Finite elastic deformations and finite rotations of 3d continuum with independent rotation field

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ABSTRACT. *Several variational principles for finite elastic deformations of a continuum with independent (finite) rotation field are constructed based on the polar decomposition theorem. Their regularized forms are then discussed and reduced to the one which is the most suitable for finite element implementation. A three-dimensional 8-node solid element with 6 degrees of freedom per node (three translational and three rotational) is developed based on the preferred variational formulation and the modified method of incompatible modes. A special care is dedicated to enhancing the computational efficiency, by considering on one hand an alternative parametrization of the finite rotation field, and on the other hand by using the operator split method in dealing with the incompatible modes. The proposed approach is evaluated on a set of challenging large displacement/large rotation problems in nonlinear elastostatics.*

RÉSUMÉ. *On considère quelques principes variationnels basés sur la factorisation polaire pour l'élasticité non linéaire avec un champ de rotations (finies) indépendantes. On donne ensuite leurs formes régularisées et on choisit celle qui est la plus favorable pour l'implantation de la méthode des éléments finis. On présente également le développement d'un élément tri-dimensionnel à 8 nœuds et 6 degrés de liberté par nœud (trois degrés de translation et trois degrés de rotation) basé sur la formulation variationnelle préférée et la méthode modifiée des modes incompatibles. On porte une attention particulière à l'amélioration de l'efficacité du calcul en considérant d'une part une autre possibilité pour le traitement des grandes rotations et d'autre part en utilisant la partition de l'opérateur agissant sur les modes icompatibles. On teste l'approche proposée sur quelques problèmes concernant les grands déplacements et grandes rotations.*

KEY WORDS : *3d continuum, finite rotation, elastic deformation, regularized variational principle, 8-node solid element, incompatible modes.*
MOTS-CLÉS : *milieu continu 3d, grande rotation, déformation élastique, principe variationnel régularisé, élément tri-dimensionnel à 8 nœuds, modes incompatibles.*

1. Introduction

Solid and membrane finite elements with rotational degrees of freedom are of great interest for engineering practice, for they can be easily combined with structural elements (see [IFR93]). No matter how complex a structural system appears to be, with the elements of this kind one can easily build its fully compatible finite element model.

Utility of the continuum elements with rotational degrees of freedom has spurred many recent research works on the subject. In summary of those efforts, one can say that it is far from trivial to construct a continuum element of this kind with high performance even for the geometrically linear theory (e.g., see [ALL84] or [BEF85] for typical attempts in that direction). The regularized variational principle of geometrically linear elastostatics given by Hughes and Brezzi [HUB89] did provide a possibility to simplify the construction of continuum elements with rotational degrees of freedom and use standard isoparametric interpolations. However, the resulting elements (see [HBM90]) are of rather poor performance when it gets to low-order interpolations and high values of regularization parameter. In trying to improve performance of a 4-node membrane element with rotational degrees of freedom and make it insensitive to the value of the regularization parameter, we have to go to non-conventional interpolations (see [ITW90]).

In this work, we aim to proceed along the same lines, i.e. addressing both a sound variational basis and its finite element approximation, into geometrically nonlinear theory. An increase of the problem complexity is very significant in a sense that, as opposed to geometrically linear theory, there exist many strain measures and energy conjugate stress tensors which can be used for such a purpose. The pioneering works of Bergan and Nygard [BEN86] and Jetteur and Frey [JEF86] on providing drilling rotations in a geometrically nonlinear membrane, tried to avoid those issues by relying on the co-rotational formulation in order to extend, respectively, the results of [BEF85] and [ALL84] obtained in geometrically linear theory. However, such an approach is not only restricted with the limitations of the co-rotational formalism, but also inherits all the deficiencies present in those works on membrane elements for geometrically linear theory (adjusted parameters, spurious modes).

In this work we take a fundamentally different approach from that in [BEN86] and [JEF86]. Namely, we concentrate directly on providing a sound variational formulation valid for geometrically nonlinear theory. We show subsequently its versatility as a starting point in the discrete approximation of the geometrically nonlinear theory. In passing we also show how a corresponding formulation valid for the geometrically linear theory can be recovered simply by the consistent linearization of our formulation for nonlinear problem.

