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Variational approaches for dynamics and time-finite-elements: numerical studies

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Abstract. This paper presents general variational formulations for dynamical problems, which are easily implemented numerically. The development presents the relationship between the very general weak formulation arising from linear and angular momentum balance considerations, and well known variational priciples. Two and three field mixed forms are developed from the general weak form. The variational principles governing large rotational motions are linearized and implemented in a time finite element framework, with appropriate expressions for the relevant "tangent" operators being derived. In order to demonstrate the validity of the various formulations, the special case of free rigid body motion is considered. The primal formulation is shown to have unstable numerical behavior, while the mixed formulation exhibits physically stable behavior. The formulations presented in this paper form the basis for continuing investigations into constrained dynamical systems and multi-rigid-body systems, which will be reported in subsequent papers.

1 Introduction

Recently there has been a renewed interest in the study of multibody dynamics and its application to a wide variety of engineering problem. Research is very active in the areas of vehicle dynamics (Agrawal and Shabana 1986; Kim and Shabana 1984; McCullough and Haug 1986), spacecraft dynamics and attitude control (Hughes 1986; Kane and Levinson 1980; Kane et al. 1983), large space structures (Meirovitch and Quinn 1987; Modi and Ibrahim 1987; Shi 1988; Amos and Atluri 1987) and machine dynamics (Haug et al. 1986; Haug and McCullough 1986; Khulief and Shabana 1986). One common interest in all these fields is the automated development and solution of the equations of motion. As discussed in Wittenburg (1985), symbolic manipulation programs are being applied to this task. The nonlinear equations of motion, in explicit form are quite complex due to the expression for the absolute acceleration. These complexities are avoided if a weak form of the dynamical equations is employed. The principle of virtual work, or Hamilton's principle is one such weak form (Borri et al. 1985). There has been a great deal of discussion in the literature concerning the equivalence of different formulations (Desloge 1987; Banerjee 1987) and the use of Hamilton's principle as a starting point for the numerical solution of dynamics problems (Bailey 1975; Baruch and Riff 1982). Some of this discussion involves the conditions under which Hamilton's principle may be stated as the stationarity condition of a scalar functional (Smith and Smith 1974). Due to the unsymmetric character of initial value problems, the governing equations are not expressible as such a condition. This fact in no way diminishes the usefulness of variational approaches for initial value problems. In fact, drawing on the mature literature concerning variational methods in the mechanics of deformable bodies, very general weak forms can be developed for dynamical systems, the most general being analogous to a Hu-Washizu type formulation. The principle of virtual work is obtainable from the general weak form by satisfying displacement compatibility (the definition of velocity) and the displacement boundary conditions *a priori*. A Hamiltonian or complementary energy approach is obtained by satisfying the constitutive relations between momentum and velocity *a priori*.

In order to establish the methodology and assess the performance of the different weak formulations, the dynamics of a single rigid body is considered. Even in its simplicity, from a theoretical viewpoint, the dynamics of a single rigid body, with its high degree of nonlinearity, consitutes a significant test for numerical procedures.

When dealing with rigid body dynamics, the choice of coordinates for finite rotation greatly influences the character of the resulting numerical procedures. As a result, many representations of finite rotation have been adopted in the literature, including: Euler angles, quaternions, Rodigues' parameters, and various rotation vectors (Geradin and Cardona 1989; Iura and Atluri 1989; Pietraszkiewicz and Badur 1983). It is difficult to establish *one* set of coordinates as the best choice for all problems. For the purposes of the present development, the finite rotation vector is chosen as the Lagrangian coordinate for the angular motion. This coordinate choice preserves the vectorial character of the formulae and results in a minimum number of independent variables. However, since any three parameter representation of rotation cannot be both global and nonsingular, an incremental approach is required to obtain a solution. The incremental displacement and rotation are measured from a reference configuration, which in general depends on time. For different choices of the reference configuration, different incremental approaches are obtained.

Moreover, depending on the form chosen for the virtual rotations (or test functions for rotational variables), different but equivalent forms of the linear and angular momentum balance conditions arise. One choice leads to a symmetric variational statement, while the other does not.

In this paper, several formulations for the dynamics of a rigid body are discussed, with the objective of developing a system of equations which may be directly implemented in the framework of time finite elements. This approach leads to a set of nonlinear equations, which are solved using Newton's method. The merits of this strategy, as related to the dynamics of constrained rigid body systems, will be discussed in a subsequent paper.

The simple example of a free tumbling rigid body is presented, and the accuracy and numerical stability of the various approaches are discussed.

The remainder of this paper is organized as follows; Sect. 2 deals with geometry and coordinate selection; Sect. 3 with the formulation of the variational principles; Sect. 4, the linearization of the resulting equations; Sect. 5, with finite element approximation; Sect. 6 deals with linearized stability analysis; Sect. 7, with numerical stability; and Sect. 8, with numerical results and Sect. 9 lists the cited references. Appendix A contains relevant formulas for rotation while the full expressions for the tangent matrices and residual vectors are presented in Appendix B.

Throughout this paper, lowercase bold roman characters will indicate a vector, while uppercase bold roman characters will indicate a tensor.

2 Coordinate selection and kinematics of a rigid body

In order to avoid redundant degrees of freedom, the finite rotation vector is chosen as rotational coordinates, which is a three parameter representation. Finite rotation vectors have also been used by Iura and Atluti (1989), Kane et al. (1983) and others. As pointed out by Struelpnagel (1964), a three parameter representation can not be both global and nonsingular. In order to overcome this, many investigators have adopted Euler parameters to uniquely describe finite rotations. However, this results in five degrees of freedom being associated with the rotation, if the constraint of unit magnitude for the Euler parameters is included through a Lagrange multiplier. Geradin and Cardona (1989) use the conformal rotation vector as a set of three rotation parameters in a global algorithm, which avoids the singularities as the rotation crosses integer multiples of π. Similarly, it is shown in Appendix A, that the finite rotation vector may be used in a similar approach if the rotation is rescaled as it passes through multiples of 2π. However, for this numerical implementation, an incremental approach is adopted, to avoid the singularities.

In order to specify the configuration of a rigid body, two orthogonal frames of reference are defined, namely $(\mathbf{O}, \boldsymbol{e}_i)$ and $(\mathbf{O}', \boldsymbol{e}'_i)$. The first frame is fixed, while the second is embedded in the body. At any given time t the embedded frame is completely identified by the position vector $\boldsymbol{x}(t) = \mathbf{O}' - \mathbf{O}$, and by the rotation vector $\boldsymbol{r}(t)$, such that $\boldsymbol{e}'_i = \boldsymbol{R}(\boldsymbol{r}) \cdot \boldsymbol{e}_i$, where $\boldsymbol{R}(\boldsymbol{r})$ denotes the rotation tensor corresponding to $\boldsymbol{r}$. The spin of the embedded fame relative to the fixed frame may be expressed by the angular velocity vector $\boldsymbol{\omega}$, such that $\boldsymbol{\omega} \times \boldsymbol{I} = \dot{\boldsymbol{R}} \cdot \boldsymbol{R}^t$ which depends linearly on $\dot{\boldsymbol{r}}$.

One common representation of the rotation vector is $\boldsymbol{r} = \phi \boldsymbol{e}$, where ϕ is the magnitude of rotation and $\boldsymbol{e}$ is the rotation axis, i.e. $\boldsymbol{R}\cdot\boldsymbol{e} = \boldsymbol{e}$. In terms of $\boldsymbol{r}$, the rotation tensor $\boldsymbol{R}$ may be conveniently expressed through the exponential map, which is the form that will be adopted here, as;

$$\boldsymbol{R}(\boldsymbol{r}) = \exp(\boldsymbol{r}(t) \times \boldsymbol{I}). \tag{2.1}$$

In Appendix A, several common rotation vectors are shown to be easily expressed in this form.

The reference configuration and incremental coordinates are now defined in the following way. Assuming that the state of the rigid body is known at some initial time t_1, the reference trajectory for the body can be defined. This reference configuration can be specified in many ways. For example, the reference could be a time varying configuration, compatible with some specified external forces and moment resultant, or the configuration corresponding to a constant linear and angular velocity, or simply held constant. Since Newton's method is used to iteratively solve the nonlinear system of equations, the reference configuration must be a reasonably good estimate of the true configuration, in order for the method to converge rapidly. At any point in time, the reference configuration is described by a position vector $\boldsymbol{x}_o(t)$, and a rotation $\boldsymbol{R}_o(t)$. The true solution will in general flow another path, with any point on the true configuration being described by a position vector $\boldsymbol{x}(t)$ and the rotation $\boldsymbol{R}(t)$. Since the reference configuration is prescribed, the true path may also be represented by the position vector $\boldsymbol{x}_*(t)$, given by $\boldsymbol{x}_*(t) = \boldsymbol{x}(t) - \boldsymbol{x}_o(t)$, and the rotation $\boldsymbol{R}_*(t)$, where $\boldsymbol{R}_*(t) = \boldsymbol{R}(t)\cdot\boldsymbol{R}_o^t(t)$. The incremental coordinates are now defined as $(\boldsymbol{x}_*, \boldsymbol{r}_*)$, where $\boldsymbol{r}_*$ is the rotation vector such that $\boldsymbol{R}_* = \boldsymbol{R}(\boldsymbol{r}_*) = \exp(\boldsymbol{r}_* \times \boldsymbol{I})$.

Henceforth, all quantities associated with the reference configuration will be designated by a subscript o and a subscript * will indicate a quantity associated with the current configuration, but referred to the reference configuration. For example, $\boldsymbol{v}_o$ and $\boldsymbol{\omega}_o$ represent the linear and angular velocity of the reference configuration, and are defined as:

$$\boldsymbol{v}_o = \dot{\boldsymbol{x}}_o, \qquad \boldsymbol{\omega}_o \times \boldsymbol{I} = \dot{\boldsymbol{R}}_o \cdot \boldsymbol{R}_o^t. \tag{2.2, 2.3}$$

Similarly, $\boldsymbol{v}_*$ and $\boldsymbol{\omega}_*$ are the linear and angular velocity of the true configuration with respect to the reference, and are defined in a consistent way:

$$\boldsymbol{v}_* = \dot{\boldsymbol{x}}_*, \qquad \boldsymbol{\omega}_* \times \boldsymbol{I} = \dot{\boldsymbol{R}}_* \cdot \boldsymbol{R}_*^t. \tag{2.4. 2.5}$$

The linear and angular velocities of the true configuration with respect to the fixed frame can now be expressed as:

$$\boldsymbol{v} = \boldsymbol{v}_* + \boldsymbol{v}_o, \qquad \boldsymbol{\omega} = \boldsymbol{\omega}_* + \boldsymbol{R}_* \cdot \boldsymbol{\omega}_o. \tag{2.6, 2.7}$$

Clearly, the angular velocity of the incremental motion, $\boldsymbol{\omega}_*$ is not the same as the relative velocity from the reference configuration, $\boldsymbol{\omega} - \boldsymbol{\omega}_o$. Having defined the angular velocity $\boldsymbol{\omega}_*$, and the rotation coordinates $\boldsymbol{r}_*$, the relationship between $\boldsymbol{\omega}_*$ and $\boldsymbol{r}_*$ may be established. Substitution of $\boldsymbol{R}_* = \exp(\boldsymbol{r}_* \times \boldsymbol{I})$ into the definition for $\boldsymbol{\omega}_*$ yields:

$$\boldsymbol{\omega}_* = \boldsymbol{\Gamma}(\boldsymbol{r}_*)\cdot\dot{\boldsymbol{r}}_*, \tag{2.8}$$

where:

$$\boldsymbol{\Gamma}(\boldsymbol{r}_*) = \boldsymbol{I} + \frac{1-\cos\phi_*}{\phi_*^2}(\boldsymbol{r}_* \times \boldsymbol{I}) + \frac{1}{\phi_*^2}\left(1 - \frac{\sin\phi_*}{\phi_*}\right)(\boldsymbol{r}_* \times \boldsymbol{I})^2, \tag{2.9}$$

and ϕ_* is the magnitude of $\boldsymbol{r}_*$. The details of this derivation are presented in Appendix A. Clearly, the operator $\boldsymbol{\Gamma}$ also relates $\boldsymbol{\omega}$ and $\boldsymbol{\omega}_o$ to $\dot{\boldsymbol{r}}$ and $\dot{\boldsymbol{r}}_o$ respectively, i.e. $\boldsymbol{\omega} = \boldsymbol{\Gamma}(\boldsymbol{r})\cdot\dot{\boldsymbol{r}}$ and $\boldsymbol{\omega}_o = \boldsymbol{\Gamma}(\boldsymbol{r}_o)\cdot\dot{\boldsymbol{r}}_o$.

This section concludes with some comments on the virtual displacement and rotation fields. The virtual displacement of the point **O**′ can be defined as the variation of its position $\delta\boldsymbol{x}(t) = \delta\boldsymbol{x}_*(t)$. However, the virtual change in the orientation of the rigid body can be represented either by the variation of the rotation vector $\delta\boldsymbol{r}_*$ or by means of a virtual rotation $\boldsymbol{\theta}_{*\delta}$ defined by:

$$\boldsymbol{\theta}_{*\delta} \times \boldsymbol{I} = \delta\boldsymbol{R}_* \cdot \boldsymbol{R}_*^t. \tag{2.10}$$

Due to the orthogonality of the rotation tensor, $\delta\boldsymbol{R}_* \cdot \boldsymbol{R}_*^t$ is skew symmetric and its correspondence with $\boldsymbol{\theta}_{*\delta} \times \boldsymbol{I}$ is always possible. Substituting for $\boldsymbol{R}_*$ in terms of $\boldsymbol{R}$ and $\boldsymbol{R}_o$, demonstrates that the total virtual rotation $\boldsymbol{\theta}_\delta$ coincides with the incremental virtual rotation $\boldsymbol{\theta}_{*\delta}$, since the reference configuration is prescribed, i.e. $\delta\boldsymbol{R}_o = 0$. In fact:

$$\begin{aligned}\boldsymbol{\theta}_{*\delta} \times \boldsymbol{I} &= \delta\boldsymbol{R}_* \cdot \boldsymbol{R}_*^t = \delta(\boldsymbol{R}\cdot\boldsymbol{R}_o^t)\cdot(\boldsymbol{R}\cdot\boldsymbol{R}_o^t)^t \\ &= \delta\boldsymbol{R}\cdot\boldsymbol{R}^t = \boldsymbol{\theta}_\delta = \boldsymbol{I}.\end{aligned} \tag{2.11}$$

The notation of subscript δ indicates that $\boldsymbol{\theta}_\delta$ and $\boldsymbol{\theta}_{*\delta}$ are not variations of true coordinates. Consequently $\boldsymbol{\theta}$ are commonly referred to as quasicoordinates. Since $\boldsymbol{\theta}$ does not exist, solution procedures cannot involve quasicoordinates exclusively.

Moreover, the virtual rotation $\boldsymbol{\theta}_\delta$ is related to the virtual change of the incremental rotation vector through the same relationship that exists between the angular velocity $\boldsymbol{\omega}$ and $\dot{\boldsymbol{r}}$ i.e.:

$$\boldsymbol{\theta}_\delta = \boldsymbol{\Gamma}(\boldsymbol{r}_*)\cdot\delta\boldsymbol{r}_*. \tag{2.12}$$

3 Weak forms for rigid body dynamics

Let $\boldsymbol{b}$ and $\boldsymbol{m}$ denote respectively the external force and moment resultants and let $\boldsymbol{l}$ and $\boldsymbol{h}$ be the linear and angular momenta, respectively, of the rigid body, with respect to the point $\mathbf{O}'$. Since the body is rigid, the velocity of any point $\tilde{\boldsymbol{v}}$, may be expressed in terms of the linear velocity of the point $\mathbf{O}'$ and the angular velocity of the body about point $\mathbf{O}'$. Thus,

$$\tilde{\boldsymbol{v}} = \boldsymbol{v} - \boldsymbol{y} \times \boldsymbol{\omega}, \tag{3.1}$$

where $\boldsymbol{y}$ is the position of the point relative to $\mathbf{O}'$. The linear and angular momenta with respect to $\mathbf{O}'$ are, respectively,

$$\begin{aligned}\boldsymbol{l} &= \int_{\mathscr{B}} \rho\tilde{\boldsymbol{v}}\,\mathrm{d}\mathscr{B} \\ &= \boldsymbol{v}\int_{\mathscr{B}} \rho\,\mathrm{d}\mathscr{B} - \boldsymbol{\omega}\int_{\mathscr{B}} \rho\boldsymbol{y} \times \boldsymbol{I}\,\mathrm{d}\mathscr{B}, \\ \boldsymbol{h} &= \boldsymbol{v}\int_{\mathscr{B}} \rho\boldsymbol{y} \times \boldsymbol{I}\,\mathrm{d}\mathscr{B} - \boldsymbol{\omega}\int_{\mathscr{B}} \rho\boldsymbol{y} \times \boldsymbol{y} \times \boldsymbol{I}\,\mathrm{d}\mathscr{B}.\end{aligned} \tag{3.2}$$

The dynamical equations, viz., the equations of linear and angular momentum balance, are written as:

$$\dot{\boldsymbol{l}} = \boldsymbol{b}, \qquad \dot{\boldsymbol{h}} + \boldsymbol{v} \times \boldsymbol{l} = \boldsymbol{m}. \tag{3.3}$$

The weak forms of these equations along with the weak forms of the natural boundary conditions can be written as:

$$\int_{t_1}^{t_2} [\boldsymbol{d}_1(t)\cdot(\dot{\boldsymbol{l}} - \boldsymbol{b}) + \boldsymbol{d}_2(t)\cdot(\dot{\boldsymbol{h}} + \boldsymbol{v} \times \boldsymbol{l} - \boldsymbol{m})]\,\mathrm{d}t = 0, \tag{3.4}$$

$$\boldsymbol{b}_1(t_k)\cdot(\boldsymbol{l}_{bk} - \boldsymbol{l}(t_k)) = 0, \qquad \boldsymbol{b}_2(t_k)\cdot(\boldsymbol{h}_{bk} - \boldsymbol{h}(t_k)) = 0 \quad (k = 1, 2), \tag{3.5}$$

where $\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{b}_1, \boldsymbol{b}_2$ are respectively, domain and boundary test functions. The subscript b indicates boundary quantities.

