but are also more easily implemented, numerically.

During the last decade the variational formulations for dynamical systems and their numerical approximations, have known a renewed interest [e.g. Bailey (1981); Simkins (1981); Baruch and Riff (1982) and others]. Borri et al. (1985) apply a weak formulation of Hamilton's principle to the dynamics of holonomic systems, using time finite elements. Although many authors, such as Neimark and Fufaev (1972), have treated nonholonomic systems, a general variational formulation suitable for a direct numerical approximation is not yet available.

As a possible solution to this problem, we suggest the adoption of a new variational principle for holonomically and nonholonomically constrained dynamical systems and show how two different time finite element approximations can be derived.

For the sake of simplicity the formulations presented here are for finite degree of freedom systems, but they can be easily extended to continuous systems as in Iura et al. (1988).

2 Different forms of Hamilton's principle

It is shown in Borri et al. (1990), that Hamilton's principle for unconstrained dynamics can be written as:

\[ \int_{t_i}^{t_f} \left[ \delta \mathcal{L}(\dot{q}, q, t) + \dot{\delta q} \cdot f \right] dt = \left. \delta q \cdot p_b \right|_i^f \]  

(1)

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where \( t_1, t_2 \) are the ends of the time interval of interest. \( q \) and \( p \) are respectively the generalized coordinates and the momenta of the system. \( \mathcal{L}(\dot{q}, q, t) \) denotes the Lagrangian function and \( f \) the external forces not included in \( \mathcal{L} \).

In the same work, it is shown that through a Lagrange transformation, Eq. (1) can be rewritten in the following mixed form:

\[
\int_{t_1}^{t_2} \left( \delta q \cdot \dot{p} - \delta \dot{q} \cdot q - \delta H + \delta q \cdot f \right) dt = (\delta q \cdot p_b - \delta \dot{q} \cdot q_b)_{t_1}^{t_2}
\]

where \( H(p, q, t) = p \cdot \dot{q} - \mathcal{L} \) denotes the Hamiltonian of the system.

Equations (1) and (2) are, respectively, primal and mixed forms of Hamilton's principle and are very suitable for numerical approximations in the context of finite elements in the time domain [e.g. Borri and Montegazza (1986); Borri and Atluri (1988)]. We note that Eq. (1) implies that displacement continuity is satisfied "a priori" while in Eq. (2) displacement continuity is enforced in a weak sense.

For purposes of illustration, we consider the class of constraints which are functions of the generalized coordinates and time, but only linear functions of the generalized velocities. As pointed out in Lanczos (1964), this class of constraints encompasses a large number of practical situations.

\[
\psi(q, q, t) = A(q, t) \cdot \dot{q} + a(t, t) = 0.
\]

If calculating the work of constraint forces is to be avoided, the virtual displacements must satisfy the constraints:

\[
A \cdot \delta q = 0.
\]

Constraints expressed in the form of Eq. (3) can be either nonholonomic, or the time derivatives of holonomic constraints. In order to enforce Eqs. (3) and (4), they are cast in weak form, with an appropriate choice of test functions. Let \( \mu \) be the Lagrange multipliers. Then, weighting Eq. (3) with the variation \( \delta \mu \) and Eq. (4) with the time derivative \( \dot{\mu} \), the following relation is obtained:

\[
\int_{t_1}^{t_2} \left( \delta \mu \cdot \dot{q} - \mu \frac{\partial \psi}{\partial q} \cdot \delta q \right) dt = 0.
\]

The benefit of this form is that it allows an integration by parts that reduces the continuity requirements for the Lagrangian multipliers. Carrying out this integration yields:

\[
\int_{t_1}^{t_2} \left[ \delta \mu \cdot \dot{q} + \mu \left( \frac{d}{dt} \left( \frac{\partial \psi}{\partial q} \right) + \frac{\partial \psi}{\partial q} \frac{d}{dt} (\delta q) \right) \right] dt = \mu \frac{\partial \psi}{\partial q} \cdot \delta q |_{t_1}^{t_2}.
\]

Combining Eq. (6) with the primal form, Eq. (1), results in a modified primal form:

\[
\int_{t_1}^{t_2} \left( \delta \mathcal{L} + \delta q \cdot \dot{f} + \delta (\mu \cdot \psi) + \mu \left( \frac{d}{dt} \frac{\partial \psi}{\partial \dot{q}} \cdot \delta q \right) \right) dt = \delta q \cdot \left( \dot{p} + \mu \frac{\partial \psi}{\partial q} \right) |_{t_1}^{t_2}.
\]

This may be written more concisely as:

\[
\int_{t_1}^{t_2} (\delta \mathcal{P} + \delta q \cdot \mathcal{f}) dt = \delta q \cdot \mathcal{P}_b |_{t_1}^{t_2},
\]

where:

\[
\mathcal{P} = \mathcal{L} + \mu \cdot \psi \quad \mathcal{P}_b = \dot{p} + \mu \frac{\partial \psi}{\partial q} \quad \mathcal{f} = \dot{f} + f_c
\]

and

\[
f_c = \mu \left( \frac{d}{dt} \frac{\partial \psi}{\partial q} - \frac{\partial \psi}{\partial \dot{q}} \right).
\]

Equation (8) is a modified primal form of Hamilton's principle for constrained systems and \( \mathcal{P}, \dot{p}, \mathcal{f} \) are respectively, the modified Lagrangian function, the modified generalized momenta, and the
external forces as modified by the reactions due to the nonholonomic constraints. The constraint reaction force \( f_c \) is typical of nonholonomic constraints, since it is identically zero for the holonomic case. In fact, the holonomic constraint implies \( \psi = \phi \) from which it is clear that:

\[
\frac{\partial \phi}{\partial q} = \frac{\partial \phi}{\partial q} = 0
\]  

so:

\[
f_c = \mu \left( \frac{d}{dt} \frac{\partial \phi}{\partial q} - \frac{\partial}{\partial q} \frac{d \phi}{dt} \right) = 0.
\]  