The basis of our work is derived from the work of Fraeijs de Veubeke [FDV72] on the complementary energy principle in geometrically nonlinear theory. Both the work of Fraeijs de Veubeke [FDV72] and related works (e.g. see [REI84], [KOI76] and [ATL83]), have concentrated mostly on establishing the validity of the complementary energy principle in geometrically nonlinear theory. In this work, however, we put the main emphasis not only on deriving the variational principles of this kind, but also on evaluating them in the context of the discrete approximation.

For a robust numerical implementation with a convenient choice of interpolations, one needs to consider a regularized form of the variational principle valid for the continuum case. Departure from a regularized form of the variational principle enables us to use, for example, the standard isoparametric interpolations. However, as already learned in the linear theory (see [ITW90]), one needs non-conventional interpolations in order to provide a geometrically nonlinear continuum element with rotational degrees of freedom of a satisfying performance. In the nonlinear Lagrangian computations one would typically opt for the solid elements with low order interpolations: first, for they have a more robust performance in the distorted configurations, and second, for these elements facilitate more convenient manipulations in the adaptive mesh refinement of h–type. However, it is well known that the standard tri-linear brick elements exhibit rather poor performance, unless additional artifices are used.

Our implementation is based on the modified method of incompatible modes (see [IBW91]), which was previously recognized (e.g., see [WTD73] and [TBW76]) as a viable alternative for improving the performance of the 8-node brick element in bending dominated problems. We show that the same robust performance carries over to the nonlinear analysis in the regime of large displacements and large rotations. Geometrically nonlinear extension of the modified method of incompatible modes [IBW91] is initially given only for two-dimensional problems (see [IBF93]). While in the present, three-dimensional case all the governing principles (see [IBF93]) remain the same, some important implementation details change rending the implementation of the method much more efficient.

Anticipating that the use of three-dimensional solid elements will gain popularity, it is worthwhile to point out some recently presented alternatives: one of Simo et al. [SAT93] who used nonlinear version of the enhanced strain method [SIR90], and another of Radovitzky and Dvorkin [RAD94] who used the method of mixed interpolations of tonsorial components (e.g., see [DVB84]) for the brick element of Wilson and Ibrahimbegović [WII91]. The element presented herein remains nevertheless unique in a sense that it possesses both translational and rotational degrees of freedom.

The outline of the paper is as follows. In Section 2 we discuss different variational principles which lead to the complementary energy principle of Fraeijs de Veubeke [FDV72]. In section 3 we discuss the discrete finite element approximation of the variational principles for the case of three-dimensional continuum. The operator split procedure used to deal with the incompatible modes is discussed in Section 4. In Section 5 we give an alternative parameterization of finite rotations which can further enhance the computation efficiency. Several illustrative examples are given in Section 6. Some closing remarks are stated in Section 7.

2. Variational Formulation

In this section we discuss the variational formulations for the continuum with independent rotation field in geometrically nonlinear theory. The starting point in our considerations can be provided by the classical potential energy principle (e.g., see [ZIT89], p. 34) for finite displacements in the form

$$\Pi(\mathbf{u}) = \int_{\mathcal{B}} W(\mathbf{H}(\mathbf{u}))\, d\mathcal{B} - \int_{\mathcal{B}} \mathbf{u}\cdot\mathbf{f}\, d\mathcal{B}\ , \qquad [1]$$

where $W(\mathbf{H}(\mathbf{u}))$ is a stored energy given as a scalar-valued function of a chosen finite strain measure. The second integral represents the external work for the Dirichlet boundary value problem we are considering herein.

Throughout this section an index-free tensor notation is utilized, such as found in modern expositions on finite elasticity (e.g. see [GUR81]), with index notation supplied only to clarify the adopted convention. So, for example,

$$\mathbf{u}\cdot\mathbf{f} = u_i f_i\ , \qquad [2]$$

denotes the inner product of displacement vector $\mathbf{u}$ and body force $\mathbf{f}$, where the standard summation convention on repeated indices is implied.