Since the expressions for $\boldsymbol{l}$ and $\boldsymbol{h}$ contain $\boldsymbol{v}$ and $\boldsymbol{\omega}$, which in turn depend on the time derivatives of the generalized coordinates $\boldsymbol{x}_*, \boldsymbol{r}_*$, the implementation of this weak form would require trial functions which are at least twice differentiable on (t_1, t_2), while the test functions $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$ have no continuity restrictions. In order to avoid higher order trial functions, the terms in Eq. (3.4) containing time derivatives are integrated by parts and combined with the boundary terms, Eq. (3.5), obtaining:

$$\int_{t_1}^{t_2} [(\dot{\boldsymbol{d}}_1 + \boldsymbol{v} \times \boldsymbol{d}_2)\cdot\boldsymbol{l} + \dot{\boldsymbol{d}}_2\cdot\boldsymbol{h} + \boldsymbol{d}_1\cdot\boldsymbol{b} + \boldsymbol{d}_2\cdot\boldsymbol{m}]\,\mathrm{d}t, = [\boldsymbol{b}_1\cdot\boldsymbol{l}_b + (\boldsymbol{d}_1 - \boldsymbol{b}_1)\cdot\boldsymbol{l} + \boldsymbol{b}_2\cdot\boldsymbol{h}_b + (\boldsymbol{d}_2 - \boldsymbol{b}_2)\cdot\boldsymbol{h}]\big|_{t_1}^{t_2}. \tag{3.6}$$

For simplicity, let the boundary test functions $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ be chosen such that they are equal to the domain test functions $(\boldsymbol{d}_1, \boldsymbol{d}_2)$ evaluated at the boundary, thus eliminating the terms in $(\boldsymbol{d}_1 - \boldsymbol{b}_1)$ and $(\boldsymbol{d}_2 - \boldsymbol{b}_2)$. Moreover, for particular choices of test functions, some of the terms in Eq. (3.6) can be made to correspond to the variation of kinetic energy (or the variation of the Lagrangian, if the conservative part of the applied loads is grouped with the kinetic energy).

In fact the kinetic energy of the rigid body may be expressed as:

$$T = \tfrac{1}{2}\boldsymbol{v}\cdot\boldsymbol{l} + \tfrac{1}{2}\boldsymbol{\omega}\cdot\boldsymbol{h}, \tag{3.7}$$

where the linear and angular momenta are related to the linear and angular velocities through the "constitutive" equations:

$$\boldsymbol{l} = \boldsymbol{M}\cdot\boldsymbol{v} + \boldsymbol{S}^T\cdot\boldsymbol{\omega}, \qquad \boldsymbol{h} = \boldsymbol{S}\cdot\boldsymbol{v} + \boldsymbol{J}\cdot\boldsymbol{\omega}. \tag{3.8}$$

Here, $\boldsymbol{M}$ is the mass, and $\boldsymbol{S}$ and $\boldsymbol{J}$ are the first and second moments of inertia, respectively, about point $\mathbf{O}'$. The definitions of $\boldsymbol{S}$ and $\boldsymbol{J}$ are clear by comparison to Eq. (3.2). In the following discussion, use will be made of the fact that the moments of inertia in the embedded frame are constant. That is to say:

$$\begin{aligned} \boldsymbol{R}^t\cdot\boldsymbol{M}\cdot\boldsymbol{R} &= \bar{\boldsymbol{M}} = \text{constant},\\ \boldsymbol{R}^t\cdot\boldsymbol{S}\cdot\boldsymbol{R} &= \bar{\boldsymbol{S}} = \text{constant},\\ \boldsymbol{R}^t\cdot\boldsymbol{J}\cdot\boldsymbol{R} &= \bar{\boldsymbol{J}} = \text{constant}. \end{aligned} \tag{3.9}$$

We define the corotational variations of $\boldsymbol{v}$ and $\boldsymbol{\omega}$ to be:

$$\begin{aligned} \delta^o\boldsymbol{v} &\overset{\text{def}}{=} \boldsymbol{R}\cdot\delta(\boldsymbol{R}^t\cdot\boldsymbol{v}) = \delta\boldsymbol{v} + \boldsymbol{v}\times\boldsymbol{\theta}_\delta = \delta\dot{\boldsymbol{x}} + \dot{\boldsymbol{x}}\times\boldsymbol{\theta}_\delta,\\ \delta^o\boldsymbol{\omega} &\overset{\text{def}}{=} \boldsymbol{R}\cdot\delta(\boldsymbol{R}^t\cdot\boldsymbol{\omega}) = \delta\boldsymbol{\omega} + \boldsymbol{\omega}\times\boldsymbol{\theta}_\delta = \dot{\boldsymbol{\theta}}_\delta. \end{aligned} \tag{3.10}$$

These are discussed further in Appendix A. With this notation in place, the variation of kinetic energy is carried out as follows:

$$\delta T = \tfrac{1}{2}(\boldsymbol{l}\cdot\delta\boldsymbol{v} + \delta\boldsymbol{l}\cdot\boldsymbol{v}) + \tfrac{1}{2}(\boldsymbol{h}\cdot\delta\boldsymbol{\omega} + \delta\boldsymbol{h}\cdot\boldsymbol{\omega}). \tag{3.11}$$

Considering the constitutive equations, and retaining the terms involving the variation of the mass (which of course is zero), $\delta\boldsymbol{l}$ and $\delta\boldsymbol{h}$ may be expressed as:

$$\begin{aligned} \delta\boldsymbol{l} &= (\delta\boldsymbol{R}\cdot\bar{\boldsymbol{M}}\cdot\boldsymbol{R}^t + \boldsymbol{R}\cdot\bar{\boldsymbol{M}}\cdot\delta\boldsymbol{R}^t)\cdot\boldsymbol{v} + \boldsymbol{M}\cdot\delta\boldsymbol{v} + (\delta\boldsymbol{R}\cdot\bar{\boldsymbol{S}}^T\cdot\boldsymbol{R}^t + \boldsymbol{R}\cdot\bar{\boldsymbol{S}}^T\cdot\delta\boldsymbol{R}^t)\cdot\boldsymbol{\omega} + \boldsymbol{S}^T\cdot\delta\boldsymbol{\omega},\\ \delta\boldsymbol{h} &= (\delta\boldsymbol{R}\cdot\bar{\boldsymbol{S}}\cdot\boldsymbol{R}^t + \boldsymbol{R}\cdot\bar{\boldsymbol{S}}\cdot\delta\boldsymbol{R}^t)\cdot\boldsymbol{v} + \boldsymbol{S}\cdot\delta\boldsymbol{v} + (\delta\boldsymbol{R}\cdot\bar{\boldsymbol{J}}\cdot\boldsymbol{R}^t + \boldsymbol{R}\cdot\bar{\boldsymbol{J}}\cdot\delta\boldsymbol{R}^t)\cdot\boldsymbol{\omega} + \boldsymbol{J}\cdot\delta\boldsymbol{\omega}. \end{aligned} \tag{3.12}$$

From the definition of $\boldsymbol{\theta}_\delta$ it is known that $\delta\boldsymbol{R} = (\boldsymbol{\theta}_\delta\times\boldsymbol{I})\cdot\boldsymbol{R}$ and $\delta\boldsymbol{R}^t = \boldsymbol{R}^t\cdot(\boldsymbol{\theta}_\delta\times\boldsymbol{I})$. Using these relations in Eq. (3.12) leads to:

$$\delta T = \boldsymbol{l}\cdot(\delta\boldsymbol{v} + \boldsymbol{v}\times\boldsymbol{\theta}_\delta) + \boldsymbol{h}\cdot(\delta\boldsymbol{\omega} + \boldsymbol{\omega}\times\boldsymbol{\theta}_\delta). \tag{3.13.}$$

In terms of the corotational variations of $\boldsymbol{v}$ and $\boldsymbol{w}$, as defined above, the variation of kinetic energy may be written concisely as:

$$\delta T = \delta^o\boldsymbol{v}\cdot\boldsymbol{l} + \delta^o\boldsymbol{\omega}\cdot\boldsymbol{h}. \tag{3.14}$$

This result is useful in selecting meaningful test functions for the linear and angular momentum balance conditions. If the test functions $(\boldsymbol{d}_1, \boldsymbol{d}_2)$ in Eq. (3.6) are taken to be $\delta\boldsymbol{x}$ and $\boldsymbol{\theta}_\delta$ respectively, the first two terms in the integrand correspond exactly with the variation of kinetic energy. Then denoting the virtual work of the external force and moment results by $L_\delta = \delta\boldsymbol{x}\cdot\boldsymbol{b} + \boldsymbol{\theta}_\delta\cdot\boldsymbol{m}$, Eq. (3.6) can be rewritten as:

$$\int_{t_1}^{t_2} (\delta T + L_\delta)\mathrm{d}t = \delta\boldsymbol{x}\cdot\boldsymbol{l}_b + \boldsymbol{\theta}_\delta\cdot\boldsymbol{h}_b\big|_{t_1}^{t_2}. \tag{3.15}$$

This combined weak form requires trial functions which are only once differentiable, at the expense of requiring differentiability of the test functions. The kinematic relations between $\boldsymbol{x}_*, \boldsymbol{r}_*$ and $\boldsymbol{v}, \boldsymbol{\omega}$

as well as the boundary conditions on $\boldsymbol{x}_*, \boldsymbol{r}_*$ are satisfied *a priori*. If the test functions in Eq. (3.15) are chosen so as to vanish the boundaries, then this reduces to the classical Hamilton's principle. Equation (3.15) will be used, in its complete form, as the basis for the numerical methods presented in the following sections.

In the interest of brevity, the following notation is introduced:

$$\begin{aligned} &\boldsymbol{q} = (\boldsymbol{x}_*, \boldsymbol{r}_*) \\ &\dot{\boldsymbol{q}} = (\dot{\boldsymbol{x}}_*, \dot{\boldsymbol{r}}_*) \qquad && \boldsymbol{w} = (\dot{\boldsymbol{x}}, \boldsymbol{\omega}) \\ &\delta\boldsymbol{q} = (\delta\boldsymbol{x}_*, \delta\boldsymbol{r}_*) && \delta\hat{\boldsymbol{q}} = (\delta\boldsymbol{x}_*, \boldsymbol{\theta}_\delta) \\ &\boldsymbol{p} = (\boldsymbol{l}, \boldsymbol{\Gamma}^t(\boldsymbol{r}_*)\cdot\boldsymbol{h}) && \hat{\boldsymbol{p}} = (\boldsymbol{l}, \boldsymbol{h}) \\ &\boldsymbol{f} = (\boldsymbol{b}, \boldsymbol{\Gamma}^t(\boldsymbol{r}_*)\cdot\boldsymbol{m}) && \hat{\boldsymbol{f}} = (\boldsymbol{b}, \boldsymbol{m}). \end{aligned} \tag{3.16}$$

It may be seen that the following relations hold:

$$\delta\boldsymbol{q} = \mathbf{X}^{-1}\cdot\delta\hat{\boldsymbol{q}}, \quad \boldsymbol{p} = \mathbf{X}^T\cdot\hat{\boldsymbol{p}}, \quad \boldsymbol{f} = \mathbf{X}^T\cdot\hat{\boldsymbol{f}} \tag{3.17}$$

where:

$$\mathbf{X} = \begin{bmatrix} \boldsymbol{I} & 0 \\ 0 & \boldsymbol{\Gamma}(\boldsymbol{r}_*) \end{bmatrix}. \tag{3.18}$$

The constitutive equation is then rewritten as:

$$\hat{\boldsymbol{p}} = \boldsymbol{M}_6\cdot\boldsymbol{w}, \tag{3.19}$$

where $\boldsymbol{M}_6 = \begin{bmatrix} \boldsymbol{M}\,\boldsymbol{S}^T \\ \boldsymbol{S} \;\; \boldsymbol{J} \end{bmatrix}$ is the generalized mass tensor. Similarly, the virtual work of the external force is rewritten as $L_\delta = \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{f}} = \delta\boldsymbol{q}\cdot\boldsymbol{f}$.

The kinematical equations then become:

$$\boldsymbol{w} = \mathbf{X}\cdot\dot{\boldsymbol{q}} + \boldsymbol{w}_n, \tag{3.20}$$

where:

$$\boldsymbol{w}_n = (\boldsymbol{v}_o, \boldsymbol{R}_*\cdot\boldsymbol{\omega}_o). \tag{3.21}$$

Finally the corotational virtual change of the generalized velocity is written as:

$$\delta^o\boldsymbol{w} = \frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{\boldsymbol{q}} - \boldsymbol{S}_1^t(\boldsymbol{w})\cdot\delta\hat{\boldsymbol{q}}, \quad \boldsymbol{S}_1(\boldsymbol{w}) = \begin{bmatrix} 0 & 0 \\ \boldsymbol{v}\times\boldsymbol{I} & 0 \end{bmatrix}, \tag{3.22}$$

where $\delta^o\boldsymbol{w} = (\delta^o\boldsymbol{v}, \delta^o\boldsymbol{\omega})$. Equation (3.15) may now be written as:

$$\int_{t_1}^{t_2} (\delta^o\boldsymbol{w}\cdot\hat{\boldsymbol{p}} + \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{f}})\mathrm{d}t = \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}}_b|_{t_1}^{t_2}, \tag{3.23}$$

where Eq. (3.19) and (Eq. (3.22) are understood.

From this variational form, two numerical approaches can be developed using the finite element method in the time domain. In the first, $\delta\hat{\boldsymbol{q}}$ is treated as an independent variation. Since the linearization process must be performed in terms of the true coordinates $\boldsymbol{q}$, the resulting tangent matrix is unsymmetric. The second approach makes use of Eq. (3.20) to express $\delta\hat{\boldsymbol{q}}$ in terms of the coordinates $\boldsymbol{q}$, and a symmetric tangent matrix results. The latter approach requires that the variation of kinetic energy by expressed in terms of $\dot{\boldsymbol{q}}$ and $\boldsymbol{q}$, and that the external force and moment resultant be expressed in a form conjugate to $\delta\boldsymbol{q}$.

$$\int_{t_1}^{t_2} (\delta T(\dot{\boldsymbol{q}}, \boldsymbol{q}, t) + \delta\boldsymbol{q}\cdot\boldsymbol{f})\mathrm{d}t = \delta\boldsymbol{q}\cdot\boldsymbol{p}_b|_{t_1}^{t_2}, \tag{3.24}$$

where $\boldsymbol{p}_b$ denotes the generalized momentum at the boundary of the time interval. Equations (3.23) and (3.24) are the primal or kinematic forms of Hamilton's law for rigid body dynamics.

In general, the primal forms are conditionally stable and may require a small step size for accurate results. Again, this behavior is the dynamical counterpart to the locking phenomenon, which is well known in elasto-statics. As with locking, the restriction on the step size can be avoided, either through selective reduced integration or by utilizing a mixed formulation [e.g. Belytschko and Hughes (1981); Kardestuncer (1987); Malkus and Hughes (1978); Zienkiewicz et al. (1971)].

By means of a Legendre transformation, the mixed form of Hamilton's law for rigid body dynamics is obtained in the following way. Let $\hat{T} = \hat{T}(\boldsymbol{w}, \boldsymbol{q}, t)$ be the kinetic energy expressed as a function of $\boldsymbol{w}$ and $\boldsymbol{q}$. The complementary Hamiltonian is defined as:

$$\hat{H}(\hat{\boldsymbol{p}}, \boldsymbol{q}, t) = \hat{\boldsymbol{p}}\cdot\boldsymbol{w}(\hat{\boldsymbol{p}}, \boldsymbol{q}, t) - \hat{T}(\boldsymbol{w}(\hat{\boldsymbol{p}}, \boldsymbol{q}, t), \boldsymbol{q}, t) = \tfrac{1}{2}\hat{\boldsymbol{p}}\cdot\boldsymbol{M}_6^{-1}\cdot\hat{\boldsymbol{p}}. \tag{3.25}$$

Then, the variational statement Eq. (3.15) may be expressed as:

$$\int_{t_1}^{t_2} (\delta(\hat{\boldsymbol{p}}\cdot\boldsymbol{w} - \hat{H}) + \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{f}})\mathrm{d}t = \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}}_b|_{t_1}^{t_2}. \tag{3.26}$$

Moreover, letting $\delta^*\boldsymbol{p} = \mathbf{X}^T\cdot(\delta\boldsymbol{l}, \delta^o\boldsymbol{h})$, and enforcing the displacement continuity *a posteriori*, Eq. (3.26) may be expressed as:

$$\int_{t_1}^{t_2} \frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}} + \delta^*\boldsymbol{p}\cdot[\dot{\boldsymbol{q}} + \mathbf{X}^{-1}\cdot(\boldsymbol{w}_n - \hat{\boldsymbol{w}})] + \delta\hat{\boldsymbol{q}}\cdot(\hat{\boldsymbol{f}} + \mathrm{S}_1(\hat{\boldsymbol{p}})\cdot\hat{\boldsymbol{w}})\mathrm{d}t = [\delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}}_b - \delta^*\boldsymbol{p}(\boldsymbol{q}_b - \boldsymbol{q})]|_{t_1}^{t_2}. \tag{3.27}$$

where: $\hat{\boldsymbol{v}} \overset{\text{def}}{=} \boldsymbol{M}_6^{-1}\cdot\hat{\boldsymbol{p}}$ and $\boldsymbol{q}_b$ denotes the coordinates at the boundary of the time domain. Finally, integrating the term in $\dot{\boldsymbol{q}}$ by parts, leads to the following:

$$\int_{t_1}^{t_2} \frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}} - \frac{\mathrm{d}}{\mathrm{d}t}\delta^*\boldsymbol{p}\cdot\boldsymbol{q} - \delta^*\boldsymbol{p}\cdot\mathbf{X}^{-1}\cdot(\hat{\boldsymbol{w}} - \boldsymbol{w}_n) + \delta\hat{\boldsymbol{q}}\cdot(\hat{\boldsymbol{f}} + \mathrm{S}_1(\hat{\boldsymbol{p}})\cdot\hat{\boldsymbol{w}})\mathrm{d}t = (\delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}}_b - \delta^*\boldsymbol{p}\cdot\boldsymbol{q}_b)|_{t_1}^{t_2}. \tag{3.28}$$

A similar procedure applied to Eq. (3.24), using the transformation:

$$H(\boldsymbol{p}, \boldsymbol{q}, t) = \boldsymbol{p}\cdot\dot{\boldsymbol{q}}(\boldsymbol{p}, \boldsymbol{q}, t) - T(\boldsymbol{p}, \boldsymbol{q}, t) \tag{3.29}$$

yields:

$$\int_{t_1}^{t_2} (\delta\dot{\boldsymbol{q}}\cdot\boldsymbol{p} - \delta\dot{\boldsymbol{p}}\cdot\boldsymbol{q} - \delta H + \delta\boldsymbol{q}\cdot\boldsymbol{f})\mathrm{d}t = (\delta\boldsymbol{q}\cdot\boldsymbol{p}_b - \delta\boldsymbol{p}\cdot\boldsymbol{q}_b)|_{t_1}^{t_2}. \tag{3.30}$$

Equations (3.28) and (3.30) are "two-field" forms, wherein the trial functions may be discontinuous.