In the nonholonomic case however, \( f_c \) is different from zero. Substituting Eq. (3) into Eq. (10), the modification of the force due to nonholonomic constraints may be written as:

\[
f_c = C \cdot \dot{q} + c, \quad C = -C'
\]

where:

\[
C_{ik} = \mu_s \left( \frac{\partial A_{xi}}{\partial q_k} - \frac{\partial A_{xk}}{\partial q_i} \right), \quad c_i = \mu_s \left( \frac{\partial}{\partial t} A_{xi} - \frac{\partial A_{xk}}{\partial q_i} \right).
\]

It is interest to note that \( \tilde{p} \) are actually the generalized momenta of the augmented Lagrangian. In fact, it can be seen that:

\[
\tilde{p} = \frac{\partial \tilde{L}}{\partial \dot{q}} = \frac{\partial \psi}{\partial q} + \mu \frac{\partial \psi}{\partial \dot{q}}.
\]

Taking this property into account, the modified Hamiltonian function can be defined as:

\[
\tilde{H} = \tilde{p} \cdot \dot{q} - \tilde{L}
\]

and Eq. (2) may be rewritten in the following modified mixed form:

\[
\int \left( \delta \dot{q} \cdot \tilde{p} - \delta \tilde{p} \cdot \dot{q} - \delta \tilde{H} + \delta q \cdot f \right) dt = \left( \delta q \cdot \tilde{p} - \delta \tilde{p} \cdot q_b \right)
\]

where the velocity \( \dot{q} \) is eliminated from the expression for \( f_c \) in favor of the momentum. It is worth emphasizing that the modified momenta \( \tilde{p} \) are no longer constrained and can be viewed as independent variables. The compatible momenta \( p \) and the Lagrangian multipliers \( \mu \) can be recovered from the modified momenta by a simple projection.

In order to better understand the role of the Lagrangian multipliers, consider the Euler equations corresponding to the principle Eq. (8). These are:

\[
\frac{d}{dt} \frac{\partial \tilde{L}}{\partial \dot{q}} - \frac{\partial \tilde{L}}{\partial q} - f + A^l \cdot \frac{d}{dt} \mu = 0, \quad A \cdot \dot{q} + a = 0.
\]

It is immediately seen that the Lagrange multipliers enter into these expressions only through their time derivatives. It is therefore only the derivative which has a meaningful physical interpretation. Therefore the initial value of modified momentum \( \tilde{p} \) may be selected in a convenient way. Specifically, a scaling approach may be used, which at the end of each integration step resets \( \mu = 0 \) and maintains \( \tilde{p} = p \). Further, the constraint equations can be written in term of the modified momentum \( \tilde{p} \) and solved for the Lagrange multipliers. In order to accomplish this, the following equations must be solved in terms of the velocity \( \dot{q} \):

\[
\tilde{p} = \frac{\partial \tilde{L}}{\partial \dot{q}}
\]

which leads to:

\[
\dot{q} = B \cdot (\tilde{p} - A^l \mu) + b.
\]
Substituting Eq. (19) back into Eq. (3) and solving for \( \mu \) results in:
\[
\mu = \mu_o + D^{-1} \cdot A \cdot B \cdot \bar{p}
\]  
(20a)

where:
\[
D = A \cdot B \cdot A^t, \quad \mu_o = D^{-1} \cdot (A \cdot b + a).
\]  
(20b)

The true momentum can then be recovered from the modified momentum through the expression:
\[
p = \bar{p} - A^t \cdot \mu,
\]  
(21)

thus obtaining:
\[
p = p_o + P \cdot \bar{p}
\]  
(22a)

where:
\[
P = I - A^t \cdot D^{-1} \cdot A \cdot B, \quad p_o = -A^t \cdot \mu_o.
\]  
(22b)

Clearly, \( P \) is a projection, since:
\[
P^2 = P.
\]  
(23)

From the knowledge of \( \bar{p} \), the corresponding \( \mu_o \) can be recovered and using Eq. (22), the boundary momentum \( p_o \) may be found.

3 Examples

In order to verify this methodology for both holonomic and nonholonomic constraints, the classical cases of a spinning top and rolling coin are considered. The mass center of the top is chosen as the reference point, so that the motion is described by six degrees of freedom, with the fixity of the suspension point being enforced as a constraint. For the coin, the mass center is again chosen as the reference, with the nonholonomic constraint of zero velocity of the contact point, enforced in weak form. In each case the constraint is put in the form of Eq. (3), and included as described above. The numerical results are compared for two, three and four noded time finite elements with various step sizes. The time finite element approach applied here, is developed in Borri et al. (1990), using the finite rotation vector as rotation coordinates. It is assumed that the reader is familiar with those results. In the following discussion, only the residual vectors and tangent matrices associated with the constraints are discussed.

3.1 Spinning top

The case of a spinning top is treated in virtually all texts on dynamics. The motion is typically described in terms of three Euler angles and the translational degrees of freedom are eliminated by using the suspension point as a reference. Since the intent of this example is to demonstrate the application of constraint equations, the mass center is chosen as the reference point. The constraint that the suspension point is fixed may then be expressed as:
\[
\dot{x} = \rho \times \omega
\]  
(24)

where \( \dot{x} \) is linear velocity of the mass center, \( \omega \) is the angular velocity of the top and \( \rho \) is the radius vector from the mass center to the suspension point.