The finite strain measure $\mathbf{H}$, often called Biot strain (see [BIO65]), can be the most explicitly defined via the polar decomposition theorem (e.g., see [GUR81], p. 14). Namely, if the deformation is a vector field $\boldsymbol{\varphi}$, which is, without loss of generality for our purposes, specified with respect to the Euclidean coordinate system with the base vectors $\mathbf{e}_i$, i.e. if

$$\mathbf{x}^{\varphi} = \boldsymbol{\varphi}(\mathbf{x})\ ;\ \mathbf{x} = x_i\mathbf{e}_i\ ;\ \boldsymbol{\varphi} = \varphi_i\mathbf{e}_i\ , \qquad [3]$$

then the deformation gradient can be written as

$$\mathbf{F} = \nabla\boldsymbol{\varphi}\ ;\ \mathbf{F} = \frac{\partial\varphi_i}{\partial x_j}\mathbf{e}_i\otimes\mathbf{e}_j\ , \qquad [4]$$

where '$\otimes$' denotes the tensor product.

Introducing the displacement vector field: $\mathbf{u} = \boldsymbol{\varphi}(\mathbf{x}) - \mathbf{x}$, the deformation gradient can be rewritten in terms of the displacement gradient $\nabla\mathbf{u}$ as

$$\mathbf{F} = \nabla\boldsymbol{\varphi} = \mathbf{I} + \nabla\mathbf{u}\ ;\ \nabla\mathbf{u} = \frac{\partial u_i}{\partial x_j}\mathbf{e}_i\otimes\mathbf{e}_j\ ;\ \mathbf{I} = \delta_{ij}\mathbf{e}_i\otimes\mathbf{e}_j\ . \qquad [5]$$

The polar decomposition theorem states that the deformation gradient can be factored in a unique way into

$$\mathbf{F} = \mathbf{R}\mathbf{U}\ , \qquad [6]$$

where $\mathbf{U}$ is a symmetric positive-definite tensor (right stretch tensor) which describes the deformation, while $\mathbf{R}$ is an orthogonal tensor which describes rotation. The Biot strain tensor is defined with

$$\mathbf{H} = \mathbf{U} - \mathbf{I}\ . \qquad [7]$$

By using the results in [5] to [7], the polar decomposition theorem can be rewritten as

$$\mathbf{I} + \nabla \mathbf{u} \;=\; \mathbf{R}(\mathbf{H} + \mathbf{I}) \,. \qquad [8]$$

By eliminating the rotation field in [8] via orthogonality of $\mathbf{R}$, we get a functional relationship between $\mathbf{H}$ and $\mathbf{u}$

$$2\mathbf{H} + \mathbf{H}^2 = \nabla \mathbf{u} + (\nabla \mathbf{u})^T + (\nabla \mathbf{u})^T \, \nabla \mathbf{u} \,, \qquad [9]$$

which is needed in [1].

We want to reformulate our problem so that the polar decomposition in [8] is recovered as the Euler-Lagrange equation of a new variational formulation rather than having it as a subsidiary condition of the variational formulation in [1]. The Lagrange multiplier procedure (e.g. see [ZIT89], p. 243) can be used to impose that condition in the form

$$PD = \int_{\mathcal{B}} \mathbf{P} \, : \, [(\mathbf{I} + \nabla \mathbf{u}) - \mathbf{R}(\mathbf{I} + \mathbf{H})] \; d\mathcal{B} \,, \qquad [10]$$

where $\mathbf{P}$ is the Lagrange multiplier and ' : ' denotes a natural inner product of two second order tensors (e.g., see [GUR81], p. 5). For clarity, if $\mathbf{A}$ and $\mathbf{B}$ are two second order tensors, then their inner product is

$$\mathbf{A} \, : \, \mathbf{B} = trace(\mathbf{A}^T \mathbf{B}) = A_{ij} B_{ij} \,. \qquad [11]$$