Relaxing the kinematic relations and considering the velocity $\boldsymbol{w}$ as an independent variable, Eq. (3.20) may be enforced in a weak sense. This leads to the most general three field form.

Modifying the Lagrangian by the weak form of the kinematic relations weighted with the momentum $\hat{\boldsymbol{p}}$, a three field variational statement can be formulated in the following way:

$$\int_{t_1}^{t_2} (\delta\bar{\mathscr{L}} + \delta\boldsymbol{q}\cdot\hat{\boldsymbol{f}})\mathrm{d}t = \delta\hat{\boldsymbol{q}}\cdot\boldsymbol{p}. \tag{3.31}$$

where:

$$\bar{\mathscr{L}} = \hat{\mathscr{L}}(\boldsymbol{w}, \boldsymbol{q}) - \hat{\boldsymbol{p}}\cdot(\boldsymbol{w} - \boldsymbol{w}_n - \mathbf{X}\cdot\dot{\boldsymbol{q}}). \tag{3.32}$$

It is clear that the momentum $\hat{\boldsymbol{p}}$ plays the role of Lagrange multiplier. In carrying out the variation of $\bar{\mathscr{L}}$, note that:

$$\delta\hat{\mathscr{L}} = \delta\boldsymbol{w}\cdot\frac{\delta\hat{\mathscr{L}}}{\delta\boldsymbol{w}} + \boldsymbol{\theta}_\delta\cdot\left(\boldsymbol{v}\times\frac{\delta\hat{\mathscr{L}}}{\delta\boldsymbol{v}} + \boldsymbol{w}\times\frac{\delta\hat{\mathscr{L}}}{\delta\boldsymbol{w}}\right), \tag{3.33}$$

and, $\delta\boldsymbol{\omega}_n = \boldsymbol{\theta}_\delta \times \boldsymbol{\omega}_n$. Then using the fundamental relation, $\delta\boldsymbol{\theta}_\mathrm{d} - \mathrm{d}\boldsymbol{\theta}_\delta = \boldsymbol{\theta}_\delta \times \boldsymbol{\theta}_\mathrm{d}$, which is established in Appendix A, and defining $\delta^*\boldsymbol{w} = (\delta\boldsymbol{v}, \delta^o\boldsymbol{\omega})$, Eq. (3.33) may be rearranged in the following way:

$$\int_{t_1}^{t_2}\left[\delta\hat{\boldsymbol{q}}\cdot\left(\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w})\cdot\frac{\delta\hat{\mathscr{L}}}{\delta\boldsymbol{w}}\right) - \delta^*\boldsymbol{w}\cdot\left(\hat{\boldsymbol{p}} - \frac{\delta\hat{\mathscr{L}}}{\delta\boldsymbol{w}}\right) - \delta^*\hat{\boldsymbol{p}}\cdot\mathbf{X}^{-1}\cdot(\boldsymbol{w} - \boldsymbol{w}_n) + \frac{\mathrm{d}}{\mathrm{d}t}(\delta\hat{\boldsymbol{q}})\cdot\hat{\boldsymbol{p}} - \frac{\mathrm{d}}{\mathrm{d}t}(\delta^*\boldsymbol{p})\cdot\boldsymbol{q}\right]\mathrm{d}t$$
$$= (\delta\boldsymbol{q}\cdot\hat{\boldsymbol{p}}_b - \delta^*\hat{\boldsymbol{p}}\cdot\boldsymbol{q}_b)|_1^{t_2}. \tag{3.34}$$

This form is very suitable for numerical implementation, since the field variables do not need to be differentiable over the time element, and the three fields, $\boldsymbol{q}, \boldsymbol{w}, \hat{\boldsymbol{p}}$ are completely independent. Therefore, very simple trial functions may be chosen. This feature arises from the particular choice of the virtual velocity $\delta^* \boldsymbol{w}$ and the virtual momentum $\delta^* \boldsymbol{p}$. The Euler–Lagrange equations and the weak forms of the boundary conditions, corresponding to Eq. (3.34) are easily obtained, by means of integrating by parts the terms envolving time derivative of $\delta^* \boldsymbol{p}$ and $\delta \hat{\boldsymbol{q}}$. In this way, the following expression is obtained:

$$\int_{t_1}^{t_2} \left[\delta\hat{\boldsymbol{q}} \cdot \left(\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w}) \cdot \frac{\delta \hat{\mathscr{L}}}{\delta \boldsymbol{w}} - \dot{\hat{\boldsymbol{p}}} \right) - \delta^* \boldsymbol{w} \cdot \left(\hat{\boldsymbol{p}} - \frac{\delta \hat{\mathscr{L}}}{\delta \boldsymbol{w}} \right) - \delta^* \hat{\boldsymbol{p}} \cdot [\mathbf{X}^{-1} \cdot (\boldsymbol{w} - \boldsymbol{w}_n) - \dot{\boldsymbol{q}}] \mathrm{d}t \right.$$
$$= \delta\hat{\boldsymbol{q}} \cdot (\hat{\boldsymbol{p}}_b - \hat{\boldsymbol{p}}) - \delta^* \hat{\boldsymbol{p}} \cdot (\hat{\boldsymbol{q}}_b - \hat{\boldsymbol{q}}) |_{t_1}^{t_2}. \tag{3.35}$$

Due to the arbitrariness of the virtual displacements $\delta\hat{\boldsymbol{q}}$, the virtual velocity $\delta^* \boldsymbol{w}$, and the virtual momentum $\delta^* \boldsymbol{p}$, Eq. (3.35) constitutes the weak form of the linear and angular momentum balance equations, the constitutive equations, the compatibility conditions and the boundary conditions. Equation (3.35) is analogous to the Hu-Washizu three field form (Washizu 1980), for rigid body dynamics. Each of the previous formulations, primal and mixed, may be obtained from this form. The primal formulation, can be obtained if the displacement field compatibility and the displacement boundary conditions are satisfied *a priori*. The mixed form arrises when the constitutive relations are satisfied *a priori*.

The drawback of this approach is that there are eighteen degrees of freedom associated with a single unconstrained rigid body. In the next section the linearization of the primal and mixed variational statements is presented.

4 Linearization

Since the variational forms developed in the previous section are nonlinear in the coordinates $\boldsymbol{q}$, a solution scheme such as a Newton or Quasi-Newton method is needed. In order to take advantage of the quadratic convergence property of the Newton method, consistent linearized expressions for the various weak forms are required. These linearizations are also useful in evaluating the stability of the system.

To illustrate the linearization, consider Eq. (3.23), written as:

$$\int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}t} \delta\hat{\boldsymbol{q}}, \delta\hat{\boldsymbol{q}} \right) \cdot (\hat{\boldsymbol{p}}, [\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w}) \cdot \hat{\boldsymbol{p}}]) \mathrm{d}t = \delta\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{p}}_b |_{t_1}^{t_2}. \tag{4.1}$$

Then, at a given state $(\dot{\boldsymbol{q}}_g, \boldsymbol{q}_g)$, the linearized form of Eq. (4.1) is:

$$\int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}t} \delta\hat{\boldsymbol{q}}, \delta\hat{\boldsymbol{q}} \right) \cdot \hat{\mathscr{T}}_p \cdot \left(\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{d}\boldsymbol{q}, \mathrm{d}\boldsymbol{q} \right) \mathrm{d}t = \delta\hat{\boldsymbol{q}} \cdot \hat{\boldsymbol{p}}_b |_{t_1}^{t_2} - \int_{t_1}^{t_2} \left(\frac{\mathrm{d}}{\mathrm{d}t} \delta\hat{\boldsymbol{q}}, \delta\hat{\boldsymbol{q}} \right) \cdot \hat{\mathscr{R}}_p \mathrm{d}t. \tag{4.2}$$

Where $\hat{\mathscr{T}}$ and $\hat{\mathscr{R}}$, are the tangent matrix and residual vector, respectively. The subscript $(\ )_p$ indicates a primal formulation and the hat indicates that $\delta\hat{\boldsymbol{q}}$ is the variation used in the weak form. The residual vector and tangent matrix are formally defined as:

$$\hat{\mathscr{R}}_p = (\hat{\boldsymbol{p}}, [\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w}) \cdot \hat{\boldsymbol{p}}])_{\substack{q = q_q \\ q = q_g}} \tag{4.3}$$

$$\hat{\mathscr{T}}_p = \begin{bmatrix} \dfrac{\partial \hat{\boldsymbol{p}}}{\partial \dot{\boldsymbol{q}}} & \dfrac{\partial \hat{\boldsymbol{p}}}{\partial \boldsymbol{q}} \\ \dfrac{\partial (\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w}) \cdot \hat{\boldsymbol{p}})}{\partial \dot{\boldsymbol{q}}} & \dfrac{\partial (\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w}) \cdot \hat{\boldsymbol{p}})}{\partial \boldsymbol{q}} \end{bmatrix}_{\substack{q = \dot{q}_g \\ q = q_g}} \tag{4.4}$$

The complete expression for $\hat{\mathscr{T}}_p$ is given in Appendix B. As mentioned previously, this matrix is not symmetric, since the weak form is not expressed in terms of the variation of the rotation coordinates.

However, if the variation of kinetic energy is expressed in terms of $\delta\dot{q}$ and δq, Eq. (3.24) may be written as:

$$\int_{t_1}^{t_2} (\delta\dot{q}, \delta q)\cdot\left(\frac{\partial T}{\partial \dot{q}}, \frac{\partial T}{\partial q} + f\right)\mathrm{d}t = dq\cdot p_b|_{t_1}^{t_2}. \tag{4.5}$$

The linearization of Eq. (4.5) about the given state is then;

$$\int_{t_1}^{t_2}\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta q, \delta q\right)\cdot\mathscr{T}_p\cdot\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}q, \mathrm{d}q\right)\mathrm{d}t = \delta q\cdot p_b|_{t_1}^{t_2} - \int_{t_1}^{t_2}\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta q, \delta q\right)\cdot\mathscr{R}_p\mathrm{d}t. \tag{4.6}$$

Here, δq is the variation used in the weak form, and consequently the part of the tangent matrix associated with the kinetic energy is symmetric. The residual vector and tangent matrix are given by;

$$\mathscr{R}_p = \left(\frac{\partial T}{\partial \dot{q}}\frac{\partial T}{\partial q} + f\right)\Bigg|_{\substack{\dot{q}=q_g\\ q=q_g}} \tag{4.7}$$

$$\mathscr{T}_p = \begin{bmatrix} \dfrac{\partial^2 T}{\partial \dot{q}^2} & \dfrac{\partial^2 T}{\partial q\,\partial \dot{q}} \\ \dfrac{\partial^2 T}{\partial \dot{q}\,\partial q} + \dfrac{\partial f}{\partial \dot{q}} & \dfrac{\partial^2 T}{\partial q^2} + \dfrac{\partial f}{\partial q} \end{bmatrix}_{\substack{\dot{q}=\dot{q}_g\\ q=q_g}}. \tag{4.8}$$

Following the same procedure, the tangent matrices for the other principles are developed in Appendix B. The results for the mixed (two field) form are sketched out briefly here. Equation (3.30) may be written as:

$$\int_{t_1}^{t_2}\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta p, \frac{\mathrm{d}}{\mathrm{d}t}\delta q\right)\cdot\mathbf{I}_S\cdot(p, q) + (\delta p, \delta q)\cdot\left(-\frac{\partial H}{\partial p}, -\frac{\partial \mathrm{H}}{\partial q} + f\right)\mathrm{d}t = (\delta p, \delta q)\cdot I_S\cdot(p_b, q_b)|_{t_1}^{t_2} \tag{4.9}$$

where $\mathbf{I}_S = \begin{bmatrix} \mathrm{P} & -I_6 \\ I_6 & 0 \end{bmatrix}$ and I_6 is the six dimensional identity. The linearization of Eq. (4.9) leads to:

$$\begin{aligned}\int_{t_1}^{t_2}&\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta p, \frac{\mathrm{d}}{\mathrm{d}t}\delta q\right)\cdot\mathbf{I}_S\cdot(\mathrm{d}p, \mathrm{d}q) + (\delta p, \delta q)\cdot\mathscr{T}_m\cdot(\mathrm{d}p, \mathrm{d}q)\right)\mathrm{d}t \\ &= (\delta p, \delta q)\cdot\mathbf{I}_S\cdot(p_b, q_b)|_{t_1}^{t_2} - \int_{t_1}^{t_2}\left[\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta p, \frac{\mathrm{d}}{\mathrm{d}t}\delta q\right)\cdot\mathbf{I}_S\cdot(p_g, q_g) + (\delta p, \delta q)\cdot\mathscr{R}_m\right]\mathrm{d}t.\end{aligned} \tag{4.10}$$

Here:

$$\mathscr{R}_m = \left(-\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q} + f\right)_{\substack{p=p_g\\ q=q_g}} \tag{4.11}$$

$$\mathscr{T}_m = \begin{bmatrix} -\dfrac{\partial^2 H}{\partial p^2} & -\dfrac{\partial^2 H}{\partial p\,\partial q} \\ \left(-\dfrac{\partial^2 H}{\partial q\,\partial p} + \dfrac{\partial f}{\partial p}\right) & \left(-\dfrac{\partial^2 H}{\partial q^2} + \dfrac{\partial f}{\partial q}\right) \end{bmatrix}_{\substack{p=p_g\\ q=q_a}} \tag{4.12}$$

are respectively, the residual vector and tangent matrix evaluated at the given state (p_g, q_g).

5 Finite element approximation

In the time finite element approximation employed in this paper, the time interval $[t_1, t_2]$ is subdivided by a number of equispaced time nodal points. The time interval $[t_1, t_2]$ may then be covered by $m < n$ consecutive non-overlapping time elements each containing two or more nodes. The shape functions used over the elements are of the piecewise Lagrange type. Once the time interval is discretized, the weak forms are applied over each element. Here only one element is considered for the primal form given in Eq. (4.1) and the mixed form given in Eq. (4.9).

5.1 Primal form

Considering the variational form Eq. (4.1) and an n noded time element, let $\boldsymbol{U} = (\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n)$ and $\boldsymbol{V} = (\delta\hat{\boldsymbol{q}}_1, \delta\boldsymbol{q}_2, \ldots, \delta\hat{\boldsymbol{q}}_n)$ be vectors of nodal values of the trial and test functions respectively. The parametric approximations for $\boldsymbol{q}$ and $\delta\hat{\boldsymbol{q}}$ are then:

$$\boldsymbol{q} = \sum_{k=1}^{n} s_k \boldsymbol{q}_k = \boldsymbol{s}\cdot\boldsymbol{U} \qquad \delta\hat{\boldsymbol{q}} = \sum_{k=1}^{n} s_k \delta\hat{\boldsymbol{q}}_k = \boldsymbol{s}\cdot\boldsymbol{V} \tag{5.1a}$$

$$\dot{\boldsymbol{q}} = \sum_{k=1}^{n} \dot{s}_k \boldsymbol{q}_k = \dot{\boldsymbol{s}}\cdot\boldsymbol{U} \quad \frac{\mathrm{d}}{\mathrm{d}t}(\delta\hat{\boldsymbol{q}}) = \sum_{k=1}^{n} \dot{s}_k \delta\hat{\boldsymbol{q}}_k = \dot{\boldsymbol{s}}\cdot\boldsymbol{V}. \tag{5.1b}$$

Moreover, the increment $\delta\boldsymbol{q}$ is approximated as:

$$\delta\boldsymbol{q} = \sum_{k=1}^{n} s_k \delta\boldsymbol{q}_k = \boldsymbol{s}\cdot\Delta\boldsymbol{U} \tag{5.2}$$

where s_k are shape functions with the property $s_k(t_j) = \delta_{kj}$ and $\Delta\boldsymbol{U}$ is the increment in the nodal values of the generalized coordinates. The nonlinear solution of Eq. (4.1) is performed using the linearized form Eq. (4.2) in an iterative procedure. The solution $\boldsymbol{U}$ is then the limit of the sequence $\boldsymbol{U}_1, \boldsymbol{U}_2, \ldots, \boldsymbol{U}_m$ as the difference between successive solutions, $\boldsymbol{U}_{m-1} - \boldsymbol{U}_m$ approaches zero. Performing the integrations in Eq. (4.2) using standard Gauss quadrature and considering $\delta\hat{\boldsymbol{q}}$ as an arbitrary variation the following is obtained, for the i^{th} solution step:

$$\mathbf{K}_i\cdot\Delta\boldsymbol{U}_i = \mathbf{B}\cdot(\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2) - \mathbf{F}_i \quad \text{(no sum on } i\text{)} \tag{5.3}$$

where:

$$\mathbf{K}_i = \int_{t_1}^{t_2} (\dot{s}, s)^t \cdot \hat{\mathscr{T}}_p(\boldsymbol{U}_i)\cdot(\dot{s}, s)\mathrm{d}t, \qquad \mathbf{F}_i = \int_{t_1}^{t_2} (\dot{s}, s)^t \cdot \hat{\mathscr{R}}_p(\boldsymbol{U}_i)\mathrm{d}t \tag{5.4, 5.5}$$

$(\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2)$ are boundary values of $\hat{\boldsymbol{p}}$ at the times t_1, t_2 respectively, and the matrix $\mathbf{B}$ is give by:

$$\mathbf{B} = \begin{bmatrix} -\boldsymbol{I}_6, 0, 0, \ldots, & 0 \\ 0, 0, 0, \ldots, & \boldsymbol{I}_6 \end{bmatrix}^t. \tag{5.6}$$

Further, the matrix $\mathbf{K}_i$ is the integrated tangent matrix at the i^{th} solution step and $\mathbf{F}_i$ is the integrated residual vector.