Following the above procedure the constraint is cast in weak form along with the constraint on virtual motion:
\[
\delta x = \rho \times \bar{\theta}_b.
\]  
(25)

Letting the multipliers be \( \mu \), Eq. (24) is weighted with the variation, \( \delta \mu \), while the virtual constraint is weighted with the time derivative, \( \dot{\mu} \). Combining the weak forms of the constraints and integrating
over the time interval leads to:
\[
\int_{t_1}^{t_2} \delta \mu \cdot (\dot{x} - \rho \times \omega) - \mu \cdot (\delta x - \rho \times \vartheta) \, dt = 0.
\] (26)

Integrating by parts the term involving \(\dot{\mu}\), results in an expression of the form:
\[
\int_{t_1}^{t_2} \delta \mu \cdot (\dot{x} - \rho \times \omega) + \mu \cdot (\delta \dot{x} - \rho \times \vartheta - \dot{\vartheta} \times \delta x) \, dt = \mu \cdot (\delta x - \rho \times \vartheta)l_{t_1}^{t_2}.
\] (27)

The residual vector contribution, due to the constraint, is then:
\[
\{(x - \rho \times \omega), \mu, (\rho \times \mu), 0, (\dot{\rho} \times \mu)\}
\] (28)
where the organization of the test functions is \((\delta \mu, \delta x, \dot{x}, \delta x, \vartheta)\).

The tangent matrix for this constraint is obtained by linearizing the residual vector. In carrying out the linearization process, the following identities are used.
\[
d\rho = \dot{\vartheta} \times \rho = -\rho \times \vartheta,
\dot{\rho} = \omega \times \rho
\] (29, 30)
\[
d\rho = \dot{\vartheta} \times \rho + \vartheta \times \dot{\rho} = -\rho \times \dot{\vartheta} - \dot{\vartheta} \times \rho,
\dot{\omega} = \dot{\vartheta} \times \omega - \vartheta \times \dot{\omega}.
\] (31, 32)

With these relations in mind, it is straightforward to write down the linearization. The first group of terms corresponding to the test functions \(\delta \mu\), leads to:
\[
\delta \mu \cdot (d \dot{x} - d \rho \times \omega - \rho \times d \omega)
\] (33)
which, in view of the above identities, simplifies to:
\[
\delta \mu \begin{bmatrix}
d\dot{x} \\
d\vartheta \\
d\omega
\end{bmatrix} = \begin{bmatrix}
d \dot{x} \\
d \vartheta \\
d \omega
\end{bmatrix}.
\] (34)

Similarly, the second group of terms in the residual vector, corresponding to the test functions \(\delta \dot{x}\), lead to:
\[
\delta \dot{x} \cdot I \cdot d \mu.
\] (35)
The terms involving the test functions \(\delta \dot{x}\) linearize as:
\[
\dot{\vartheta} \left(\delta \rho \times \mu + \rho \times d \mu\right)
\] (36)
which reduces to:
\[
\dot{\vartheta} \begin{bmatrix}
d \mu \\
d \vartheta
\end{bmatrix}.
\] (37)

Finally, the last group of terms in the residual vector leads to:
\[
\dot{\vartheta} \left(\delta \rho \times \mu + \dot{\rho} \times d \mu\right)
\] (38)
which may be written as:
\[
\dot{\vartheta} \begin{bmatrix}
d \mu \\
d \vartheta
\end{bmatrix}.
\] (39)

Combining these relations provides the tangent matrix for the constraint. The resulting tangent matrix is then:
\[
\mathcal{T}_{\text{tang}} = \begin{bmatrix}
0 & -\rho \times I & 0 & \dot{\rho} \times I \\
I & 0 & 0 & 0 \\
\rho \times I & 0 & 0 & \mu \times \rho \times I \\
0 & 0 & 0 & 0
\end{bmatrix}
\] (40)
The exact solution for a spinning top involves the evaluation of an elliptic integral. This is not done here. Rather, the regions of different behavior are explored. Initial conditions for the top are altered, in order to produce the following three situations (Fig. 1). Case 1 exhibits precession which is always in the same direction throughout the motion. Case 2 exhibits precession which changes sign during the motion. Case 3 does not reverse its direction of precession but does stop precessing at points in its motion (cuspidal motion).

For each of these cases, the problem is solved with different time steps and with two, three and four noded time elements. The input data for each case are given as:

**Case 1:**
- The mass is 1.0.
- The axial moment of inertia is 0.40.
- The transverse moment of inertia is 0.75.
- The initial orientation is in the yz plane, included 10° from vertical.
- The initial angular velocity is (0, 0.9888, 7.5167) rad/s.
- The distance from the mass center to the support is 0.2.
- Gravity is 3.0.

**Case 2:**
- The initial angular velocity is (0.020905, 6.2964) rad/s.
- All other data are the same.

**Case 3:**
- The initial angular velocity is (0, 0, 6.3794) rad/s.
- All other data are the same.

The solutions obtained by time finite elements are compared to the solution found by integrating the equations of motion in terms of Euler angles, using the fourth order Runge–Kutta integrator RKM45. The allowable error per step, used in the Runge–Kutta integration was $10^{-10}$, and this solution will be referred to as the exact solution in the following comparisons.

Figure 2 shows the results for case 1, using two noded elements and with the maximum time step restricted to 0.06 s. This represents about 28° of proper rotation per step. For a direct comparison, Fig. 3 shows the result for three noded elements with the step size restricted to 0.06 s. Even though a three model element spans twice the time of a two noded elements, the improvement in the solution is clear. Figure 4 presents the results for the four noded elements, which are also quite good. The three and four noded elements are very accurate and demonstrate superior performance compared to the two noded elements. The errors in the $x$, $y$ and $z$ coordinates of the mass center, at the end of the simulation, were (0.976%, 1.345%, 0.0539%) for the two noded elements, (0.308%, 0.176%, 0.0068%) for the three noded elements and (0.068%, 0.095%, 0.00022%) for the four noded elements.