That Lagrange multiplier $\mathbf{P}$ is actually the non-symmetric Piola-Kirchhoff stress tensor follows directly from a result on energy conjugate pairs (e.g., see [GUR81], p. 185). The non-symmetric Piola-Kirchhoff tensor $\mathbf{P}$ is related to the Cauchy (true) stress tensor $\boldsymbol{\sigma}$ via Piola transform

$$\mathbf{P} = J \boldsymbol{\sigma} \mathbf{F}^{-T} \; ; \; J = det \mathbf{F} \,. \qquad [12]$$

If one is to introduce the pull-back of $\mathbf{P}$ performed with the rotation part $\mathbf{R}$ of the deformation gradient, we obtain the new stress tensor

$$\mathbf{T} = \mathbf{R}^T \mathbf{P} = J \mathbf{R}^T \boldsymbol{\sigma} \mathbf{F}^{-T} \,, \qquad [13]$$

which is also non-symmetric.

By using the properties of inner product and result in [13], we can rewrite result in [10] in the form

$$PD = \int_{\mathcal{B}} \mathbf{T} \, : \, [\mathbf{R}^T (\mathbf{I} + \nabla \mathbf{u}) - (\mathbf{I} + \mathbf{H})] \; d\mathcal{B} \,. \qquad [14]$$

The weak form of the polar decomposition in [14] can be added to the variational formulation in [1] to get a general Hu-Washizu type variational formulation which is valid for geometrically nonlinear theory

$$\Pi(\mathbf{u}, \mathbf{R}, \mathbf{T}, \mathbf{H}) = \int_{\mathcal{B}} \{ W(\mathbf{H}) - \mathbf{T} \, : \, \mathbf{H} + \mathbf{T} \, : \, [\mathbf{R}^T (\mathbf{I} + \nabla \mathbf{u}) - \mathbf{I})] \} \; d\mathcal{B} - \int_{\mathcal{B}} \mathbf{u} \cdot \mathbf{f} \; d\mathcal{B} \,. \qquad [15]$$

The associated variational equations and the Euler-Lagrange equations can be obtained by taking the directional derivative (see [GUR81], p. 21) in the direction of virtual displacements $\delta\mathbf{u}$, virtual rotations $\delta\mathbf{R}$, virtual stresses $\delta\mathbf{T}$ and virtual strains $\delta\mathbf{H}$. We get, respectively:
(i) The linear momentum balance equations

$$\begin{aligned} &\int_{\mathcal{B}} \{\mathbf{T} \; : \; [\mathbf{R}^T(\nabla\,\delta\mathbf{u})] - \delta\mathbf{u}\cdot\mathbf{f}\}\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow \int_{\mathcal{B}} \{\delta\mathbf{u}\cdot[div(\mathbf{RT}) + \mathbf{f}]\}\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow div(\mathbf{RT}) + \mathbf{f} = \mathbf{0} \;;\; div\mathbf{A} = \frac{\partial A_{ij}}{\partial x_j}\mathbf{e}_i \;, \end{aligned} \qquad [16]$$

where we used integration by parts on the first integral;
(ii) The angular momentum balance

$$\begin{aligned} &\int_{\mathcal{B}} \mathbf{T} \; : \; [\mathbf{R}^T\;(\mathbf{R}\,\delta\mathbf{R}^T)(\mathbf{I}+\nabla\mathbf{u})]\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow \int_{\mathcal{B}} [\mathbf{RT}(\mathbf{I}+\nabla\mathbf{u})^T] \; : \; (\mathbf{R}\,\delta\mathbf{R}^T)\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow \mathbf{RT}(\mathbf{I}+\nabla\mathbf{u})^T = (\mathbf{I}+\nabla\mathbf{u})(\mathbf{RT})^T \;, \end{aligned} \qquad [17]$$

where the skew-symmetry of $(\mathbf{R}\;\delta\mathbf{R}^T)$ is utilized;
(iii) The definition of strains $\mathbf{H}$ and rotations $\mathbf{R}$