In the case of an initial value problem, $\boldsymbol{q}_1$ and $\hat{\boldsymbol{p}}_1$ are prescribed so that the components of $\Delta\boldsymbol{U}$ associated with the first node are always zero. Since the equations for $\hat{\boldsymbol{p}}_1$ and $\hat{\boldsymbol{p}}_2$ are decoupled, the iteration scheme may be carried out considering a reduced problem. The final momentum $\hat{\boldsymbol{p}}_2$ need only be calculated after the iterations have converged. This is a simple matter, since at the converged solution $\Delta\boldsymbol{U}$ is zero, to within some prescribed tolerance. The final momentum is then obtained by computing the residual vector at the converged solution.

5.2 Mixed form

For the mixed form Eq. (4.9), a different approach is required. Continuity of the coordinates $(\boldsymbol{p}, \boldsymbol{q})$ is not satisfied "a priori" over the time element, while at the boundary, continuity of $(\delta\boldsymbol{p}, \delta\boldsymbol{q})$ is required. It is therefore important to understand $(\delta\boldsymbol{p}, \delta\boldsymbol{q})$ to be a virtual state vector rather than a mere variation of $(\boldsymbol{p}, \boldsymbol{q})$. Since the trial and test functions may be chosen independently, they may be approximated as:

$$(\boldsymbol{p},\boldsymbol{q}) = \sum_{k=1}^{n-1} s_k \boldsymbol{U}_k = \boldsymbol{s}_a \cdot \boldsymbol{U}, \quad (\delta\boldsymbol{p},\delta\boldsymbol{q}) = \sum_{k=1}^{n} s_k \boldsymbol{V}_k = \boldsymbol{s}_b \cdot \boldsymbol{V} \tag{5.7}$$

where $\boldsymbol{U}_k = (\boldsymbol{p}_k, \boldsymbol{q}_k)$ and $\boldsymbol{V}_k = (\delta\boldsymbol{p}_k, \delta\boldsymbol{q}_k)$ are vectors of nodal values. The expression for $(\delta\boldsymbol{p},\delta\boldsymbol{q})$ contains one more term than that for $(\boldsymbol{p},\boldsymbol{q})$. Further, the values $(\boldsymbol{p},\boldsymbol{q})$ evaluated at the boundary are not required to be equal to $(\boldsymbol{p}_b, \boldsymbol{q}_b)$. The linearized form Eq. (4.10) is then:

$$\mathbf{K}_i \cdot \Delta \boldsymbol{U}_i = \mathbf{B} \cdot (\boldsymbol{p}_1, \boldsymbol{q}_1, \boldsymbol{p}_2, \boldsymbol{q}_2) - \mathbf{F}_i, \tag{5.8}$$

where $\mathbf{K}_i$ and $\mathbf{F}_i$ are given by:

$$\mathbf{K}_i = \int_{t_1}^{t_2} (\dot{\boldsymbol{s}}_b^t \cdot \mathbf{I}_S \cdot \boldsymbol{s}_a + \boldsymbol{s}_b^t \cdot \mathscr{T}_{rm}(\boldsymbol{U}_i) \cdot \boldsymbol{s}_a)\,\mathrm{d}t, \quad \mathbf{F}_i = \int_{t_1}^{t_2} (\dot{\boldsymbol{s}}_b^t \cdot \mathbf{I}_S \cdot \boldsymbol{s}_a \cdot \boldsymbol{U}_i + \boldsymbol{s}_b^t \cdot \mathscr{R}_{rm}(\boldsymbol{U}_i))\,\mathrm{d}t. \tag{5.9a, b}$$

In this case the matrix $\mathbf{B}$ is defined as:

$$\mathbf{B} = \begin{bmatrix} \mathbf{I}_S, & 0, 0, \ldots, & 0 \\ 0, & 0, 0, \ldots, & -\mathbf{I}_S \end{bmatrix}^t \quad \mathbf{I}_S = \begin{bmatrix} 0 & -\mathbf{I}_6 \\ \mathbf{I}_6 & 0 \end{bmatrix}. \tag{5.10}$$

For the initial value problem $(\boldsymbol{p}_1, \boldsymbol{q}_1)$ is prescribed and we can solve for $\Delta \boldsymbol{U}_i$ and $(\boldsymbol{p}_2, \boldsymbol{q}_2)$. In this case the increments in the variables $\boldsymbol{p}$ and $\boldsymbol{q}$ are not zero at the first time node.

6 Linearized stability analysis

In dynamical problems, a stability analysis, even in linearized form, is useful in evaluating the behavior of the system. Further, a stability analysis, for a problem where the solution is known in advance, is valuable in assessing the performance of the numerical approximation scheme. Rearranging Eq. (5.3) so that the boundary nodes and interior nodes are grouped together i.e. $\boldsymbol{U} = (\boldsymbol{U}_B, \boldsymbol{U}_I)$ and performing the same partitioning on $\mathbf{K}, \mathbf{F}$ and $\mathbf{B}$, Eq. (5.3) becomes:

$$\begin{aligned} &\mathbf{K}_{BB} \cdot \Delta \boldsymbol{U}_B + \mathbf{K}_{BI} \cdot \Delta \boldsymbol{U}_I = \mathbf{B}_{BB} \cdot (\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2) - \mathbf{F}_B, \\ &\mathbf{K}_{IB} \cdot \Delta \boldsymbol{U}_B + \mathbf{K}_{II} \cdot \Delta \boldsymbol{U}_I = \mathbf{B}_{IB} \cdot (\hat{\boldsymbol{p}}_1, \hat{\boldsymbol{p}}_2) - \mathbf{F}_I. \end{aligned} \tag{6.1}$$

Since, by definition $\mathbf{B}_{IB} = 0$, this is equivalent to:

$$\tilde{\mathbf{K}}_{BB} \cdot \Delta \boldsymbol{U}_B = \mathbf{B}_{BB} \cdot (\boldsymbol{p}_1, \boldsymbol{p}_2) - \tilde{\mathbf{F}}_B, \tag{6.2}$$

where:

$$\tilde{\mathbf{K}}_{BB} = \mathbf{K}_{BB} - \mathbf{K}_{BI} \cdot \mathbf{K}_{II}^{-1} \cdot \mathbf{K}_{IB}, \qquad \tilde{\mathbf{F}}_B = \mathbf{F}_B - \mathbf{K}_{BI} \cdot \mathbf{K}_{II}^{-1} \cdot \mathbf{F}_I. \tag{6.3, 6.4}$$

In the case of a two noded time element there are no interior nodes, so that $\tilde{\mathbf{K}}_{BB}$ and $\tilde{\mathbf{F}}_B$ reduce to $\mathbf{K}_{BB}$ and $\mathbf{F}_B$ respectively.

Equation (6.2) is also useful in a perturbation analysis. If we consider a perturbation of a dynamical solution, we have the following equations:

$$\tilde{\mathbf{F}}_B - \mathbf{B}_{BB} \cdot (\boldsymbol{p}_1, \hat{\boldsymbol{p}}_2) = 0, \quad \tilde{\mathbf{K}}_{BB} \cdot \mathrm{d}\boldsymbol{U}_B - \mathbf{B}_{BB} \cdot (\mathrm{d}\hat{\boldsymbol{p}}_1, \mathrm{d}\hat{\boldsymbol{p}}_2) = 0. \tag{6.5}$$

Since $\mathbf{B}_{BB} = \begin{bmatrix} -I_6 & 0 \\ 0 & I_6 \end{bmatrix}$ the second of Eq. (6.5) becomes:

$$\tilde{\mathbf{K}}_{11} \cdot \mathrm{d}\boldsymbol{q}_1 + \tilde{\mathbf{K}}_{12} \cdot \mathrm{d}\boldsymbol{q}_2 + \mathrm{d}\hat{\boldsymbol{p}}_1 = 0, \quad \tilde{\mathbf{K}}_{21} \cdot \mathrm{d}\boldsymbol{q}_1 + \tilde{\mathbf{K}}_{22} \cdot \mathrm{d}\boldsymbol{q}_2 - \mathrm{d}\hat{\boldsymbol{p}}_2 = 0, \tag{6.6}$$

where the subscripts 1 and 2 refer to nodes at times t_1 and t_2 and the subscript $(\ )_{BB}$ is dropped for simplicity of notation. Equation (6.6) can be put in the form of a transition matrix, which maps the perturbation of the initial state vector $(\mathrm{d}\hat{\boldsymbol{p}}_1, \mathrm{d}\boldsymbol{q}_1)$ into the perturbation of the final state vector $(\mathrm{d}\hat{\boldsymbol{p}}_2, \mathrm{d}\boldsymbol{q}_2)$ i.e.:

$$(\mathrm{d}\hat{\boldsymbol{p}}_2, \mathrm{d}\boldsymbol{q}_2) = \mathbf{T} \cdot (\mathrm{d}\hat{\boldsymbol{p}}_1, \mathrm{d}\boldsymbol{q}_1). \tag{6.7}$$

The transition matrix $\mathbf{T}$ has the following expression:

$$\mathbf{T}=\begin{bmatrix} -\tilde{\mathbf{K}}_{22}\cdot\tilde{\mathbf{K}}_{12}^{-1} & \tilde{\mathbf{K}}_{21}-\tilde{\mathbf{K}}_{22}\cdot\tilde{\mathbf{K}}_{12}^{-1}\cdot\tilde{\mathbf{K}}_{11} \\ -\tilde{\mathbf{K}}_{12}^{-1} & -\tilde{\mathbf{K}}_{12}^{-1}\cdot\mathbf{K}_{11} \end{bmatrix}. \tag{6.8}$$

It may be seen that the above transition matrix is a function of the time step t_2-t_1 and is problem dependent. Here the eigenvalues of $\mathbf{T}$ are denoted by λ. If any of the eigenvalues have moduli greater than 1, the corresponding eigensolution will increase exponentially, and the solution step is not stable. If the eigenvalues of the true transition matrix are known, comparison with those of the approximated matrix will provide a measure of the accuracy of the numerical method. Some examples of this are given in the next section.

Proceeding in a similar fashion for the mixed form, the linearized expression Eq. (5.8) may be partitioned such that $V=(V_i, V_m, V_f)$ where the subscripts i, m, f refer to initial, middle, and final nodes. Equation (5.8) then take the form:

$$\mathbf{K}_i\cdot\Delta U=-\mathbf{I}_S\cdot(\boldsymbol{p}_1,\boldsymbol{q}_1)-\mathbf{F}_i,\quad \mathbf{K}_m\cdot\Delta U=-\mathbf{F}_m,\quad \mathbf{K}_f\cdot\Delta U=\mathbf{I}_S\cdot(\boldsymbol{p}_2,\boldsymbol{q}_2)-\mathbf{F}_f. \tag{6.9}$$

Solving the first two expressions for ΔU, and substituting into the last expression, the transition matrix for the mixed form is calculated. In the case of a two noded element, there are no middle nodes, leading to:

$$\Delta U=-\mathbf{K}_i^{-1}\cdot(\mathbf{I}_S\cdot(\boldsymbol{p}_1,\boldsymbol{q}_1)+\mathbf{F}_i). \tag{6.10}$$

Recalling that $\mathbf{I}_S^{-1}=-\mathbf{I}_S$, the final state $(\boldsymbol{p}_2,\boldsymbol{q}_2)$ is:

$$(\boldsymbol{p}_2,\boldsymbol{q}_2)=\mathbf{T}\cdot(\boldsymbol{p}_1,\boldsymbol{q}_1)-\tilde{\mathbf{F}}_f, \tag{6.11}$$

where:

$$\mathbf{T}=\mathbf{I}_S\cdot\mathbf{K}_f\cdot\mathbf{K}_i^{-1}\cdot\mathbf{I}_S,\quad \tilde{\mathbf{F}}_f=\mathbf{I}_S\cdot(\mathbf{F}_f+\mathbf{K}_f\cdot\mathbf{K}_i^{-1}\cdot\mathbf{F}_i). \tag{6.12}$$

The perturbed state equation is then

$$(\mathrm{d}\boldsymbol{p}_2,\mathrm{d}\boldsymbol{q}_2)=\mathbf{T}\cdot(\mathrm{d}\boldsymbol{p}_1,\mathrm{d}\boldsymbol{q}_1). \tag{6.13}$$

7 Numerical stability considerations

In order to understand the behavior of the various approaches, the stability of a vertical spinning top is evaluated. Even though it is quite simple, this example will show the different behavior of the primal and mixed forms. For simplicity, the development presented is for the two noded element only and the time step t_2-t_1 is denoted by Δt. Numerical comparisons are given for the three and four node elements.

Let us consider the vertical spinning top rotating about the vertical axis $\boldsymbol{e}_3$ at a constant rate Ω and acted upon by gravity. Let $\boldsymbol{d}$ be the distance from the center of gravity to the suspension point. The steady rotation about the vertical axis is taken as a reference configuration.

$$\boldsymbol{R}_0=\boldsymbol{R}(\Omega t\boldsymbol{e}_3). \tag{7.1}$$

First consider the primal form. Eliminating the translational degrees of freedom, it is easily seen that the tangent matrices $\hat{\mathscr{T}}$ and $\mathscr{T}$, become:

$$\hat{\mathscr{T}}=\begin{bmatrix}\boldsymbol{J} & -\boldsymbol{h}\times\boldsymbol{I}\\ 0 & \boldsymbol{L}\end{bmatrix}\quad \mathscr{T}=\begin{bmatrix}\boldsymbol{J} & -\frac{1}{2}\boldsymbol{h}\times\boldsymbol{I}\\ \frac{1}{2}\boldsymbol{h}\times\boldsymbol{I} & \boldsymbol{L}\end{bmatrix}, \tag{7.2}$$

where:

$$\boldsymbol{J}=\mathscr{I}_a\boldsymbol{e}_3\cdot\boldsymbol{e}_3^t+\mathscr{I}_t(\boldsymbol{I}-\boldsymbol{e}_3\cdot\boldsymbol{e}_3^t),\quad \boldsymbol{h}=\mathscr{I}_a\Omega\boldsymbol{e}_3,\quad \boldsymbol{L}=(\boldsymbol{I}-\boldsymbol{e}_3\cdot\boldsymbol{e}_3^t)mgd. \tag{7.3}$$

$\mathscr{I}_a$ and $\mathscr{I}_t$ are respectively the axial and transverse moments of inertia referred to the suspension point, and d and g are the moduli of $\boldsymbol{d}$ and $\boldsymbol{g}$. The vertical component of rotation is decoupled from the others. Therefore, the transverse rotation is denoted by ψ and the stability of transverse motion only is analysed. Representing $\psi = \psi_a + i\psi_b$, where $i = \sqrt{-1}$, the reduced tangent matrices in terms of $\dot{\psi}$ and ψ, are:

$$\hat{\mathscr{T}}_r = \begin{bmatrix} \mathscr{I}_t & -i\Omega\mathscr{I}_a \\ 0 & mgd \end{bmatrix} \quad \mathscr{T}_r = \begin{bmatrix} \mathscr{I}_t & -\frac{1}{2}i\Omega\mathscr{I}_a \\ \frac{1}{2}i\Omega\mathscr{I}_a & mgd \end{bmatrix}. \tag{7.4}$$

Assuming linear shape functions for the virtual rotation, and the rotation itself, leads to:

$$\hat{\mathbf{K}}_{BB} = \begin{bmatrix} A & -B+iC \\ -B-iC & A \end{bmatrix} \quad \mathbf{K}_{BB} = \begin{bmatrix} A+iC & -B+iC \\ -B-iC & A-iC \end{bmatrix}, \tag{7.5}$$

where:

$$A = \frac{\mathscr{I}_t}{\Delta t} + \frac{amgd}{2}\Delta t, \quad B = \frac{\mathscr{I}_t}{\Delta t} - \frac{bmgd}{2}\Delta t, \quad C = \frac{\Omega\mathscr{I}_a}{2}. \tag{7.6}$$

An exact integration of the tangent matrices leads to $a = \frac{2}{3}$, $b = \frac{1}{3}$. Reduced order integration using only one Gauss point yields $a = b = \frac{1}{2}$. The transition matrices for quasi coordinates and full Lagrange coordinates are then:

$$\hat{\mathbf{T}} = \frac{B+iC}{B^2+C^2}\left[\begin{array}{c|c} A-iC & A^2-B^2 \\ \hline 1 & A+iC \end{array}\right] \quad \mathbf{T} = \frac{B+iC}{B^2+C^2}\left[\begin{array}{c|c} A & \dfrac{A^2-(B^2+C^2)}{A} \\ \hline 1 & \end{array}\right]. \tag{7.7}$$

Both of these matrices have the same eigenvalues, λ. Letting $\lambda = \frac{B+iC}{(B^2+C^2)^{1/2}}\mu$ the characteristic equation will be:

$$\mu^2 - \frac{2A}{(B^2+C^2)^{1/2}}\mu + 1 = 0. \tag{7.8}$$

Since λ and μ differ by a unit complex factor, they gain the same stability limits. It is interesting to note that when using a reduced order integration, the stability boundary is indepentent of the time step Δt, and coincides with the physical stability boundary. In fact, solving Eq. (7.8) results in:

$$\mu = \frac{1}{(B^2+C^2)^{1/2}}(A \pm D^{1/2}), \tag{7.9}$$

where:

$$\begin{aligned} D &= A^2 - B^2 - C^2 \\ &= -\frac{1}{4}\left[(\mathscr{I}_a\Omega)^2 - (2\mathscr{I}_t\omega)^2\left(1 - \frac{a^2-b^2}{4}\omega^2\Delta t^2\right)\right], \end{aligned} \tag{7.10}$$

and:

$$\omega = \left(\frac{mgd}{\mathscr{I}_t}\right)^{1/2}. \tag{7.11}$$

For reduced order integration, D becomes negative when $\Omega = \Omega_c = \frac{2\mathscr{I}_t\omega}{\mathscr{I}_a}$ which is also the physical stability limit. On the other hand with exact integration, D becomes negative when $\Omega = \Omega_c\sqrt{1 + \frac{(\omega\Delta t)^2}{12}}$. In this case, the stability limit is dependent on the step size and approaches the physical limit only as $\Delta t \to 0$.