The same type of behavior is exhibited in the other two motion cases. Figures 5 and 6 show the results for case 2, by three-noded and four-noded elements, respectively. The cuspidal motion is shown in Figs. 7 and 8.
3.2 Rolling coin

As an example of a nonholonomic or velocity constraint, the classic problem of a rolling coin is considered (Fig. 9). Here again the mass center is taken as the reference point. The constraint equations, enforcing zero velocity of the contact point, appear identical to those for the top.
However, the radius vector from the mass center to the contact point is not embedded in the body fixed frame, as it was for the top.

\[ \dot{x} = \rho \times \omega \]  

(41)

where \( \dot{x} \) is linear velocity of the mass center, \( \omega \) is the angular velocity of the coin and \( \rho \) is the instantaneous radius vector from the mass center to the contact point.

The constraint is again cast in a weak form, along with the constraint on virtual motion:

\[ \delta x = \rho \times \theta_b. \]  

(42)

The results is identical to Eq. 26.

\[ \int_{t_1}^{t_2} \delta \mu \cdot (\dot{x} - \rho \times \omega) - \dot{\mu} \cdot (\delta x - \rho \times \theta_b) dt = 0. \]  

(43)

Integrating by parts the term involving \( \dot{\mu} \) results in an expression of the form

\[ \int_{t_1}^{t_2} \delta \mu \cdot (\dot{x} - \rho \times \omega) + \mu \cdot (\delta \dot{x} - \rho \times \dot{\theta}_b - \dot{\rho} \times \theta_b) dt = \mu \cdot (\delta x - \rho \times \theta_b) |_{t_1}^{t_2}. \]  

(44)

Before Eq. (44) can be simplified further, the radius must be expressed in terms of known directions. This can be done by first denoting the unit vector in the direction of gravity by \( e_g \), the unit vector normal to the plane of the coin by \( e_n \) and the unit vector along the line of the radius as \( e_p \). The unit vector \( e_p \) is then written as:

\[ e_p = \frac{(I - e_n \cdot e_n') e_g}{\sqrt{e_g^2 (I - e_n \cdot e_n')}} = \frac{e_g}{\sqrt{c \cdot c}} \]  

(45)

where \( c = (I - e_n \cdot e_n') e_g \). The variation and the time derivative of \( e_p \) can then be expressed as:

\[ \delta e_p = -\frac{1}{\sqrt{c \cdot c}} \left[ I - \frac{c \cdot c'}{c' \cdot c} \right] \delta c = A \cdot B \cdot \theta_b \]  

(46)

\[ \dot{e}_p = \frac{1}{\sqrt{c \cdot c}} \left[ I - \frac{c \cdot c'}{c' \cdot c} \right] \dot{c} = A \cdot B \cdot \omega \]  

(47)

where:

\[ A = \frac{1}{\sqrt{c' \cdot c}} [I - e_n \cdot e_p'], \quad B = [e_n^2 e_g \times I - e_n \cdot e_n' e_g \times I]. \]  

(48, 49)
Using these relations in Eq. (44), the residual vector for the rolling constraint is expressed as:

\[
\{(\dot{x} - \rho \times \omega), \mu, (\rho \times \mu), 0, (\dot{\rho} \times \mu)\}
\]

where, again, the organization of the test functions is \((\delta \mu, \delta x, \delta \mu, \delta x, \delta \mu)\). In Eq. (50) \(\dot{\rho}\) is understood to be \(\rho \dot{e}\), with \(\dot{e}\) given by Eq. (47) and \(\rho\) being the modulus of \(\rho\).

The tangent matrix for the rolling constraint is obtained by linearizing the residual vector. In carrying out the linearization, the following identities and notations are used.

\[
\begin{align*}
d\omega &= \dot{\theta} - \omega \times \theta, & d\rho &= \rho de = \rho A \cdot B \cdot \theta \\
\dot{\rho} &= \rho \dot{e}, & \dot{\rho} &= \rho A \cdot B \dot{\theta} + (A \cdot B + A \cdot \dot{B}) \cdot \theta \\
\end{align*}
\]

where:

\[
\begin{align*}
\dot{A} &= -\frac{c \cdot \dot{B} \cdot \omega}{c \cdot c} A - \frac{1}{c \cdot c}(\dot{e}_\rho \cdot \dot{e}_\rho + \dot{e}_\mu \cdot \dot{e}_\mu) \\
\dot{B} &= e_\rho \cdot \omega \times e_n \times I + e_\mu \cdot \omega \times e_n \times I + e_\mu \cdot e_n \cdot \omega \times e_n \times I = \omega \times e_n \cdot e_n \times I.
\end{align*}
\]

In view of the above relations, the development of the tangent matrix for this constraint proceeds in exactly the same way as for the top. The details of the algebra are omitted, but the steps are...
straightforward to verify. The resulting tangent matrix is given by:

\[
\mathcal{F}_{\text{coin}} = \begin{bmatrix}
0 & I & -\rho \times I & 0 & \rho \times \omega \times I + \omega \times \rho A \cdot B \\
I & 0 & 0 & 0 & 0 \\
\rho \times I & 0 & 0 & 0 & -\mu \times \rho A \cdot B \\
0 & 0 & 0 & 0 & 0 \\
\rho A \cdot B \cdot \omega \times I & 0 & -\mu \times \rho A \cdot B & 0 & -\mu \times \rho (A \cdot B + A \cdot \dot{B})
\end{bmatrix}
\]  

(57)

The problem definition for the rolling coin example is as follows: The coin was started with an initial angular velocity of \(-2\) radians/s about the axis of symmetry of the coin, and an initial velocity of the mass center of 0.4 units/s in the positive X direction. The coin has unit mass and axial and transverse moments of inertia given by 0.4 and 0.75, respectively. The coin has a radius of 0.2 units, and is initially inclined at 45°.