$$\begin{aligned} &\int_{\mathcal{B}} symm\,\delta\mathbf{T} \; : \; [-\mathbf{H} + symm[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u}) - \mathbf{I}]\; d\mathcal{B} \\ &+ \int_{\mathcal{B}} skew\,\delta\mathbf{T} \; : \; skew\,[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u}) - \mathbf{I}]\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow \mathbf{H} = symm[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u}) - \mathbf{I}] \;, \\ &\Longrightarrow skew\,[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u})] = \mathbf{0} \;, \end{aligned} \qquad [18]$$

where we used the fact that $\mathbf{H}$ is a symmetric tensor;
(iv) The constitutive equations

$$\begin{aligned} &\int_{\mathcal{B}} \delta\mathbf{H} \; : \; [\frac{\partial W(\mathbf{H})}{\partial \mathbf{H}} - symm\mathbf{T}]\; d\mathcal{B} = 0 \;, \\ &\Longrightarrow symm\mathbf{T} = \frac{\partial W(\mathbf{H})}{\partial \mathbf{H}} \;. \end{aligned} \qquad [19]$$

In equations [18] and [19] we have introduced the Euclidean decomposition for a second order tensor into its symmetric and skew-symmetric part. For example, for stress tensor $\mathbf{T}$, we have

$$\mathbf{T} = symm\mathbf{T} + skew\mathbf{T} \;;\; symm\mathbf{T} = \frac{1}{2}(\mathbf{T}+\mathbf{T}^T) \;;\; skew\mathbf{T} = \frac{1}{2}(\mathbf{T}-\mathbf{T}^T) \;. \qquad [20]$$

The work of Fraeijs de Veubeke and most of the works related to it (e.g. see [KOI76], [ATL83] and [REI84]) have concentrated on establishing the validity of the complementary energy principle in the regime of large displacements. Therein, the crucial assumption is that the complementary energy $\Sigma(symm\mathbf{T})$ exists, and that it can be recovered by the Lagendre transform

$$-\mathbf{H} \ : \ symm\mathbf{T} + W(\mathbf{H}) = -\Sigma(symm\mathbf{T}) \ . \qquad [21]$$

By introducing the transformation in [21] into the variational formulation in [15], we can eliminate the strain field $\mathbf{H}$ to get the three-field variational formulation

$$\Pi(\mathbf{u},\mathbf{R},\mathbf{T}) = \int_{\mathcal{B}} \{-\Sigma(symm\mathbf{T})+\mathbf{T} \ : \ [\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u})-\mathbf{I}]\} \, d\mathcal{B} - \int_{\mathcal{B}} \mathbf{u}\cdot\mathbf{f} \, d\mathcal{B} \ . \qquad [22]$$

The Euler-Lagrange equations of linear and angular momentum balance, given in [16] and in [17], remain preserved, while the definition of strains in [18] and the constitutive equations in [19] give rise to a new Euler-Lagrange equation, which connects directly the stresses with the displacements and rotations

$$\begin{aligned} &\int_{\mathcal{B}} symm\,\delta\mathbf{T} \ : \ [-\frac{\partial\Sigma(symm\mathbf{T})}{\partial\, symm\mathbf{T}} + symm[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u}) - \mathbf{I}] \, d\mathcal{B} \\ &\qquad + \int_{\mathcal{B}} skew\,\delta\mathbf{T} \ : \ skew\,[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u})] \, d\mathcal{B} = 0 \ , \qquad [23] \\ &\qquad \Longrightarrow \frac{\partial\Sigma(symm\mathbf{T})}{\partial\, symm\mathbf{T}} = symm[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u}) - \mathbf{I}] \ , \\ &\qquad\qquad \Longrightarrow skew\,[\mathbf{R}^T(\mathbf{I}+\nabla\mathbf{u})] = \mathbf{0} \ . \end{aligned}$$

In the work of Fraeijs de Veubeke, an additional step is taken to eliminate the displacement field via picking up the stress field which satisfies linear momentum balance equations in [16], so that in the final form of the complementary energy principle only stress and rotation fields are retained. We do not follow this procedure to devise the variational principles, because the absence of the displacement field can be undesirable in the solution to a practical problem.