8 Numerical examples

In order to demonstrate numerical stability and to show how reduced order integration affects this behavior, the vertical spinning top is solved numerically. The problem is solved using two,

Table 1. Eigenvalues for vertical top-exact integration

	Eigenvalues for exact integration					
	Two nodes		Three nodes		Four nodes	
Δt	Real	Imag	Real	Imag	Real	Imag
0.02	1.6031E-02	1.6663	2.7599E-04	1.6666	1.7240E-05	1.6666
0.04	3.2027E-02	1.6654	1.1032E-03	1.6666	4.1751E-05	1.6666
0.06	4.7952E-02	1.6638	2.4795E-03	1.6666	1.4113E-04	1.6666
0.08	6.3772E-02	1.6617	4.4010E-03	1.6666	3.3443E-04	1.6666
0.10	7.9453E-02	1.6590	6.8623E-03	1.6665	6.5150E-04	1.6666
0.12	9.4963E-02	1.6557	9.8564E-03	1.6664	1.1222E-03	1.6666
0.14	0.1102	1.6518	1.3374E-02	1.6663	1.7753E-03	1.6666
0.16	0.1253	1.6474	1.7404E-02	1.6661	2.6385E-03	1.6666
0.18	0.1401	1.6424	2.1934E-02	1.6658	3.7381E-03	1.6666
0.20	0.1546	1.6370	2.6949E-02	1.6653	5.0991E-03	1.6666

Table 2. Eigenvalues for vertical top-under integration

	Eigenvalues for reduced integration					
	Two nodes		Three nodes		Four nodes	
Δt	Real	Imag	Real	Imag	Real	Imag
0.02	2.3881E-05	1.6665	2.3261E-05	1.6666	1.6713E-05	1.6666
0.04	2.3211E-05	1.6660	1.0527E-05	1.6666	1.3681E-05	1.6666
0.06	1.6634E-05	1.6652	1.3681E-05	1.6666	7.9443E-06	1.6666
0.08	1.0443E-05	1.6642	7.7153E-06	1.6666	8.0284E-06	1.6666
0.10	1.2153E-05	1.6628	8.0605E-06	1.6666	7.6044E-06	1.6666
0.12	1.3460E-05	1.6611	8.0266E-06	1.6666	7.4198E-06	1.6666
0.14	7.2016E-06	1.6591	7.7597E-06	1.6665	8.3770E-06	1.6666
0.16	7.5157E-06	1.6568	7.4664E-06	1.6664	6.2104E-06	1.6666
0.18	7.6967E-06	1.6543	7.4116E-06	1.6663	6.1258E-06	1.6666
0.20	7.7657E-06	1.6514	7.8648E-06	1.6662	6.0095E-06	1.6666

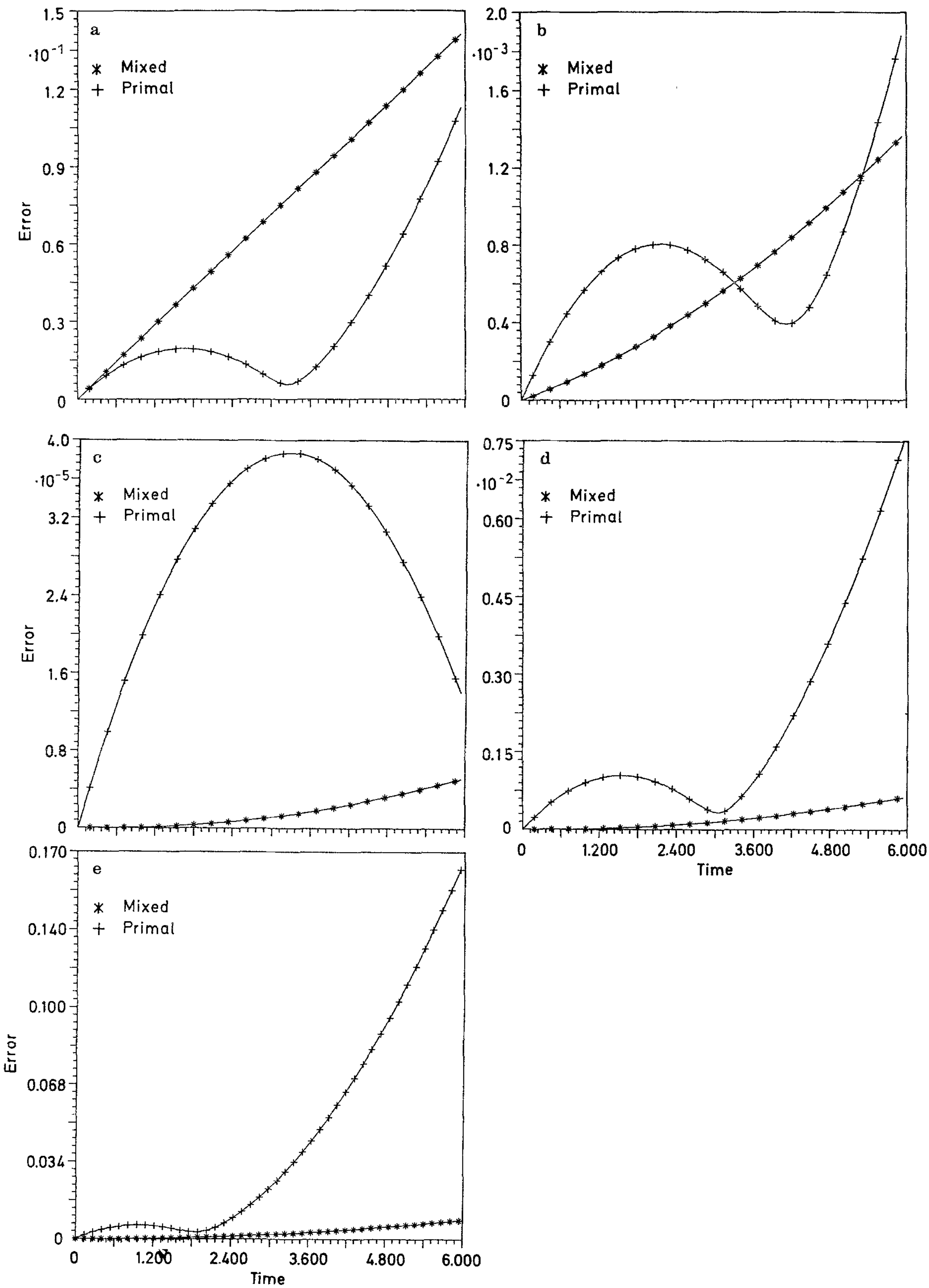
three and four noded time elements. For a top spinning at its critical speed, the eigenvalues of the system are purely imaginary. The exact eigenvalues of the system considered are $\pm i\frac{5}{3}$. Table 1 summarizes the numerical results obtained at the critical speed for exact integration. The influence of time step on the real part of the eigenvalues is clear. While the effect is not as strong in the higher order elements, the trend is the same.

The results for reduced order integration are presented in Table 2. It should be noted that the real parts of the eigenvalues are essentially zero, and are insensitive to the time step. For the case of a vertical spinning top or other simple system, it is straightforward to choose the degree of reduced integration required to follow the physics of the problem. However this is not the case in general.

For the mixed form, the stability boundary obtained numerically coincides with the physical boundary, without resorting to reduced order integration.

8.1 "Torque-free" body

In this section, the numerical resuts for a "torque-free" rigid body having one axis of symmetry are compared with the exact solution. Numerical studies of the accuracy, when using two, three and four noded elements, are summarized.



Figs. 1 a–e. Absolute error 2, **b** error 3, **c–e** error 4 noded elements

In order to compare the different formulations and check their accuracy, the very simple problem of a torque free rigid body with an axis of material symmetry is studied. This is a convenient problem for checking the methods since the closed form solution is well known. If we choose the reference point to coincide with the center of mass, the linear and angular degrees of freedom are coupled only by the external force, which in this case is zero. The exact solution of this problem is briefly summarized here.

If $\boldsymbol{a}$ denotes the axis of symmetry, the moment of inertia has the form:

$$\boldsymbol{J} = \mathscr{I}_a \boldsymbol{a} \otimes \boldsymbol{a} + \mathscr{I}_t (\boldsymbol{I} - \boldsymbol{a} \otimes \boldsymbol{a}). \tag{8.1}$$

One of the peculiarities of the symmetrical inertia is that the vectors $\boldsymbol{h}, \boldsymbol{\omega}$, and $\boldsymbol{a}$ are coplanar, i.e. $\boldsymbol{\omega} \cdot \boldsymbol{a} \times \boldsymbol{h} = 0$. In fact $\boldsymbol{\omega} \cdot \boldsymbol{a} \times \boldsymbol{h} = \boldsymbol{\omega} \cdot \boldsymbol{a} \times \boldsymbol{J} \cdot \boldsymbol{\omega}$ which is zero due to the skew symmetry of $\boldsymbol{a} \times \boldsymbol{J} \equiv \mathscr{I}_t \boldsymbol{a} \times \boldsymbol{I}$.

The angular momentum balance equation, referred to the center of gravity, is simply that $\dot{\boldsymbol{h}} = 0$. This leads to:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{h} \cdot \boldsymbol{a}) = \boldsymbol{h} \cdot \boldsymbol{\omega} \times \boldsymbol{a} \equiv 0, \qquad \frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{h} \times \boldsymbol{a}) = \boldsymbol{h} \times \dot{\boldsymbol{a}} = \boldsymbol{h} \times (\boldsymbol{\omega} \times \boldsymbol{a}) = \frac{\boldsymbol{h}}{\mathscr{I}_t} \times (\boldsymbol{h} \times \boldsymbol{a}), \tag{8.2a, b}$$

where the fact that $\dot{\boldsymbol{a}} = \boldsymbol{\omega} \times \boldsymbol{a}$ and $\boldsymbol{\omega} \times \boldsymbol{a} = \frac{\boldsymbol{h}}{\mathscr{I}_t} \times \boldsymbol{a}$ are used. The ratio $\frac{\boldsymbol{h}}{\mathscr{I}_t} = \boldsymbol{\omega}_p$, called the precession angular velocity, represents the angular velocity of the plane containing $\boldsymbol{a}, \boldsymbol{h}$, and $\boldsymbol{\omega}$. If $\boldsymbol{n}$ is the normal to this plane, then:

$$\dot{\boldsymbol{n}} = \boldsymbol{\omega}_p \times \boldsymbol{n}. \tag{8.3}$$

The corotational time derivative of $\boldsymbol{n}$ is:

$$\frac{d^o}{\mathrm{d}t}\boldsymbol{n} = -\boldsymbol{\omega}_r \times \boldsymbol{n}, \tag{8.4}$$

where:

$$\boldsymbol{\omega}_r = \boldsymbol{\omega} - \boldsymbol{\omega}_p = \frac{\mathscr{I}_t - \mathscr{I}_a}{\mathscr{I}_t \mathscr{I}_a}(\boldsymbol{h} \cdot \boldsymbol{a})\boldsymbol{a} \tag{8.5}$$

which is called the relative spin. The vector $\boldsymbol{\omega}_p$ is constant while $\boldsymbol{\omega}_r$ is time-variant, with:

$$\dot{\boldsymbol{\omega}}_r = \frac{\mathscr{I}_t - \mathscr{I}_a}{\mathscr{I}_t \mathscr{I}_a}(\boldsymbol{h} \cdot \boldsymbol{a})\dot{\boldsymbol{a}} = \boldsymbol{\omega}_p \times \boldsymbol{\omega}_r. \tag{8.6}$$

Denoting the value of $\boldsymbol{\omega}_r$ at time t_o by $\boldsymbol{\omega}_{r_o}$ results in:

$$\boldsymbol{\omega}_r = \exp((t - t_o)\boldsymbol{\omega}_p \times \boldsymbol{I}) \cdot \boldsymbol{\omega}_{r_o}. \tag{8.7}$$

If $\boldsymbol{R}(t_o)$ is the rotation from some fixed reference to the orientation at time t_o, then the rotation at any later time is:

$$\boldsymbol{R}(t) = \exp((t - t_o)\boldsymbol{\omega}_p \times \boldsymbol{I}) \cdot \exp((t - t_o)\boldsymbol{\omega}_r(t_o) \times \boldsymbol{I}) \cdot \boldsymbol{R}(t_o). \tag{8.8}$$

Since $\boldsymbol{\omega} = \boldsymbol{\omega}_p + \boldsymbol{\omega}_r$, Eq. (8.7) and Eq. (8.8) constitute the integral of the motion.

The numerical solution has been computed using two, three, and four noded time finite elements, for both primal and mixed forms. Several nodal spacings are investigated, for a body with a ratio of transverse to axial inertia of 1.875. The initial conditions are, angular velocity of 15 rad/s about the axis of symmetry and 10 rad/s about one transverse axis. The results are shown in Figs. 1a–e. The total rotation of the body after 6 s is roughly 100 radians. The errors plotted in figures are absolute errors. That is to say, the error is the magnitude, in radians, of the difference in rotation between the calculated solution and the exact solution. Figure 1a compares the error of the two noded primal and mixed elements. The time between nodes is 0.015 s. Figure 1b shows the three noded elements with the same time between the nodes, which means that the time elements in this case are 0.030 s long. Figure 1c compares results for the four noded elements. Again, the same time (0.015 s) between nodes is used, so the four noded element is 0.045 s in length.

Figure 1d and e compare the four noded elements at different time steps. Figure 1d contains plots of the error for a time between nodes of 0.030 s, while Fig. 1e shows the results for a time of 0.045 s between nodes. Therefore, the elements for Fig. 1d–e are, 0.090 s long and 0.135 s long, respectively. The behavior of the error in the mixed form is clearly more stable than the primal form. Comparing the primal curves in Figs. 1a and 1e, shows that the use of a four noded element with a total length of 0.135 s results in about the same error as the two noded element of length 0.015 s. However the mixed four noded element has an order of magnitude improvement in error. It is interesting to note that the maximum error in all of the test cases is less that 0.2 radians out of about 100 radians total rotation. It is difficult to genealize based on this simple, yet numerically significant, test case; but the behavior of the mixed formulation is very encouraging.

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Appendix A – relevant formulas for rotation

This appendix reports some fundamental formulas related to the three dimensional parametrization of the finite rotation tensor.

A.1 Exponential representation and its tangent map

Let $\boldsymbol{a}$ be an arbitrary vector undergoing a rotation to a new orientation $\hat{\boldsymbol{a}}$. This proper rotation may be expressed as $\boldsymbol{r} = \phi \boldsymbol{e}$, where ϕ is the magnitude of ratation and $\boldsymbol{e}$ defines the ratation axis. This constitutes a three dimensional parametrization of the rotation and is therefore not unique. Expressing $\hat{\boldsymbol{a}}$ in terms of its components in the basis $\boldsymbol{e}, \boldsymbol{t}, \boldsymbol{s}$, respectively defined as $\boldsymbol{e}, \boldsymbol{e} \times \boldsymbol{a}, \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{a})$, leads to:

$$\hat{\boldsymbol{a}} = [\boldsymbol{I} \cos \phi + (\boldsymbol{e} \times \boldsymbol{I}) \sin \phi + (1 - \cos \phi) \boldsymbol{e} \cdot \boldsymbol{e}^t] \cdot \boldsymbol{a}. \tag{A.1}$$

The term in brackets is the familiar form of the rotation tensor $\boldsymbol{R}$. Making use of the fact that $\boldsymbol{e} \cdot \boldsymbol{e}^t = \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{I}) + \boldsymbol{I}$, the rotation tensor may be written as:

$$\boldsymbol{R} = \boldsymbol{I} + \sin \phi (\boldsymbol{e} \times \boldsymbol{I}) + (1 - \cos \phi) \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{I}) \tag{A.2}$$

or in terms of $\boldsymbol{r}$ as:

$$\boldsymbol{R} = \boldsymbol{I} + \frac{\sin \phi}{\phi} (\boldsymbol{r} \times \boldsymbol{I}) + \frac{(1 - \cos \phi)}{\phi^2} \boldsymbol{r} \times (\boldsymbol{r} \times \boldsymbol{I}). \tag{A.3}$$

Expanding $\sin \phi$ and $\cos \phi$ in power series and substituting in the above expression, leads to:

$$\boldsymbol{R} = \boldsymbol{I} + \left[\phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} - \frac{\phi^7}{7!} + \cdots \right] (\boldsymbol{e} \times \boldsymbol{I}) + \left[\frac{\phi^2}{2!} - \frac{\phi^4}{4!} + \frac{\phi^6}{6!} - \frac{\phi^8}{8!} \right] \boldsymbol{e} \times (\boldsymbol{e} \times \boldsymbol{I}). \tag{A.4}$$

Making use of the fact that $\boldsymbol{e} \times \boldsymbol{e} \times \boldsymbol{e} \times \boldsymbol{I} = -\boldsymbol{e} \times \boldsymbol{I}$ and $\boldsymbol{r} = \phi \boldsymbol{e}$ we may rewrite this expression in the following form:

$$\boldsymbol{R} = \boldsymbol{I} + (\boldsymbol{r} \times \boldsymbol{I}) + \frac{1}{2!} \boldsymbol{r} \times (\boldsymbol{r} \times \boldsymbol{I}) + \frac{1}{3!} \boldsymbol{r} \times [\boldsymbol{r} \times (\boldsymbol{r} \times \boldsymbol{I})] + \cdots \text{h.o.t.} \tag{A.5}$$

This has the form of an exponential in $\boldsymbol{r} \times \boldsymbol{I}$, so the rotation tensor may be written concisely as:

$$\boldsymbol{R} = \exp (\boldsymbol{r} \times \boldsymbol{I}). \tag{A.6}$$

Other common rotation vectors such as $\boldsymbol{r}_s = \sin \phi \boldsymbol{e}$ and $\boldsymbol{r}_t = 2 \tan (\phi/2) \boldsymbol{e}$ give rise to completely equivalent representations for $\boldsymbol{R}$. In the former case, substituting $\boldsymbol{r}_s = \sin\phi \boldsymbol{e}$ into Eq. (A.3) and using the trigonometric half angle relations results in an expression for $\boldsymbol{R}$ of the form:

$$\boldsymbol{R} = \boldsymbol{I} + \boldsymbol{r}_s \times \boldsymbol{I} + \frac{1}{2\cos\frac{\phi}{2}} \boldsymbol{r}_s \times \boldsymbol{r}_s \times \boldsymbol{I}. \tag{A.7}$$