Just as with the top, the solution for the rolling coin was evaluated with the integrator RKM45, imposing an accuracy requirement of \(10^{-10}\) to establish an “exact” solution. The same type of behavior observed in the top problem is found here. The two-noded elements produced good results for reasonably small time steps, while the three, and four-noded elements were much more accurate. Figures 10 through 12 shows the plots of the mass center, indicated by circles and the contact point, indicated by plus signs. The two noded elements used a time step of 0.3s which corresponds to approximately 35° of proper rotation per element. The three and four noded elements were similarly restricted to a maximum time step of 0.3s and clearly produce much more accurate solutions.

4 Rigid body dynamics using quaternions

The methodology for including constraints presented above, may be applied when using quaternions as rotation parameters. The use of quaternions as a four dimensional parametrization of rotation is well known. However, their use in a time finite element approximation, has not been reported. Quaternions, used in this context result in a very simple expression for the linearization of the governing equations, as will be shown in the following discussion. This simplicity may justify the increased number of parameters. For this choice of rotation coordinates, a free tumbling body constitutes a constrained problem, if the restriction that the quaternion have unit magnitude, is enforced in a weak sense.

For the case of a free tumbling body, attention is focused on the angular motion. The rotation tensor \(R\), which describes the orientation of a body fixed frame, may be expressed in terms of a unit quaternion. This is demonstrated in Appendix A, along with some other fundamental relations in quaternion algebra.

A generic quaternion is indicated by \(q\) and has a scalar part \(q_s\) and a vector part \(q_v\). In this case, the quaternion constitutes the generalized coordinates. A unit quaternion has a scalar part \(q_s = \cos \phi/2\) and a vector part \(q_v = \sin \phi/2\). Where \(\phi\) is the magnitude of rotation and \(\mathbf{e}\) is the unit vector along the axis of rotation. As shown in Appendix A, a four dimensional angular velocity is defined as \(\dot{\omega} = 2B(q) \cdot \dot{q}\). Expressed in reference coordinates, the pull back of the angular velocity is \(\dot{\omega} = 2A(q) \cdot \dot{q}\). When \(q\) is a unit quaternion, \(\omega_q = \omega_q^f = 0\) and the vectorial part \(\omega_v \equiv R \cdot \dot{\omega}_v\) coincides with the three dimensional angular velocity. An a priori satisfaction of the unit condition on the quaternion is not convenient in a finite element context. This is due to the fact that polynomial interpolation of unit quaternions does not result in a unit quaternion. The unity constraint that \(q \cdot q = 1\) will be put in the differential form, \(2\dot{q} \cdot q = 0\) and enforced in a weak sense.

As with the angular velocity, we define a four dimensional momentum \(h\) as \(h = J \cdot \omega\), where \(J\) is a four dimensional inertia tensor which can be defined in a number of ways. The simplest is:

\[
J = \begin{bmatrix}
J_s & 0 \\
0 & J_s
\end{bmatrix}
\]  

(58)
where $J_3$ is the three dimensional inertia tensor and the scalar $J_s$ in an arbitrary constant, different from zero. With this definition, the scalar part of $\mathbf{h}$ is zero for a unit quaternion. The vectorial part then coincides with the usual three dimensional momentum regardless of the value of $J_s$. Choosing $J_s \neq 0$ allows the calculation of the inverse relation $\omega = J^{-1} \mathbf{h}$.

The high degree of nonlinearity in rigid body dynamics arise from the fact that $J_3$ is not constant but satisfies the following:

$$ J_3 = R \cdot \tilde{J}_3 \cdot R^t $$

(59)

where $\tilde{J}_3$ is constant. The four dimensional inertia tensor is then defined as:

$$ J = G \cdot \tilde{J} \cdot G^t $$

(60)

where:

$$ G = \begin{bmatrix} 1 & 0 \\ 0 & R \end{bmatrix} \quad \text{and} \quad \tilde{J} = \begin{bmatrix} J_s & 0 \\ 0 & J_3 \end{bmatrix} $$

(61)

Two matrices, $A(q)$ and $B(q)$, which will be used extensively in this section, are defined to be:

$$ A(q) = \begin{bmatrix} q_s & -q_v \\ q_v & q_s I + q_v \times I \end{bmatrix} = [q] A_s(q) $$

(62)

$$ B(q) = \begin{bmatrix} q_s & -q_v \\ q_v & q_s I - q_v \times I \end{bmatrix} = [q] B_s(q) $$

(63)

The modified primal form, Eq. (7), and the modified mixed form, Eq. (16), may now be written in terms of the quaternion parameters.

### 4.1 Primal form

In the case of the free tumbling body, the kinetic energy is the Lagrangian and may be written as:

$$ T = \frac{1}{2} \omega^* \cdot \tilde{J} \cdot \omega^* = 2 \dot{q} \cdot A(q) \cdot \tilde{J} \cdot A(q) \cdot \dot{q} = 2 q \cdot C(q) \cdot \tilde{J} \cdot C'(q) \cdot q. $$

(64)

The momentum, $p$, which is conjugate to $\dot{q}$, is defined as:

$$ p = \frac{\partial T}{\partial \omega} = 2 A(q) \cdot \dot{h}^* = 2 B(h^*) \cdot q. $$

(65)

The modified kinetic energy is then:

$$ \tilde{T} = T + 2 \mu_\ast q \cdot \dot{q} $$

(66)

and the modified momentum is:

$$ \tilde{p} = \frac{\partial \tilde{T}}{\partial \omega} 2 \mu_\ast q = 2 A(q) \cdot \dot{h}^* + 2 \mu_\ast q = 2 A(q) \cdot \tilde{h}^* = 2 B(\tilde{h}^*) \cdot q $$