In the remaining part of this section, we want to make a small digression from the main body of this paper and look at the geometrically linear theory. For that purpose, we simply use the consistent linearization of the preceding results around the reference configuration, which is assumed free of initial stress and initial deformation. For example, by using the result of Argyris [ARG82], we can linearize an orthogonal tensor to get

$$\mathbf{R} \xrightarrow{lin.} \mathbf{I} + \boldsymbol{\Omega} \ ; \ \boldsymbol{\Omega}^T = -\boldsymbol{\Omega} \ . \qquad [24]$$

From the finite strain measure $\mathbf{H}$ in $[18]_2$ we recover a standard definition of infinitesimal strain as the symmetric part of displacement gradient

$$\mathbf{H} \xrightarrow{lin.} \epsilon = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \; , \qquad [25]$$

and from $[18]_3$ and result in [24] we recover the definition of infinitesimal rotation field $\boldsymbol{\Omega}$ as the skew-symmetric part of the deformation gradient

$$\boldsymbol{\Omega} = \frac{1}{2}(\nabla \mathbf{u} - (\nabla \mathbf{u})^T) \; . \qquad [26]$$

The stress tensor is assumed to remain non-symmetric

$$\mathbf{T} \xrightarrow{lin.} \boldsymbol{\sigma} \; ; \; \boldsymbol{\sigma}^T \neq \boldsymbol{\sigma} \; . \qquad [27]$$

If these results are introduced into the variational formulation in [15], and higher order terms are neglected, we get

$$\Pi(\mathbf{u}, \boldsymbol{\Omega}, \boldsymbol{\sigma}, \epsilon) = \int_{\mathcal{B}} \{W(\epsilon) - \boldsymbol{\sigma} \; : \; \epsilon + \boldsymbol{\sigma} \; : \; (\nabla \mathbf{u} - \boldsymbol{\Omega})\} \; d\mathcal{B} - \int_{\mathcal{B}} \mathbf{u} \cdot \mathbf{f} \; d\mathcal{B} \; . \quad [28]$$

Similarly, by the consistent linearization of the variational formulation in [22], we get

$$\Pi(\mathbf{u}, \boldsymbol{\Omega}, \boldsymbol{\sigma}) = \int_{\mathcal{B}} \{-\Sigma(symm\boldsymbol{\sigma}) + \boldsymbol{\sigma} \; : \; (\nabla \mathbf{u} - \boldsymbol{\Omega})\} \; d\mathcal{B} - \int_{\mathcal{B}} \mathbf{u} \cdot \mathbf{f} \; d\mathcal{B} \; . \qquad [29]$$

The variational principles [28] and [29] both appear in our earlier developments in geometrically linear theory (see [ITW90], [IFR93]). It is this link with the geometrically linear theory that guides us in proposing the regularized forms of the variational principles for the geometrically nonlinear theory which are discussed next.

3. Finite element approximation

In this section we discuss the regularized form of the variational principles within the framework of the finite-dimensional discrete approximation, constructed by using the finite element procedure. The field variables in the discrete approximation carry a superscript $'h'$, which denotes the finite element mesh parameter.

It proves convenient to switch to the matrix notation (e.g., [ZIT89]). If we denote

$$\mathbf{R}^h = [\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3] \; ; \; \mathbf{I} + \nabla \mathbf{u}^h = [\mathbf{y}_1(\mathbf{u}^h); \mathbf{y}_2(\mathbf{u}^h); \mathbf{y}_3(\mathbf{u}^h)] \; , \qquad [30]$$

then the symmetric part of the strain tensor can be mapped into a 6-dimensional vector

$$symm[\mathbf{R}(\mathbf{I} + \nabla \mathbf{u}) - \mathbf{I}] \longrightarrow \mathbf{e}(\mathbf{u}^h, \mathbf{R}^h) := \boldsymbol{\Lambda}(\mathbf{R}^h)\mathbf{y}(\mathbf{u}^h) - \mathbf{1} \; , \qquad [31]$$