Substitution of $\boldsymbol{r}_t = 2\tan(\phi/2)\boldsymbol{e}$ into Eq. (A.3) and again using the half angle relations yield an expression for $\boldsymbol{R}$ which is:

$$\boldsymbol{R} = \boldsymbol{I} + \frac{1}{1 + \frac{1}{4}\boldsymbol{r}_t \cdot \boldsymbol{r}_t} \boldsymbol{r}_t \times (\boldsymbol{I} + \tfrac{1}{2}\boldsymbol{r}_t \times \boldsymbol{I}). \tag{A.8}$$

These two forms and the form of Eq. (A.3) are the most common finite rotation vectors. The following properties of the rotation tensor are well known and easily verified.

$$\boldsymbol{R}^t \cdot \boldsymbol{R} = \boldsymbol{R} \cdot \boldsymbol{R}^t = \boldsymbol{I}, \quad \det \boldsymbol{R} = 1, \quad \det(\boldsymbol{R} - \boldsymbol{I}) = 0. \tag{A.9}$$

The last of these properties shows that the rotation tensor has one real unit eigenvalue, where the corresponding eigenvector is the axis of rotation. Differentiation of Eq. (A.9) with respect to time yields:

$$\dot{\boldsymbol{R}} \cdot \boldsymbol{R}^t = -\boldsymbol{R} \cdot \dot{\boldsymbol{R}}^t. \tag{A.10}$$

This skew symmetric tensor may be represented by a spin vector $\boldsymbol{\omega}$ defined by:

$$\boldsymbol{\omega} \times \boldsymbol{I} = \dot{\boldsymbol{R}} \cdot \boldsymbol{R}^t. \tag{A.11}$$

The spin, or angular velocity, vector $\boldsymbol{\omega}$ is not the rate of the rotation vector $\dot{\boldsymbol{r}}$, but is related to $\dot{\boldsymbol{r}}$ through the tensor $\boldsymbol{\Gamma}$, which itself depends on $\boldsymbol{r}$, i.e. $\boldsymbol{\omega} = \boldsymbol{\Gamma}(\boldsymbol{r})\dot{\boldsymbol{r}}$. Since this relationship is essential for constructing the tangent matrices in Appendix B, its derivation is briefly sketched out here. From Eq. (A.2) it is clear that $\boldsymbol{R}^t$ is:

$$\boldsymbol{R}^t = \boldsymbol{I} - \sin\phi(\boldsymbol{e} \times \boldsymbol{I}) + (1 - \cos\phi)\boldsymbol{e} \times \boldsymbol{e} \times \boldsymbol{I} \tag{A.12}$$

and that $\dot{\boldsymbol{R}}$ may be written as:

$$\dot{\boldsymbol{R}} = \cos\phi\dot{\phi}(\boldsymbol{e} \times \boldsymbol{I}) + \sin\phi(\dot{\boldsymbol{e}} \times \boldsymbol{I}) + \sin\phi\dot{\phi}(\boldsymbol{e} \times \boldsymbol{e} \times \boldsymbol{I}) + (1 - \cos\phi)(\dot{\boldsymbol{e}} \times \boldsymbol{e} \times \boldsymbol{I} + \boldsymbol{e} \times \dot{\boldsymbol{e}} \times \boldsymbol{I}). \tag{A.13}$$

Substituting Eq. (A.12) and Eq. (A.13) into Eq. (A.11) and making use of the fact that $\dot{\boldsymbol{e}} \cdot \boldsymbol{e} = 0$, and $\boldsymbol{e} \times \dot{\boldsymbol{e}} \times \boldsymbol{e} \times \boldsymbol{I} = 0$, results in:

$$\boldsymbol{\omega} \times \boldsymbol{I} = \dot{\phi}(\boldsymbol{e} \times \boldsymbol{I}) + \sin\phi(\dot{\boldsymbol{e}} \times \boldsymbol{I}) + (1 - \cos\phi)(\boldsymbol{e} \times \dot{\boldsymbol{e}} \times \boldsymbol{I}). \tag{A.14}$$

With the use of the definition of $\boldsymbol{r}$, this expression may be written as:

$$\boldsymbol{\omega} \times \boldsymbol{I} = \left[\dot{\boldsymbol{r}} + \frac{1 - \cos\phi}{\phi^2}(\boldsymbol{r} \times \dot{\boldsymbol{r}}) + \frac{1}{\phi^2}\left(1 - \frac{\sin\phi}{\phi}\right)(\boldsymbol{r} \times \boldsymbol{r} \times \dot{\boldsymbol{r}}) \right] \times \boldsymbol{I}. \tag{A.15}$$

Then:

$$\boldsymbol{\omega} = \left[\boldsymbol{I} + \frac{1 - \cos\phi}{\phi^2}(\boldsymbol{r} \times \boldsymbol{I}) + \frac{1}{\phi^2}\left(1 - \frac{\sin\phi}{\phi}\right)(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}) \right] \cdot \dot{\boldsymbol{r}}. \tag{A.16}$$

This leads directly to the definition of $\boldsymbol{\Gamma}$.

$$\begin{aligned} \boldsymbol{\Gamma}(\boldsymbol{r}) &= \left[\boldsymbol{I} + \frac{1 - \cos\phi}{\phi^2}(\boldsymbol{r} \times \boldsymbol{I}) + \frac{1}{\phi^2}\left(1 - \frac{\sin\phi}{\phi}\right)(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}) \right] \\ &= \boldsymbol{I} + \sum_{k=1}^{\infty} \frac{(\boldsymbol{r} \times \boldsymbol{I})^k}{(k+1)!}. \end{aligned} \tag{A.17}$$

Clearly the above argument, which establish the relationship between $\boldsymbol{\omega}$ and $\dot{\boldsymbol{r}}$, are equally valid for the virtual rotations $\boldsymbol{\theta}_\delta$ and $\delta \boldsymbol{r}$, where:

$$\boldsymbol{\theta}_\delta \times \boldsymbol{I} = \delta \boldsymbol{R} \cdot \boldsymbol{R}^t \tag{A.18}$$

and we may write:

$$\boldsymbol{\theta}_\delta = \boldsymbol{\Gamma}(r) \cdot \delta \boldsymbol{r}. \tag{A.19}$$

Starting with the expression for $\boldsymbol{\Gamma}$ in Eq. (A.17) it is staightforward to verify that:

$$\boldsymbol{\Gamma}^t = \boldsymbol{I} - a_1(\boldsymbol{r} \times \boldsymbol{I}) + b_1(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}) \tag{A.20}$$

$$\boldsymbol{\Gamma}^{-1} = \boldsymbol{I} - \frac{1}{2}(\boldsymbol{r} \times \boldsymbol{I}) + \frac{1}{\phi^2}\left(1 - \frac{a_o}{2b_1}\right)(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}) \tag{A.21}$$

$$\boldsymbol{\Gamma}^{-t} = \boldsymbol{I} - \frac{1}{2}(\boldsymbol{r} = \boldsymbol{I}) + \frac{1}{\phi^2}\left(1 - \frac{a_o}{2b_1}\right)(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}), \tag{A.22}$$

where:

$$a_o = \frac{\sin\phi}{\phi}, \quad a_1 = \frac{1-\cos\phi}{\phi^2}, \quad b_1 = \frac{1}{\phi^2}(1 - a_o). \tag{A.23}$$

Further, the tensors $\boldsymbol{\Gamma}$ and $\boldsymbol{R}$ are related by:

$$\boldsymbol{R} = \boldsymbol{\Gamma}^{-t} \cdot \boldsymbol{\Gamma} = \boldsymbol{\Gamma} \cdot \boldsymbol{\Gamma}^{-t}, \tag{A.24}$$

and

$$\boldsymbol{\Gamma}^{-t} - \boldsymbol{\Gamma}^{-1} = \boldsymbol{r} \times \boldsymbol{I}. \tag{A.25}$$

Then multiplying Eq. (A.25) by $\boldsymbol{\Gamma}$ and taking Eq. (A.24) into account leads to:

$$\boldsymbol{R} = \boldsymbol{I} + \boldsymbol{\Gamma} \cdot \boldsymbol{r} \times \boldsymbol{I} = \boldsymbol{I} + \boldsymbol{r} \times \boldsymbol{\Gamma}. \tag{A.26}$$

It is important to recognize that $\boldsymbol{\Gamma}$ is singular for certain values of ϕ. From the general expresion for the determinant of a 3×3 matrix it is seen that:

$$\operatorname{der} \boldsymbol{\Gamma} = \tfrac{1}{3} \operatorname{tr} \boldsymbol{\Gamma}^3 - \tfrac{1}{2} \operatorname{tr} \boldsymbol{\Gamma}^2 \cdot \operatorname{tr} \boldsymbol{\Gamma} - \tfrac{1}{6}(\operatorname{tr} \boldsymbol{\Gamma})^3. \tag{A.27}$$

Then, considering Eq. (A.17), the determinant is:

$$\det \boldsymbol{\Gamma}(\boldsymbol{r}) = \frac{2(1-\cos\phi)}{\phi^2}. \tag{A.28}$$

Clearly, $\boldsymbol{\Gamma}$ is singular when $\phi = 2n\pi \; n = 1, 2, 3, \ldots$, but is not singular for $\phi = 0$. In order to avoid this problem of singularity an incremental approach is adopted. A more general rescaling process may also be used to avoid this singularity and it is briefly shown here; see also Geradin and Cardona (1989).

Let:

$$\boldsymbol{r}_p = \boldsymbol{r} - 2n\pi \boldsymbol{e} \quad n = int\left(\frac{\phi}{2\pi}\right), \tag{A.29}$$

and

$$\phi_p = \boldsymbol{e} \cdot \boldsymbol{r}_p = \phi - 2n\pi. \tag{A.34}$$

Then from Eq. (A.29):

$$\boldsymbol{\theta}_\delta = \boldsymbol{\Gamma}(\boldsymbol{r}) \cdot \delta \boldsymbol{r} = \boldsymbol{\Gamma}(\boldsymbol{r}_p) \cdot \delta \boldsymbol{r}_p, \tag{A.31}$$

This equation and the Eq. (A.29) constitute the rescaling process. Proving Eq. (A.31) is easy since from Eq. (A.29):

$$\delta \boldsymbol{r}_p = \delta \boldsymbol{r} - 2n\pi \delta \boldsymbol{e} \tag{A.32}$$

and since $\boldsymbol{e} = \boldsymbol{r}/\phi$:

$$\delta \boldsymbol{e} = \frac{\boldsymbol{I} - \boldsymbol{e}\cdot\boldsymbol{e}^t}{\phi}\delta \boldsymbol{r} = -\frac{\boldsymbol{e} \times \boldsymbol{e} \times \delta \boldsymbol{r}}{\phi}. \tag{A.33}$$

Substituting back into Eq. (A.32) yields:

$$\delta \boldsymbol{r}_p = \left[\boldsymbol{I} + \frac{2n\pi}{\phi}(\boldsymbol{e} \times \boldsymbol{I})\cdot(\boldsymbol{e} \times \boldsymbol{I}) \right]\cdot \delta \boldsymbol{r}. \tag{A.34}$$

Further, since:

$$\boldsymbol{\Gamma}(\boldsymbol{r}_p)\cdot\left[\boldsymbol{I} + \frac{2n\pi}{\phi}(\boldsymbol{e} \times \boldsymbol{I})\cdot(\boldsymbol{e} \times \boldsymbol{I}) \right] = \boldsymbol{\Gamma}(\boldsymbol{r}) \tag{A.35}$$

from Eq. (A.34) and Eq. (A.35) it is seen that:

$$\boldsymbol{\Gamma}(\boldsymbol{r}_p)\cdot \delta \boldsymbol{r}_p = \boldsymbol{\Gamma}(\boldsymbol{r})\cdot \delta \boldsymbol{r} \tag{A.36}$$

which proves Eq. (A.31).

A.2 Properties of the tangent map

In this section, some identities associated with the tangent map of rotation are presented. These will be necessary in the development of expressions for the tangent matrices in Appendix B.

In the space of the rotations $\boldsymbol{r}$, consider two arbitrary infinitesimal variations $\delta \boldsymbol{r}$ and $\mathrm{d}\boldsymbol{r}$ and let $\delta \boldsymbol{R}$ and $\mathrm{d}\boldsymbol{R}$ be the associated variations on $\boldsymbol{R}$. The corresponding virtual rotation vectors $\boldsymbol{\theta}_\delta$ and $\boldsymbol{\theta}_\mathrm{d}$ are, respectively defined through:

$$\boldsymbol{\theta}_\delta \times \boldsymbol{I} = \delta \boldsymbol{R}\cdot\boldsymbol{R}^t \quad \text{and} \quad \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{I} = \mathrm{d}\boldsymbol{R}\cdot\boldsymbol{R}^t. \tag{A.37}$$

As shown in the preceding section, $\boldsymbol{\theta}_\delta$ and $\boldsymbol{\theta}_\mathrm{d}$ are related to $\delta \boldsymbol{r}$ and $\mathrm{d}\boldsymbol{r}$ by:

$$\boldsymbol{\theta}_\delta = \boldsymbol{\Gamma}(\boldsymbol{r})\cdot \delta \boldsymbol{r} \quad \boldsymbol{\theta}_\mathrm{d} = \boldsymbol{\Gamma}(\boldsymbol{r})\cdot \mathrm{d}\boldsymbol{r}. \tag{A.38}$$

Using the fact that $\mathrm{d}\delta \boldsymbol{R} = \delta \mathrm{d}\boldsymbol{R}$ and considering Eq. (A.37) leads to:

$$\mathrm{d}\delta \boldsymbol{R} = \mathrm{d}\boldsymbol{\theta}_\delta \times \boldsymbol{R} + \boldsymbol{\theta}_\delta \times \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{R}, \quad \delta \mathrm{d}\boldsymbol{R} = \delta \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{R} + \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{\theta}_\delta \times \boldsymbol{R}. \tag{A.39}$$

Post-multiplication of Eq. (A.39) by $\boldsymbol{R}^t$ yields:

$$\mathrm{d}\boldsymbol{\theta}_\delta \times \boldsymbol{I} - \delta \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{I} + \boldsymbol{\theta}_\delta \times \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{I} - \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{\theta}_\delta \times \boldsymbol{I} = 0 \tag{A.40}$$

from which:

$$\mathrm{d}\boldsymbol{\theta}_\delta = \delta \boldsymbol{\theta}_\mathrm{d} + \boldsymbol{\theta}_\mathrm{d} \times \boldsymbol{\theta}_\delta. \tag{A.41}$$

This result indicates that, in general $\mathrm{d}\boldsymbol{\theta}_\delta \neq \delta \boldsymbol{\theta}_\mathrm{d}$ (i.e. when $\boldsymbol{\theta}_\mathrm{d}$ and $\boldsymbol{\theta}_\delta$ are not parallel), which is a direct consequence of the noncommutative nature of sequential rotations.

In order to better understand implications for this result consider the vectors:

$$\boldsymbol{h}_k = \boldsymbol{\Gamma}(\boldsymbol{r})\cdot \boldsymbol{e}_k. \tag{A.42}$$

Since in general $\det \boldsymbol{\Gamma}(\boldsymbol{r}) \neq 1$, the three vectors $\boldsymbol{h}_k$ are not orthogonal. Now representing $\boldsymbol{r} = r^k \boldsymbol{e}_k$, from Eq. (A.41):

$$\frac{\partial \boldsymbol{h}_k}{\partial r^i} - \frac{\partial \boldsymbol{h}_i}{\partial r^k} = \boldsymbol{h}_i \times \boldsymbol{h}_k. \tag{A.43}$$

This clearly shows that the matrix $\boldsymbol{\Gamma}$ cannot be understood as a deformation gradient or as the Jacobian of any coordinate transformation. Therefore the virtual rotation $\boldsymbol{\theta}_\delta$ can not be expressed as a variation of any coordinate, i.e. it is not an exact differential. In the same way, the integral of the angular velocity is path dependent.