(67)

where:

$$ \tilde{h}^* = (h^\mu_\ast, h^\ast_\mu) $$

(68)

is the modified four dimensional angular momentum. The form of Hamilton’s principle, with a quaternion parametrization of rotation, may be linearized quite simply as:

$$ \int_{t1}^{t2} \delta(q, q, \mu) \cdot \mathcal{T}_q \cdot d(q, q, \mu) = \int_{t1}^{t2} \delta q \cdot \tilde{p}_q |_{t1}^{t2} - \int_{t1}^{t2} \delta(q, q, \mu) \cdot \mathcal{R}_q \cdot dt $$

(69)

where:

$$ \mathcal{R}_q = (2 B(\tilde{h}^*) \cdot q, 2 B(\tilde{h}^*) \cdot \dot{q} + f, 2 \dot{q}^t \cdot q) $$

(70)
\[ \mathcal{F}_q = \begin{bmatrix} A(q) \cdot \mathcal{J} \cdot A'(q) & 2B(\mathcal{J}^*) + 4A(q) \cdot \mathcal{J} \cdot C(q) & 2q \\ 2B' (\mathcal{J}^*) + 4C(q) \cdot \mathcal{J} \cdot A'(q) + f_q & 4C(q) \cdot \mathcal{J} \cdot C'(q) + f_q & 2q \\ 2q' & 2q' & 0 \end{bmatrix} \] (71)

4.2 Mixed form

The discussion of the mixed formulation begins with the definition of the modified Hamiltonian:

\[ \mathcal{H} = \frac{1}{2} \mathcal{H}^* \cdot J^* \cdot \mathcal{H}^* \] (72)

where \( \mathcal{H}^* \) is given by the following expression:

\[ \mathcal{H}^* = (\mathcal{J}^* t - \mu, \mathcal{H}^* s) = \frac{1}{2} A(q) \cdot (\mathcal{J}^* - 2\mu \mathcal{q}) = \frac{1}{2} C'(\mathcal{J}^* - 2\mu \mathcal{q}) \mathcal{q} \] (73)

It is interesting in this case to see the Euler equations corresponding to the mixed form. They are:

\[ \dot{q} = \frac{1}{2} B(w^*) \cdot \mathcal{J} \mathcal{q} \]
\[ \dot{\mathcal{p}} = -\frac{1}{2} B(\mathcal{w}^*) \cdot \mathcal{J} \mathcal{p} + 2\mu \mathcal{q} \mathcal{q} + f \]
\[ 0 = \frac{1}{2} q^2 \cdot B(\mathcal{w}^*) \mathcal{J} + B(\mathcal{w}^*) \cdot \mathcal{J} \mathcal{q} = q^2 \omega_s \] (74)

where \( \omega_s = \frac{1}{2} J^{-1} \cdot A'(q) \cdot (\mathcal{J}^* - 2\mu \mathcal{q}) \). From the last equation it is immediately clear that \( \omega_s = 0 \). The equations can then be reduced to the first two sets in terms of \( \mathcal{p} \) and \( \mathcal{q} \) leading to:

\[ \dot{q} = \frac{1}{2} B(\mathcal{w}^*) \cdot \mathcal{J} \mathcal{q}, \quad \dot{\mathcal{p}} = -\frac{1}{2} B(\mathcal{w}^*) \cdot \mathcal{J} \mathcal{p} + f. \] (75)

Solving for \( \mu \) from the equation \( \omega_s = 0 \) leads to:

\[ \mu = \frac{1}{2} q^{-2} \mathcal{q} \cdot \mathcal{p}. \] (76)

Clearly, the multiplier, \( \mu \), is independent of \( J^* \). Moreover, by substitution into the definition \( \mathcal{p} = \mathcal{p} - 2\mu \mathcal{q} \), the true momentum may be written as:

\[ \mathcal{p} = P \cdot \mathcal{p} \] (77)

where:

\[ P = \mathcal{I}_s - q^{-2} \mathcal{q} \cdot \mathcal{q} \] (78)

is the projection for the present case. This projection is not required during the solution process, but only when the true momentum must be recovered.

The linearization of the modified mixed principle, around a given state \((\mathcal{p}_0, \mathcal{q}_0)\), can be written as:

\[ \frac{d}{dt} \left[ I_s \left[ \frac{d}{dt} (\delta \mathcal{p}, \delta \mathcal{q}) \cdot I_s \left[ \delta \mathcal{p}, \delta \mathcal{q} \right] - \delta (\mathcal{p}, \mathcal{q}, -) \cdot \mathcal{F}_s \cdot \delta (\mathcal{p}, \mathcal{q}, \mu) \right] dt = (\delta \mathcal{p}, \delta \mathcal{q}) \cdot I_s \left[ \delta (\mathcal{p}, \mathcal{q}, \mu) \cdot \mathcal{S}_s \right] \cdot dt \] (79)

where:

\[ I_s = \begin{bmatrix} 0 & -I_s \\ I_s & 0 \end{bmatrix}, \quad \mathcal{S}_s = \left( \frac{1}{2} B(\mathcal{w}^*) \cdot \mathcal{J} + B(\mathcal{w}^*) \cdot \mathcal{J} \mathcal{q} - 2\mu \mathcal{q} \mathcal{q}, -q^{-2} \omega_s^* \right) \] (80, 81)

\[ \mathcal{F}_s = \begin{bmatrix} \frac{1}{4} A(q) \cdot J^{-1} \cdot A(q) & 2B(\mathcal{J}^*) + 4A(q) \cdot \mathcal{J} \cdot C(q) & \frac{1}{2} q^2 J_s^{-1} q \\ \frac{1}{2} A(q) \cdot J^{-1} \cdot A(q) + 2B'(\mathcal{w}^*) + f_q & \frac{1}{2} A(q) \cdot J^{-1} \cdot \frac{\partial h}{\partial q} + \frac{1}{2} B(\mathcal{w}^*) & 0 \\ -\frac{1}{2} q^2 J_s^{-1} q' & -\frac{1}{2} q^2 J_s^{-1} q + f_s & 0 \end{bmatrix} \] (82)
in which:
\[
\frac{\partial h}{\partial q} = \frac{1}{2} \left[ C'(p) - 2 \mu A'(q) \right], \quad \frac{\partial h}{\partial \mu} = -A'(q) \cdot q. \tag{83, 84}
\]

These tangent matrices and residual vectors have been verified by numerical studies. The formulations for a free tumbling body, using quaternions, produce the same results as reported in Borri et al. (1990), were the finite rotation vector is employed.