while the skew-symmetric part of the strain tensor is mapped into a 3-dimensional vector

$$skew[\mathbf{R}(\mathbf{I}+\nabla\mathbf{u})] \longrightarrow \omega(\mathbf{u}^h,\mathbf{R}^h) := \Xi(\mathbf{R}^h)\mathbf{y}(\mathbf{u}^h) \ , \qquad [32]$$

where

$$\Lambda(\mathbf{R}^h) = \begin{bmatrix} \mathbf{r}_1^T & \mathbf{0}^T & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{r}_2^T & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{0}^T & \mathbf{r}_3^T \\ \mathbf{r}_2^T & \mathbf{r}_1^T & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{r}_3^T & \mathbf{r}_2^T \\ \mathbf{r}_3^T & \mathbf{0}^T & \mathbf{r}_1^T \end{bmatrix} ; \ \Xi(\mathbf{R}^h) = \begin{bmatrix} \mathbf{r}_2^T & -\mathbf{r}_1^T & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{r}_3^T & -\mathbf{r}_2^T \\ -\mathbf{r}_3^T & \mathbf{0}^T & \mathbf{r}_1^T \end{bmatrix} ; \ \mathbf{y}(\mathbf{u}^h) = \begin{pmatrix} \mathbf{y}_1(\mathbf{u}^h) \\ \mathbf{y}_2(\mathbf{u}^h) \\ \mathbf{y}_3(\mathbf{u}^h) \end{pmatrix} . \qquad [33]$$

The corresponding symmetric and skew-symmetric parts of the stress tensor are also mapped into the vectors

$$symm\mathbf{T} \longrightarrow \mathbf{t}^h \ , \ skew\mathbf{T} \longrightarrow \mathbf{p}^h \ , \qquad [34]$$

with the components ordered so as to preserve the energy-conjugate pairs.

In the foregoing we will focus upon so-called semi-linear material (e.g., see [KOI76]) for which the complementary energy is a quadratic form

$$\Sigma(\mathbf{t}^h) = \frac{1}{2}\mathbf{t}^h \cdot \mathbf{D}^{-1}\mathbf{t}^h \ , \qquad [35]$$

where $\mathbf{D}$ is the elastic modulus of a standard form (e.g., see [ZIT89], p. 94) for an isotropic material.

Hence, the discrete approximation of the variational principle in [22] can be written in matrix notation as

$$\Pi(\mathbf{u}^h,\mathbf{R}^h,\mathbf{t}^h,\mathbf{p}^h) = \int_{\mathcal{B}^h} \{-\frac{1}{2}\mathbf{t}^h \cdot \mathbf{D}^{-1}\mathbf{t}^h + \mathbf{t}^h \cdot \mathbf{e}(\mathbf{u}^h,\mathbf{R}^h)$$

$$+\mathbf{p}^h \cdot \omega(\mathbf{u}^h,\mathbf{R}^h)\} \ d\mathcal{B} - \int_{\mathcal{B}^h} \mathbf{u}^h \cdot \mathbf{f} \ d\mathcal{B} \ . \qquad [36]$$

Within the framework of geometrically linear theory, Hughes and Brezzi [HUB89] proposed a regularized form of the variational principle. The corresponding generalization of their proposal for the present, geometrically nonlinear case can be written down as

$$\Pi_\gamma(\mathbf{u}^h,\mathbf{R}^h,\mathbf{t}^h,\mathbf{p}^h) = \Pi(\mathbf{u}^h,\mathbf{R}^h,\mathbf{t}^h,\mathbf{p}^h) - \int_{\mathcal{B}^h} \{\frac{1}{2}\mathbf{p}^h \cdot \gamma^{-1}\mathbf{p}^h\} \ d\mathcal{B} \ , \qquad [37]$$

where γ is a regularization parameter. While an optimal value of γ, $\gamma = \mu$, was identified in the infinitesimal theory on the basis of convergence analysis of the discrete problem (see [HUB89]), no such conclusion appears to be possible to draw for the finite deformation case. One indication for keeping the same choice of γ in the nonlinear as in the linear case follows from the fact that the linearized form of [37] reduces to the regularized form of Hughes and Brezzi [HUB89].