Equation (A.41) is very general, in fact if $\boldsymbol{\theta}_d$ is just the infinitesimal rotation associated with the angular velocity $\boldsymbol{\omega}$ acting over the time interval dt, then $\boldsymbol{\theta}_d = \boldsymbol{\omega}\mathrm{d}t$, and:

$$\frac{\mathrm{d}\boldsymbol{\theta}_\delta}{\mathrm{d}t} = \delta\boldsymbol{\omega} + \boldsymbol{\omega} \times \boldsymbol{\theta}_\delta = \delta\boldsymbol{\omega} - \boldsymbol{\theta}_\delta \times \boldsymbol{\omega} = \delta^o\boldsymbol{\omega} \tag{A.44}$$

which shows that the absolute time derivative of the virtual rotation coincides with the corotational variation of the angular velocity. In the same way if the cross product term in Eq. (A.44) is moved to the left hand side, it is recognized that the corotational time derivative of the virtual rotation coincides with the absolute variation of the angular velocity, i.e.:

$$\frac{\mathrm{d}^o\boldsymbol{\theta}_\delta}{\mathrm{d}t} = \frac{\mathrm{d}\boldsymbol{\theta}_\delta}{\mathrm{d}t} - \boldsymbol{\omega}\boldsymbol{\theta}_\delta = \delta\boldsymbol{\omega}. \tag{A.45}$$

In order to cast this result in a form which will be useful in Appendix B, consider the application of $\mathrm{d}\boldsymbol{\theta}_\delta$ to an arbitrary vector $\boldsymbol{b}$.

$$\mathrm{d}\boldsymbol{\theta}_\delta \cdot \boldsymbol{b} = \delta\boldsymbol{r} \cdot \mathrm{d}\boldsymbol{\Gamma}^t(\boldsymbol{r}) \cdot \boldsymbol{b} = \delta\boldsymbol{r} \cdot \mathbf{H}(\boldsymbol{r}, \boldsymbol{b}) \cdot \mathrm{d}\boldsymbol{r} \tag{A.46}$$

where $\mathbf{H}(\boldsymbol{r}, \boldsymbol{b})$ depends linearly on $\boldsymbol{b}$ and is obtained by taking a variation of $\boldsymbol{\Gamma}^t$. The development of this expression is straightforward and it may be verified that:

$$\mathbf{H}(\boldsymbol{r}, \boldsymbol{b}) = -a_1 \boldsymbol{b} \times \boldsymbol{I} + b_1[(\boldsymbol{b} \times \boldsymbol{r}) \times \boldsymbol{I} + \boldsymbol{b} \times \boldsymbol{r} \times \boldsymbol{I}] + c_1 \boldsymbol{b} \times \boldsymbol{r} \cdot \boldsymbol{r}^t - d_1(\boldsymbol{b} \times \boldsymbol{r}) \times \boldsymbol{r} \cdot \boldsymbol{r}^t. \tag{A.47}$$

The constants, a_1 and b_1 are defined in the preceding section, and are repeated here along with there variations c_1 and d_1, respectively:

$$a_1 = \frac{1 - \cos\phi}{\phi^2} \qquad c_1 = \frac{1}{\phi^2}\left(\frac{\sin\phi}{\phi} - \frac{2(1 - \cos \mathrm{Y})}{\phi^2}\right)$$
$$b_1 = \frac{1}{\phi^2}\left(1 - \frac{\sin\phi}{\phi}\right) \quad d_1 = \frac{1}{\phi^2}\left[\frac{1 - \cos\phi}{\phi^2} - \frac{3}{\phi^2}\left(1 - \frac{\sin\phi}{\phi}\right)\right]. \tag{A.48}$$

As a consequence of Eq. (A.41), $\mathbf{H}$ is not symmetric.

$$\mathbf{H}(\boldsymbol{r}, \boldsymbol{b}) = \mathbf{H}^t(\boldsymbol{r}, \boldsymbol{b}) + \boldsymbol{\Gamma}^t(\boldsymbol{r}) \cdot \boldsymbol{b} \times \boldsymbol{\Gamma}(\boldsymbol{r}). \tag{A.49}$$

Moreover, since $\boldsymbol{\Gamma}^t(\boldsymbol{r}) \cdot \boldsymbol{b} \times \boldsymbol{\Gamma}(\boldsymbol{r}) = \det \boldsymbol{\Gamma}(\boldsymbol{r}) \cdot (\boldsymbol{\Gamma}^{-1}(\boldsymbol{r}) \cdot \boldsymbol{b}) \times \boldsymbol{I}$ it is easily seen that $\mathbf{H}(\boldsymbol{r}, \boldsymbol{b})$ will not be symmetric for any choice of rotation parameters.

The corotational increment of the virtual rotation follows from Eq. (A.45), multiplying by the time increment dt:

$$\mathrm{d}^o\boldsymbol{\theta}_\delta = \mathrm{d}\boldsymbol{\theta}_\delta - \boldsymbol{\theta}_d \times \boldsymbol{\theta}_\delta = \delta\boldsymbol{\theta}_d. \tag{A.50}$$

From this equation and Eq. (A.46) it follows that:

$$\mathrm{d}^o\boldsymbol{\theta}_\delta \cdot \boldsymbol{b} = \delta\boldsymbol{r} \cdot \mathbf{H}^t(\boldsymbol{r}, \boldsymbol{b}) \cdot \mathrm{d}\boldsymbol{r}. \tag{A.51}$$

As will be shown later, the development of the tangent matrix for the symmetric primal form, requires an expression for $(\mathrm{d}/\mathrm{d}t)\mathbf{H}(\boldsymbol{r}, \mathbf{b})$. Similarly in developing the tangent matrix for the symmetric mixed form, expressions for $\delta\boldsymbol{\Gamma}^{-1}$ and $\mathrm{d}\delta\boldsymbol{\Gamma}^{-1}$ are needed. Two other expressions which will also be needed are, $\dot{\boldsymbol{\Gamma}}$ and $\dot{\boldsymbol{\Gamma}}^{-1}$. These can be easily computed recognizing that:

$$\dot{a}_1 = c_1\dot{\phi} \quad \dot{b}_1 = d_1\phi\dot{\phi} \quad \dot{c}_1 = \tfrac{1}{\phi}(b_1 - a_1 - 4c_1)\dot{\phi} \quad \dot{d}_1 = \tfrac{1}{\phi}(c_1 - 5d_1)\dot{\phi} \tag{A.52}$$

and $\phi\dot{\phi} = \boldsymbol{r} \cdot \dot{\boldsymbol{r}}$. Then the time derivative of $\boldsymbol{\Gamma}$ is:

$$\dot{\boldsymbol{\Gamma}} = \dot{a}_1(\boldsymbol{r} \times \boldsymbol{I}) + \dot{\boldsymbol{b}}_1(\boldsymbol{r} \times \boldsymbol{r} \times \boldsymbol{I}) + a_1(\dot{\boldsymbol{r}} \times \boldsymbol{I}) + b_1(\dot{\boldsymbol{r}} \times \boldsymbol{r} \times \boldsymbol{I} + \boldsymbol{r} \times \dot{\boldsymbol{r}} \times \boldsymbol{I}). \tag{A.53}$$

The expression for $\dot{\boldsymbol{\Gamma}}^{-1}$ is then:

$$\dot{\boldsymbol{\Gamma}}^{-1} = \frac{1 - 2a_1}{\phi^3(2a_1)}\dot{\phi}(\boldsymbol{r} \times \boldsymbol{I}) \cdot (\boldsymbol{r} \times \boldsymbol{I}) - \frac{1}{2}(\dot{\boldsymbol{r}} \times \boldsymbol{I}) + \frac{1}{\phi^2}\left(1 - \frac{a_o}{2b_1}\right)(\dot{\boldsymbol{r}} \times \boldsymbol{r} \times \boldsymbol{I} + \boldsymbol{r} \times \dot{\boldsymbol{r}} \times \boldsymbol{I}). \tag{A.54}$$

Since in each of Eq. (A.53) and Eq. (A.54) the time derivatives may be replaced by variations, $\delta\boldsymbol{\Gamma}^{-1}$ operating on an arbitrary vector $\boldsymbol{b}$ may be written as:

$$\delta\boldsymbol{\Gamma}^{-1}\cdot\boldsymbol{b} = \mathbf{K}(\boldsymbol{r},\boldsymbol{b})\cdot\delta\boldsymbol{r} \tag{A.55}$$

where:

$$\mathbf{K}(\boldsymbol{r},\boldsymbol{b}) = \tfrac{1}{2}\boldsymbol{b}\times\boldsymbol{I} + a_2[(\boldsymbol{b}\times\boldsymbol{r})\times\boldsymbol{I} - \boldsymbol{r}\times\boldsymbol{b}\times\boldsymbol{I}] + b_2(\boldsymbol{r}\times\boldsymbol{b}\times\boldsymbol{r})\cdot\boldsymbol{r}^t \tag{A.56}$$

where ϕ is the magnitude of $\boldsymbol{r}$, and:

$$a_2 = \frac{1}{\phi^2}\left(1 - \frac{\dfrac{\sin\phi}{\phi}}{\dfrac{2(1-\cos\phi}{\phi}}\right) = \frac{1}{\phi^2}\left(1 - \frac{a_o}{2b_o}\right)$$

$$b_2 = \frac{1}{\phi^4}\left(2 - \frac{1+a_o}{2b_o}\right). \tag{A.57}$$

Finally, taking the variation of Eq. (A.54) we can write the expression for $\mathrm{d}\delta\boldsymbol{\Gamma}^{-1}$ acting on two arbitrary vectors $\boldsymbol{b}$ and $\boldsymbol{c}$ as:

$$\boldsymbol{c}\cdot\mathrm{d}\delta\boldsymbol{\Gamma}^{-1}\cdot\boldsymbol{b} = \mathrm{d}\boldsymbol{r}\cdot\mathbf{L}(\boldsymbol{c},\boldsymbol{r},\boldsymbol{b})\cdot\delta\boldsymbol{r}, \tag{A.58}$$

where:

$$\mathbf{L}(\boldsymbol{c},\boldsymbol{r},\boldsymbol{b}) = a_2\mathbf{L}_a + b_2\mathbf{L}_b + c_2\mathbf{L}_c, \tag{A.59}$$

and

$$c_2 = \left(6 - \frac{1+a_o}{b_o} - \frac{a_o}{2b_o^2}\right),$$

$$\mathbf{L}_a = \boldsymbol{c}\times\boldsymbol{b}\times\boldsymbol{I} + \boldsymbol{b}\times\boldsymbol{c}\times\boldsymbol{I},$$

$$\mathbf{L}_b = \mathbf{L}_a\cdot\boldsymbol{r}\cdot\boldsymbol{r}^t + \boldsymbol{r}\cdot\boldsymbol{r}^t\cdot\mathbf{L}_a^t + \frac{\boldsymbol{r}\cdot\mathbf{L}_a\cdot\boldsymbol{r}}{\phi^2}\cdot(\boldsymbol{r}\times\boldsymbol{r}\times\boldsymbol{I}),$$

$$\mathbf{L}_c = (\boldsymbol{r}\cdot\mathbf{L}_a\cdot\boldsymbol{r})\cdot\boldsymbol{r}\cdot\boldsymbol{r}^t. \tag{A.60}$$

The complexity of these relations increases the computations required to calculate symmetric tangent matrices, to no apparent advantage for initial value problems. However, if the symmetry of the tangent matrices can be exploited, the effort required to calculate **H** and **J** or **K** and **L** may lead to significant savings in the solution process.

Appendix B – tangent matrices

In this appendix the expressions for the tangent maps of the various variational principles are obtained. In the following paragraphs several notations are introduced, involving very sparse matrices. While the notation makes the discussion simpler, this sparsity must be recognized and taken into account in the programming of the residual vectors and tangent matrices.

B.1 Primal form – unsymmetric approach

The first form considered is the unsymmetric, primal formulation. In this case the variational statement is given by Eq. (3.48), which is repeated here for convenience:

$$\int_{t_1}^{t_2}\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{\boldsymbol{q}},\delta\hat{\boldsymbol{q}}\right)\cdot(\hat{\boldsymbol{p}},(\hat{\boldsymbol{f}} - \boldsymbol{S}_1(\boldsymbol{w})\cdot\hat{\boldsymbol{p}}))\mathrm{d}t = \delta\hat{\boldsymbol{q}}\cdot\hat{\boldsymbol{p}}_b|_{t_1}^{t_2} \tag{B.1}$$

where $\hat{p} = M_6 \cdot w$. The linearized form reads:

$$\int_{t_1}^{t_2} \left(\frac{d}{dt} \delta\hat{q}, \delta\hat{q} \right) \cdot \hat{\mathscr{T}}_p \cdot \left(\frac{d}{dt} dq, dq \right) dt = \delta\hat{q} \cdot \hat{p}_b |_{t_1}^{t_2} - \int_{t_1}^{t_2} \left(\frac{d}{dt} \delta\hat{q}, \delta\hat{q} \right) \cdot \hat{\mathscr{R}}_p dt \tag{B.2}$$

where $\hat{\mathscr{T}}_p$ and $\hat{\mathscr{R}}_p$ are respectively the tangent matrix and the residual vector for the unsymmetric primal approach. The hat indicates that the variational statement employs the test functions $(d/dt)\delta\hat{q}$ and $\delta\hat{q}$, and the subscript p indicates a primal formulation. Then, directly:

$$\hat{\mathscr{R}}_p = (\hat{p}, \hat{f} - S_1(w) \cdot \hat{p}). \tag{B.3}$$

Separating the contributions due to kinetic energy and external loads, leads to, $\hat{\mathscr{R}}_{pk} = (\hat{p}, -S_1(w) \cdot \hat{p})$ and $\hat{\mathscr{R}}_{pe} = (0, \hat{f})$. Similarly, let $\hat{\mathscr{T}}_p = \hat{\mathscr{T}}_{pk} + \hat{\mathscr{T}}_{pe}$. The derivation of the tangent matrix is considerably simplified if use is made of the relation, $((d/dt)\,d\hat{q}, d\hat{q}) = \mathbf{Y} \cdot ((d/dt)dq, dq)$, where $\mathbf{Y}$ is:

$$\mathbf{Y} = \begin{bmatrix} \mathbf{X} & \dot{\mathbf{X}} \\ 0 & \mathbf{X} \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} I & 0 \\ 0 & \Gamma \end{bmatrix}. \tag{B.4}$$

Then, $\hat{\mathscr{T}}_{pk} = \tilde{\mathscr{T}}_{pk} \cdot \mathbf{Y}$, and:

$$\tilde{\mathscr{T}}_{pk} = \begin{bmatrix} M_6 & (S_2(\hat{p}) - S_1(w) \cdot M_6)^t \\ S_1(\hat{p}) - S_1(w) \cdot M_6 & -S_1(w) \cdot (S_2(\hat{p}) - S_1(w) \cdot M_6)^t \end{bmatrix} \tag{B.5}$$

$$\hat{\mathscr{T}}_{pe} = \begin{bmatrix} 0 & 0 \\ \dfrac{\partial \hat{f}}{\partial \dot{q}} & \dfrac{\partial \hat{f}}{\partial q} \end{bmatrix}. \tag{B.6}$$

where:

$$S_1(\hat{p}) = \begin{bmatrix} 0 & 0 \\ l \times I & 0 \end{bmatrix}, \quad S_2(\hat{p}) = \begin{bmatrix} 0 & 0 \\ l \times I & h \times I \end{bmatrix}. \tag{B.7}$$

For a general six dimensional vector $z = (z_L, z_A)$ the linear operators $S_1(z)$ and $S_2(z)$ are defined as:

$$S_1(z) = \begin{bmatrix} 0 & 0 \\ z_L \times I & 0 \end{bmatrix}, \quad S_2(z) = \begin{bmatrix} 0 & 0 \\ z_L \times I & z_A \times I \end{bmatrix}. \tag{B.8}$$

For the following discussion it is useful to also define S_3 as: $S_2(\cdot) - S_1(\cdot)$.

By inspection of Eq. (B.5) it is clear that even referring to the center of gravity the tangent matrix is greatly simplified, since M_6 is block diagonal and $S_1(\hat{p}) - S_1(w) \cdot M_6 = 0$. Even with this simplification, however, the tangent matrix is not symmetric.

B.2 Primal form – symmetric approach

Next, consider the symmetric primal form,

$$\int_{t_1}^{t_2} [\delta T(\dot{q}, q, t) + \delta q \cdot f] dt = \delta q \cdot p_b |_{t_1}^{t_2}. \tag{B.9}$$

Which in linearized form may be written as:

$$\int_{t_1}^{t_2} \left(\frac{d}{dt} \delta q, \delta q \right) \cdot \mathscr{T}_p \cdot \left(\frac{d}{dt} dq, dq \right) dt = \delta q \cdot p_b |_{t_1}^{t_2} - \int_{t_1}^{t_2} \left(\frac{d}{dt} \delta q, \delta q \right) \cdot \mathscr{R}_p dt. \tag{B.10}$$

Again the residual vector and the tangent matrix may be thought of as begin composed of contributions from the kinetic energy and external forces.

$$\mathscr{R}_p = \mathscr{R}_{pk} + \mathscr{R}_{pe}, \quad \mathscr{T}_p = \mathscr{T}_{pk} + \mathscr{T}_{pe}. \tag{B.11}$$

Obviously $\mathscr{R}_{pk} = \left(\frac{\partial T}{\partial \dot{q}}, \frac{\partial T}{\partial q}\right)$, $\mathscr{R}_{pe} = (0, f)$ and:

$$\mathscr{T}_{pk} = \begin{bmatrix} \frac{\partial^2 T}{\partial \dot{q}^2} & \frac{\partial^2 T}{\partial \dot{q}\partial q} \\ \frac{\partial^2 T}{\partial \dot{q}\partial q} & \frac{\partial^2 T}{\partial q^2} \end{bmatrix}, \qquad \mathscr{T}_{pe} = \begin{bmatrix} 0 & 0 \\ \frac{\partial f}{\partial \dot{q}} & \frac{\partial f}{\partial q} \end{bmatrix}. \tag{B.12, 13}$$

Working in this way, $\mathscr{T}_{pk}$ is found to be symmetric.

Performing these derivatives is not a simple matter. However, the expression for $\mathscr{T}_{pk}$ may be obtained from $\tilde{\mathscr{T}}_{pk}$ and $\hat{\mathscr{R}}_{pk}$ which have already been presented. In fact:

$$\mathrm{d}\delta T = \left(\frac{\mathrm{d}}{\mathrm{d}t}\delta q, \delta q\right). \quad \mathscr{T}_{pk}\cdot\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}q, \mathrm{d}q\right) \tag{B.14}$$

which must also be given by:

$$\mathrm{d}\delta T = \left(\frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{q}, \delta\hat{q}\right)\cdot\tilde{\mathscr{T}}_{pk}\cdot\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}\hat{q}, \mathrm{d}\hat{q}\right) + d\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta\hat{q}, \delta\hat{q}\right).\hat{\mathscr{R}}_{pk}. \tag{B.15}$$

Comparison of the last two expressions leads to:

$$\mathscr{T}_{pk} = \mathbf{Y}^t\cdot\tilde{\mathscr{T}}_{pk}\cdot\mathbf{Y} + \left(\frac{\partial(\mathbf{Y}^t\cdot\hat{\mathscr{R}}_{pk})}{\partial\dot{q}}, \frac{\partial(\mathbf{Y}^t\cdot\hat{\mathscr{R}}_{pk})}{\partial q}\right) \tag{B.16}$$

where $\hat{\mathscr{R}}_{pk}$ is held constant and is equal to the value corresponding to the given state.