It is straightforward to incorporate the translational degrees of freedom and impose physical constraints, as was done for the top and coin in the previous discussion. The results obtained are identical to those presented above. One difference worth noting is that the quaternion approach was much faster for the simple single body problems considered. While extensive timing studies were not made, the quaternion approach for simulating the spinning top required approximately 45\% of the time required by the finite rotation vector approach. One factor in this "speed-up" is the simplicity of forming the tangent matrices. Another is the fact that an incremental approach is not required since the four parameter representation of rotation is not singular. This cuts down on the amount of internal book keeping required by the program.

5 Conclusions

A consistent variational approach to both holonomic and nonholonomic constraints is presented. The methodology is demonstrated for both types of constraint, through numerical simulations. It is also shown that this approach may be used to develop primal and mixed time finite elements, using a quaternion representation for finite rotation. For the single rigid-body problems investigated, the quaternion formulations are approximately twice as fast as those using the finite rotation vector.

Appendix. A relevant formulae on quaternions

Let \( q \) be a quaternion, and \( q_s \) and \( q_v \) be respectively the scalar and vectorial parts. In the following \( q = (q_s, q_v) \) is understood. Provided \( q \neq 0 \), it may be normalized to a unit quaternion. Let \( q^* \), be the unit quaternions associate with \( q \) i.e. \( q^* = \frac{q}{|q|} \), where \( |q| = (q \cdot q)^{1/2} \) is the modulus of \( q \). Moreover, let \( \bar{q} \) be the quaternion conjugate to \( q \), i.e., \( q_s = \bar{q}_s \) and \( q_v = -\bar{q}_v \).

It is well known that quaternion multiplication can be cast in the following way. Let \( q, r, s \) be quaternions and \( s = qr \) \( (s = r \bar{q}) \). This multiplication may be expressed as:

\[
s = A(q) \cdot r = B(r)q \tag{85}
\]

where the operators \( A(\cdot) \) and \( B(\cdot) \), for a given quaternion \( q \) are defined as:

\[
A(q) = \begin{bmatrix} q_s & -q_v' \\ q_v & q_s I + q_v \times I \end{bmatrix}, \quad B(q) = \begin{bmatrix} q_s & -q_v' \\ q_v & q_s I - q_v \times I \end{bmatrix} = [q] B_s(q). \tag{86}
\]

It is interesting to note that \( A_s(q) \) and \( B_s(q) \) are orthogonal to \( q \), i.e., \( q \cdot A_s(q) = q \cdot B_s(q) = 0 \forall q \). The \( \cdot \) denotes the four dimensional dot product. The operators \( A(\cdot) \) and \( B(\cdot) \) follows some rules that are reported here for convenience:

\[
A(\bar{q}) = A(q), \quad B(q) = B^*(q) \quad A(q) B(r) = B^*(r) \cdot A(q) \tag{87}
\]

\[
A'(q) \cdot r = C(r) \cdot q, \quad B'(q) \cdot r = C(r) \cdot q \tag{88}
\]

where \( C(\cdot) \) is defined as:

\[
C(q) = [q] - A_s(q), \quad C'(q) = [q'] - B_s(q). \tag{89}
\]
Moreover, the following relation hold:

\[ A'(q) \cdot A(q) = A(q) \cdot A'(q) = q^2 I_4 \]
\[ B'(q) \cdot B(q) = A(q) \cdot B'(q) = q^2 I_4 \]
\[ C'(q) \cdot C(q) = C(q) \cdot C'(q) = q^2 I_4 \]  

(90)

while:

\[ A_1(q) \cdot A'_1(q) = q^2 I, \quad B'_2(q) \cdot B'_2(q) = q^2 I \]  

(91)

where \( q^2 = q \cdot q \) and \( I \) and \( I_4 \) denote respectively the three-dimensional and four-dimensional identity tensors.

It is well known that a unit quaternions may represent a rotation. In fact consider the following quaternion product:

\[ n = q^{*} m q^{*} = A(q^{*}) \cdot A(m) \cdot q^{*} = A(q^{*}) \cdot B(q^{*}) \cdot m = A(q^{*}) \cdot B'(q^{*}) \cdot m. \]  

(92)

It is easily shown that \( n \cdot n = m \cdot m \) which means that \( n \) may be obtained from \( m \) by a rotation. Clearly this rotation may be expressed as \( A(q^{*}) \cdot B'(q^{*}) \). Then in general, we can write:

\[ G(q^{*}) = A(q^{*}) \cdot B'(q^{*}) = B'(q^{*}) \cdot A(q^{*}) = C(q^{*}) \cdot C(q^{*}) = \begin{bmatrix} 1 & 0 \\ 0 & R \end{bmatrix} \]  

(93)

where \( R = B'_2(q^{*}) \cdot A_1(q^{*}) \) is a proper three dimensional rotation tensor, i.e. \( R R^{T} = R^{T} R = I \) and \( \det R = 1 \).