Recalling the definition of the map $\mathbf{H}(r, b) = \frac{\partial \boldsymbol{\Gamma}^t\cdot b}{\partial r}$ for an arbitrary constant vector b and defining, $\mathbf{J}(\dot{r}, r, b) = \frac{\partial \dot{\boldsymbol{\Gamma}}^t\cdot b}{\partial r}$, the last term in Eq. (B.16) may be expressed as:

$$\left(\frac{\partial(\mathbf{Y}^t\cdot\hat{\mathscr{R}}_{pk})}{\partial\dot{q}}, \frac{\partial(\mathbf{Y}^t\cdot\hat{\mathscr{R}}_{pk})}{\partial q}\right) = \begin{bmatrix} 0 & \mathbf{H}_6(q, \hat{p}) \\ \mathbf{H}_6(q, \hat{p}) & \mathbf{J}_6(\dot{q}, q, \hat{p}) + \mathbf{H}_6(q, -S_1(w)\cdot\hat{p}) \end{bmatrix}. \tag{B.17}$$

Whereas the operators $\mathbf{H}_6$ and $\mathbf{J}_6$ applied to a general six component vector $z = (z_L, z_A)$ are defined as:

$$\mathbf{H}_6(q, z) = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{H}(r, z_A) \end{bmatrix}, \quad \mathbf{J}_6(\dot{q}, q, z) = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{J}(\dot{r}, r, z_A) \end{bmatrix}. \tag{B.18}$$

The map $\mathbf{J}(\dot{r}, r, b)$ is obtained by taking the time derivative of $\mathbf{H}(r, b)$, while considering b constant. Making use of Eq. (A.48) leads to:

$$\mathbf{J}(\dot{r}, r, b) = \mathbf{J}'(\dot{r}, r, b) + \boldsymbol{\Gamma}^t\cdot b \times \dot{\boldsymbol{\Gamma}} + \dot{\boldsymbol{\Gamma}}^t\cdot b \times \boldsymbol{\Gamma}. \tag{B.19}$$

Taking these properties into account, the symmetry of $\mathscr{T}_{pk}$ can be easily demonstrated.

B.3 Mixed form – unsymmetric approach

In linearizing the unsymmetric mixed formulation, it is convenient to rewrite Eq. (3.40) as:

$$\int_{t_1}^{t_2}\left[\frac{\mathrm{d}}{\mathrm{d}t}(\delta^* p, \delta\hat{q})\cdot\mathbf{I}_S\cdot(\hat{p}, q) + (\delta^* p, \delta\hat{q})\cdot(\mathbf{X}^{-1}\cdot(w_n - \hat{w}), \hat{f} + S_1(\hat{p})\cdot\hat{w})\right]\mathrm{d}t = (\delta^* p, \delta\hat{q})\cdot\mathbf{I}_S\cdot(p_b, q_b)|_{t_1}^{t_2} \tag{B.20}$$

where $\hat{w} = M_6^{-1}\cdot\hat{p}$. The linearization of Eq. (B.20) leads to:

$$\int_{t_1}^{t_2}\left[\frac{\mathrm{d}}{\mathrm{d}t}(\delta^* p, \delta\hat{q})\cdot\mathbf{I}_S\cdot(\mathrm{d}\hat{p}, \mathrm{d}q) + (\delta^* p, \delta\hat{q})\cdot\hat{\mathscr{T}}_m\cdot(\mathrm{d}\hat{p}, \mathrm{d}\hat{q})\right]\mathrm{d}t$$
$$= (\delta^* p, \delta\hat{q})\cdot\mathbf{I}_S\cdot(\hat{p}_b, q_b)|_{t_1}^{t_2} - \int_{t_1}^{t_2}\left[\frac{\mathrm{d}}{\mathrm{d}t}(\delta^* p, \delta\hat{q})\cdot\mathbf{I}_S\cdot(\hat{p}_g, q_g) + (\delta^* p, \delta\hat{q})\cdot\hat{\mathscr{R}}_m\right]\mathrm{d}t \tag{B.21}$$

where:

$$\hat{\mathscr{R}}_m = (\mathbf{X}^{-1}\cdot(w_n - \hat{w}), \hat{f} + S_1(\hat{p})\cdot\hat{w}). \tag{B.22}$$

The residual vector and the tangent matrix may be separated into contributions from the Hamiltonian function and the external force.

$$\hat{\mathscr{R}}_m = \hat{\mathscr{R}}_{mh} + \hat{\mathscr{R}}_{me}, \quad \hat{\mathscr{T}}_m = \hat{\mathscr{T}}_{mh} + \hat{\mathscr{T}}_{me}. \tag{B.23}$$

Clearly, $\hat{\mathscr{R}}_{me} = (0, \hat{f})$. The tangent matrix $\hat{\mathscr{T}}_{mh}$ is obtained by taking the variation of $\hat{\mathscr{R}}_{mh}$, and is given by:

$$\hat{\mathscr{T}}_{mh} = \begin{bmatrix} -\mathbf{X}^{-1}\cdot M_6^{-1} & \begin{matrix}\mathbf{K}_6(q, w_n - \hat{w}) \\ -\mathbf{X}^{-1}\cdot(S_3(w_n) - S_2^t(\hat{w}) - M_6^{-1}\cdot S_2^t(\hat{p}))\cdot\mathbf{X}\end{matrix} \\ S_1(\hat{p})\cdot M_6^{-1} - S_1(\hat{w}) & S_1(\hat{p})\cdot(S_2^t(\hat{w}) - M_6^{-1}\cdot S_2^t(\hat{p}))\cdot\mathbf{X} \end{bmatrix}. \tag{B.24}$$

Both $\hat{\mathscr{R}}_{mh}$ and $\hat{\mathscr{T}}_{mh}$ are evaluated at the given state $(\hat{p}_g, q_g)$. The linear operators S_1, S_2 and S_3 are as defined previously and the operator $\mathbf{K}_6(q, z)$, applied to an arbitrary vector $z = (z_L, z_A)$ is given by:

$$\mathbf{K}_6(q, z) = \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{K}(r, z_A) \end{bmatrix}. \tag{B.25}$$

The full expression for $\mathbf{K}(r, z_A)$ is given in Appendix A.

B.4 Mixed form-symmetric approach

Now consider the tangent map given by Eq. (3.42) in order to find the expressions for the residual vector $\mathscr{R}_m$ and the tangent matrix $\mathscr{T}_m$. Again the vector $\mathscr{R}_m$ and the matrix $\mathscr{T}_m$ have contributions due to the Hamiltonian function as well as the external force i.e.:

$$\mathscr{R}_m = \mathscr{R}_{mh} + \mathscr{R}_{me}, \quad \mathscr{T}_m = \mathscr{T}_{mh} + \mathscr{T}_{me}. \tag{B.26}$$

Since the expressions for $\mathscr{R}_{me}$ and for $\mathscr{T}_{me}$ depend on the specific nature of the external forces, only the expressions for $\mathscr{R}_{mh}$ and for $\mathscr{T}_{mh}$ are developed here.

Starting from Eq. (3.37), the Hamiltonian function may be expressed as:

$$H(p, q, t) = \tfrac{1}{2}\hat{p}\cdot M_6^{-1}\cdot\hat{p} - \hat{p}\cdot w_n. \tag{B.27}$$

Using the relationship between $\hat{p}$ and p, leads to:

$$\delta\hat{p} = \mathbf{X}^{-t}\cdot\delta p + \delta\mathbf{X}^{-t}\cdot p = \mathbf{X}^{-t}(\delta p - \delta\mathbf{X}^t\cdot\hat{p}) \tag{B.28}$$

which may be written as:

$$(\delta\hat{p}, \delta\hat{q}) = Z\cdot(\delta p, \delta q), \quad Z = \begin{bmatrix} \mathbf{X}^{-t} & \mathbf{X}^{-t}\cdot\mathbf{H}_6(q, \hat{p}) \\ 0 & \mathbf{X} \end{bmatrix}. \tag{B.29}$$

Then the virtual change of the Hamiltonian function can be stated equivalently as:

$$\delta H = (\delta\hat{p}, \delta\hat{q})\cdot\hat{\mathscr{R}}_{mh} = (\delta p, \delta q)\cdot\mathscr{R}_{mh}, \tag{B.30}$$

and the vectors $\hat{\mathscr{R}}_{mh}$ and $\mathscr{R}_{mh}$ can be seen to be related by: $\hat{\mathscr{R}}_{mh} = Z^t\cdot\mathscr{R}_{mh}$.

The linearization of the virtual change of the Hamiltonian can then be written as:

$$\begin{aligned} \mathrm{d}\delta H &= (\delta\hat{p}, \delta\hat{q})\cdot\hat{\mathscr{T}}_{mh}\cdot(\mathrm{d}\hat{p}, \mathrm{d}\hat{q}) + (\mathrm{d}\delta\hat{p}, \mathrm{d}\delta\hat{q})\cdot\hat{\mathscr{R}}_{mh} \\ &= (\delta p, \delta q)\cdot\mathscr{T}_{mh}\cdot(\mathrm{d}p, \mathrm{d}q) \end{aligned} \tag{B.31}$$

where $(\mathrm{d}\hat{p}, \mathrm{d}\hat{q}) = Z\cdot(\mathrm{d}p, \mathrm{d}q)$. By comparison, then:

$$\mathscr{T}_{mh} = Z^t\cdot\hat{\mathscr{T}}_{mh}\cdot Z + \left(\frac{\partial(Z^t\cdot\hat{\mathscr{R}}_{mh})}{\partial p}, \frac{\partial(Z^t\cdot\hat{\mathscr{R}}_{mh})}{\partial q}\right). \tag{B.32}$$

In the last expression $\hat{\mathscr{R}}_{mh}$ is the value of the residual evaluated at the given state $(\hat{p}_g, \hat{q}_g)$, and is considered constant. The definitions of $\mathscr{R}_{mh}$ and $\mathscr{T}_{mh}$, are not the same as in the previous section, but are consistent with the notation that $(\hat{\ })$ indicates test functions which are variations of $\hat{p}$ and $\hat{q}$.

The expressions for $\hat{\mathscr{R}}_{mh}$ and for $\hat{\mathscr{T}}_{mh}$, are now developed. The virtual change of the Hamiltonian function is expressed by:

$$\delta H = \delta^o \hat{p} \cdot (\hat{w} - w_n) - \delta^o w_n \cdot \hat{p} \tag{B.33}$$

where $\hat{w} = M_6^{-1} \cdot \hat{p}$. Since it is known that:

$$\delta^o \hat{p} = \delta \hat{p} - S_2^t(\hat{p}) \cdot \delta \hat{q}, \quad \delta^o w_n = -S_1^t(w_n) \cdot \delta \hat{q} \tag{B.34}$$

Eq. (B.33) can be rewritten as:

$$\delta H = \delta \hat{p} \cdot (\hat{w} - w_n) - \delta \hat{q} \cdot [S_3(\hat{p}) \cdot w_n - S_2(\hat{p}) \cdot \hat{w}], \tag{B.35}$$

then the vector $\mathscr{R}_{mh}$ has the following expression:

$$\mathscr{R}_{mh} = (\hat{w} - w_n, S_3(\hat{p}) \cdot w_n - S_2(\hat{p}) \cdot \hat{w}). \tag{B.36}$$

From this, it is straightforward to find the expression of the tangent matrix $\hat{\mathscr{T}}_{mh}$, which has the form:

$$\hat{\mathscr{T}}_{mh} = \begin{bmatrix} M_6^{-1} & \begin{matrix} S_2^t(\hat{w}) - S_3^t(w_n) \\ - M_6^{-1} \cdot S_2^t(\hat{p}) \end{matrix} \\ \begin{matrix} S_2(\hat{w}) - S_3(w_n) \\ - S_2(\hat{p}) \cdot M_6^{-1} \end{matrix} & \begin{matrix} S_2(\hat{p}) \cdot M_6^{-1} \cdot S_2^t(\hat{p}) - \\ S_2(\hat{p}) \cdot S_2^t(\hat{w}) + S_3(\hat{p}) \cdot S_3^t(w_n) \end{matrix} \end{bmatrix}. \tag{B.37}$$

In order to compute the terms $(\mathrm{d}\delta\hat{p}, \mathrm{d}\delta\hat{q}) \cdot \hat{\mathscr{R}}_{mh}$ recall the expressions for $\delta \boldsymbol{\Gamma}^{-1}$ and $\mathrm{d}\delta \boldsymbol{\Gamma}^{-1}$ that are computed in Appendix A. Specifically:

$$\delta \boldsymbol{\Gamma}^{-1} \cdot b = \mathrm{K}(r, b) \cdot \delta r \tag{B.38}$$

and:

$$c \cdot \mathrm{d}\delta \boldsymbol{\Gamma}^{-1} \cdot b = \mathrm{d}r^t \cdot \mathrm{L}(c, r, b) \cdot \delta r, \tag{B.39}$$

The map $\mathrm{K}_6(q, z)$ is defined in the previous section. In a similar way, $\mathrm{L}_6(x, q, z)$ is defined, considering two general six dimensional vectors, x and z.

$$\mathrm{K}_6(q, z) = \begin{bmatrix} 0 & 0 \\ 0 & \mathrm{K}(r, z_A) \end{bmatrix}, \quad \mathrm{L}_6(x, q, z) = \begin{bmatrix} 0 & 0 \\ 0 & \mathrm{L}(x_A, r, z_A) \end{bmatrix}. \tag{B.40}$$

With the use of these definitions the last term in Eq. (B.32) can be written as:

$$\left(\frac{\partial (Z^t \cdot \mathscr{R}_{mh})}{\partial p}, \frac{\partial (Z^t \cdot \mathscr{R}_{mh})}{\partial q} \right) = \begin{bmatrix} 0 & \mathrm{K}_6(q, \hat{w} - w_n) \\ \mathrm{K}_6^t(q, \hat{w} - w_n) & \begin{matrix} \mathrm{L}_6(\mathrm{X}^t \cdot \hat{p}, \hat{q}, \hat{w} - w_n) + \\ \mathrm{H}_6(q, \hat{p}) \cdot (S_3(\hat{p}) \cdot w_n - S_2(\hat{p}) \cdot \hat{w}) \end{matrix} \end{bmatrix}. \tag{B.41}$$

Even if the programming of the tangent matrix can be optimized, the fully symmetric mixed method requires a great deal of computations.

Three field form

The linearization of the three field principle Eq. (3.46) is much more straightforward. For convenience the three field form is recalled here:

$$\int_{t_1}^{t_2}\left[\delta\hat{q}\cdot\left(\hat{f}-S_1(w)\cdot\frac{\delta\hat{\mathscr{L}}}{\delta w}\right)-\delta^*w\cdot\left(\hat{p}-\frac{\delta\hat{\mathscr{L}}}{\delta w}\right)-\delta^*\hat{p}\cdot\mathbf{X}^{-1}\cdot(w-w_n)\right.$$
$$\left.+\frac{d}{dt}(\delta\hat{q})\cdot\hat{p}-\frac{d}{dt}(\delta^*p)\cdot q\right]dt=(\delta\hat{q},\hat{p}_b-\delta^*\hat{p}\cdot q_b)|_{t_1}^{t_2}. \quad (B.42)$$

Grouping the test functions into a single vector, Eq. (B.42) may be rewritten as:

$$\int_{t_1}^{t_2}\left[(\delta\hat{q},\delta^*w,\delta^*\hat{p})\cdot\left(\hat{f}-\mathbf{S}_1(w)\cdot\frac{\delta\hat{\mathscr{L}}}{\delta w},-\hat{p}+\frac{\delta\hat{\mathscr{L}}}{\delta w},-\mathbf{X}^{-1}\cdot(w-w_n)\right)dt\right.$$
$$+\int_{t_1}^{t_2}\left(\frac{d}{dt}\delta^*p,\frac{d}{dt}\delta\hat{q}\right)\cdot\mathbf{I}_S\cdot(\hat{p},q)\,dt=(\delta\hat{q}\cdot\hat{p}_b-\delta^*\hat{p}\cdot q_b)|_{t_1}^{t_2}. \quad (B.43)$$

The linearization is then given by:

$$\int_{t_1}^{t_2}\left[\frac{d}{dt}(\delta^*p,\delta\hat{q})\cdot\mathbf{I}_S\cdot(d\hat{p},d\hat{q})\,dt+\int_{t_1}^{t_2}(\delta\hat{q},\delta^*w,\delta^*p)\cdot\hat{\mathscr{T}}_3\cdot(dq,dw,d\hat{p})\right]dt$$
$$=(\delta^*p,\delta\hat{q})\cdot\mathbf{I}_S\cdot(p_b,q_b)|_{t_1}^{t_2}-\int_{t_1}^{t_2}\frac{d}{dt}(\delta^*p,\delta\hat{q})\cdot\mathbf{I}_S\cdot(\hat{p}_g,q_g)\,dt+\int_{t_1}^{t_2}(\delta\hat{q},\delta^*w,\delta^*p)\cdot\hat{\mathscr{R}}_3\,dt \quad (B.44)$$

where:

$$\hat{\mathscr{R}}_3=\left(\hat{f}-S_1(w)\cdot\frac{\delta\hat{\mathscr{L}}}{\delta w},-\hat{p}+\frac{\delta\hat{\mathscr{L}}}{\delta w},-\mathbf{X}^{-1}\cdot(w-w_n)\right). \quad (B.45)$$

Once more, it is a simple matter to separate the contribution from the external force. The variation of the residual, neglecting the external force terms leads to the tangent matrix for the three field approach.

$$\hat{\mathscr{T}}_3=\begin{bmatrix} S_1(w)\cdot\dfrac{\delta^2\hat{\mathscr{L}}}{\delta w\delta q} & S_1(M_6\cdot w)-S_1(w)\cdot M_6 & 0\\ \dfrac{\delta^2\hat{\mathscr{L}}}{\delta w\delta q} & M_6 & -I_6\\ \mathbf{K}_6(q,w-w_n)-S_3(w_n)\cdot\mathbf{X} & -\mathbf{X}^{-1} & 0\end{bmatrix} \quad (B.46)$$

The first and second partial derivative of $\hat{\mathscr{L}}$ are given by:

$$\frac{\partial\hat{\mathscr{L}}}{\partial w}=M_6\cdot w,\quad \frac{\partial^2\hat{\mathscr{L}}}{\partial w\partial q}=[S_2^t(M_6\cdot w)-M_6\cdot S_2(w)]\cdot\mathbf{X}, \quad (B.47)$$

and the partial derivative of w_n with respect to q is $\frac{\partial w_n}{\partial q}=S_3^t(w_n)\cdot\mathbf{X}$. The simplicity of this tangent matrix, combined with the fact that for initial value problems symmetry of the tangent matrix is not easily exploited, makes this a an attractive formulation, with the obvious drawback of increased degrees of freedom.

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