In terms of the rotation vector \( r = \phi e \) the unit quaternion of Euler parameters are defined as:

\[ q_1 = \cos \phi / 2, \quad q_2 = \sin \phi / 2 e. \]  

(94)

In the previous section it is shown that the rotation tensor may be expressed as:

\[ R = I + \sin \phi e \times I + (1 - \cos \phi) e \times e \times I. \]  

(95)

Recalling the following trigonometric identities:

\[ \sin \phi = 2 \sin \frac{\phi}{2} \cos \frac{\phi}{2}, \quad 1 - \cos \phi = 2 \sin^2 \frac{\phi}{2} \]  

(96)

the rotation tensor is expressed as:

\[ R = I + 2 q_1 q_1^{*} e \times I + 2 q_2 q_2^{*} e \times I. \]  

(97)

Successive rotations can be easily handled with quaternions. Suppose that: \( R(r_3) = R(r_2) \cdot R(r_1) \) where \( r_3 \) is the rotation vector associated with the total rotation resulting from the sequence of rotations, \( r_1 \) followed by \( r_2 \). Then let \( q_1^{*}, q_2^{*}, q_3^{*} \) be the unit quaternions corresponding to \( r_1, r_2 \) and \( r_3 \) respectively. For each of them, a relation of the form Eq. (93) holds. This leads to the relation \( G(q_3^{*}) = G(q_2^{*}) \cdot G(q_1^{*}) \). The expansion of \( r_3 \) in terms of \( r_1 \) and \( r_2 \) is very involved but the relation between \( q_3^{*} \) and \( q_1^{*} \) and \( q_2^{*} \) is simply a multiplication. In fact \( q_3^{*} = q_2^{*} q_1^{*} \), which in matrix form is:

\[ q_3^{*} = B(q_2^{*}) \cdot q_1^{*}. \]  

(98)

Moreover, in this case the following relations hold:

\[ B(q_3^{*}) = B(q_1^{*}) \cdot B(q_2^{*}), \quad A(q_3^{*}) = A(q_2^{*}) \cdot A(q_1^{*}). \]  

(99)

The composite rotation is then easily obtained.

\[ G(q_3^{*}) = A(q_3^{*}) \cdot B'(q_3^{*}) \]  

(100)

then Eq. (93) yields:

\[ G(q_3^{*}) = A(q_2^{*}) \cdot A(q_1^{*}) \cdot B'(q_2^{*}) \cdot B'(q_1^{*}) = A(q_2^{*}) \cdot B'(q_1^{*}) \cdot A(q_1^{*}) \cdot B'(q_1^{*}) = G(q_2^{*}) \cdot G(q_1^{*}) \].  

(101)
Quaternions and angular velocity

Let \( \omega_e \) be the spinning velocity of \( \mathcal{R} \) defined through \( \omega_e \times l = \mathcal{R}(r) \dot{r} \) then using the relations developed above:

\[
\omega_e = \mathcal{R}(r) \dot{r}, \quad \omega_e^* = \mathcal{R}(r) \dot{e}
\]

where \( \omega_e^* = \mathcal{R}^* \omega_e \) and:

\[
\mathcal{R}(r) = I + \frac{1}{\phi^2} r \times I + \frac{1}{\phi^2} \left( 1 - \frac{\sin \phi}{\phi} \right) r \times r \times I
\]

\[
= I + \frac{1}{\phi} e \times I + \left( 1 - \frac{\sin \phi}{\phi} \right) e \times e \times I
\]

\[
= \frac{\sin \phi}{\phi} I + \frac{1 - \cos \phi}{\phi} e \times I + \left( 1 - \frac{\sin \phi}{\phi} \right) e \cdot e'
\]

and \( r = \phi e \). Taking into account the following identities:

\[
\dot{e} = \dot{\phi} e + \dot{\phi} e, \quad e \cdot e = 1, \quad \dot{e} \cdot e = 0, \quad \frac{\phi}{2} \sin \frac{\phi}{2} = \frac{\phi}{2} \cos \frac{\phi}{2}
\]

into Eq. (102) and Eq. (103) leads to:

\[
\omega_e = 2B' (q^*) \dot{q}^*, \quad \omega_e^* = 2A' (q^*) \dot{q}^*
\]

Equation (105) can be written in four dimensional form as follows:

\[
\omega = 2B' (q) \dot{q}, \quad \omega^* = 2A' (q^*) \dot{q}^*
\]

where \( \omega = (\omega_3, \omega_s, \omega_e, \omega_e^*) \) and \( \omega_s = 2q^* \dot{q} \). It is recognized that \( \omega_s = \frac{d}{dt} (q, q) \) which is zero when \( q \) is a unit quaternion. If \( q \) is not unit quaternion then \( \omega_s = 0 \) may be interpreted as the differential form of the constraint of unit magnitude. The four dimensional vector \( \omega \) is the spinning velocity corresponding to \( q \), and \( \omega^* \) is its pullback that can be performed by the tensor \( G(q) \) through the relation:

\[
\omega^* = G(q) \omega.
\]

Composition of angular velocity can be handled easily. In fact, supposing \( q_3^* = q_2^* q_1^* \) then:

\[
q_3^* = B(q_1^*) q_2^* = A(q_2^*) q_1^*.
\]

Further, let \( \omega_1, \omega_2, \omega_3 \) be the corresponding velocities defined through the Eq. (106), that are related by the formula:

\[
\omega_3 = \omega_2 + G(q_2^*) \omega_1.
\]

Which, in terms of derivatives may be written as:

\[
\omega_3 = 2B' (q_2^*) (q_2^* + A(q_2^*) B'(q_1^*) \dot{q}_1^*)
\]

\[
= 2G(q_2^*) (A(q_2^*) q_2^* + B(q_2^*) \dot{q}_1^*)
\]

and also:

\[
G'(q_3^*) \omega_3 = 2G'(q_1^*) (A'(q_2^*) q_2^* + B'(q_2^*) \dot{q}_1^*).
\]
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References


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