The regularized form of the variational principle preserves the Euler-Lagrange equations [16], [17] and [23], only now written in the matrix form, while producing an additional Euler-Lagrange equation which is given as

$$\mathbf{p}^h = \gamma\boldsymbol{\omega}(\mathbf{u}^h, \mathbf{R}^h) \ . \qquad [38]$$

Different versions of the regularized variational principle in [37] are possible to use for the finite element implementation. For example, we can insert in [37] the Euler-Lagrange equations for $\mathbf{t}^h$, $\mathbf{t}^h = \mathbf{D}\mathbf{e}(\mathbf{u}^h, \mathbf{R}^h)$, in order to produce a mixed-type variational principle with $\mathbf{u}^h$, $\mathbf{R}^h$ and $\mathbf{p}^h$ as the dependent variables (e.g., see [IBR93]). Moreover, if we also insert the Euler-Lagrange equation [38], we get the simplest form of the regularized variational principle with kinematic variables only

$$\Pi(\mathbf{u}^h, \mathbf{R}^h) = \int_{\mathcal{B}^h} \frac{1}{2}\{\mathbf{e}(\mathbf{u}^h, \mathbf{R}^h)\cdot\mathbf{D}\mathbf{e}(\mathbf{u}^h, \mathbf{R}^h) + \boldsymbol{\omega}(\mathbf{u}^h, \mathbf{R}^h)\cdot\gamma\boldsymbol{\omega}(\mathbf{u}^h, \mathbf{R}^h)\}\, d\mathcal{B}$$
$$- \int_{\mathcal{B}^h} \mathbf{u}^h\cdot\mathbf{f}\, d\mathcal{B} \ . \qquad [39]$$

4. Incompatible modes and operator split

In the foregoing, we will drop the superscript $'h'$ in order to alleviate the notation. A theoretical framework for addition of incompatible modes (see [IBF93]) can be provided though the additive split of the displacement gradient, i.e. by adding an enhanced displacement gradient $[\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3]$ to the existing displacement gradient $[\nabla\mathbf{u}]$. The variational formulation now becomes

$$\Pi(\mathbf{u}, \mathbf{R}, \mathbf{d}) := \int_{\mathcal{B}} \{\frac{1}{2}[\mathbf{e}(\mathbf{u}, \mathbf{R}, \mathbf{d})\cdot\mathbf{C}\mathbf{e}(\mathbf{u}, \mathbf{R}, \mathbf{d}) + \boldsymbol{\omega}(\mathbf{u}, \mathbf{R}, \mathbf{d})\cdot\gamma\boldsymbol{\omega}(\mathbf{u}, \mathbf{R}, \mathbf{d})] - \tilde{\mathbf{p}}\cdot\mathbf{d}\}\, d\mathcal{B}$$
$$- \int_{\mathcal{B}} \mathbf{u}\cdot\mathbf{f}\, d\mathcal{B} \ , \qquad [40]$$

where $\mathbf{d}^T = \langle \mathbf{d}_1^T \mathbf{d}_2^T \mathbf{d}_3^T \rangle$ and $\tilde{\mathbf{p}}$ is the set of Lagrange multipliers[1].

In the modified method of incompatible modes (see [IBW91] or [IBF93]), the interpolations for the enhanced displacement gradient,

$$\mathbf{d} = \widehat{\mathbf{G}}\boldsymbol{\alpha} \ ; \ \widehat{\mathbf{G}} = [\widehat{\mathbf{G}}_1, \widehat{\mathbf{G}}_2, \widehat{\mathbf{G}}_3] \ ; \ \widehat{\mathbf{G}}_I = \begin{bmatrix} \frac{\partial \widehat{M}_I}{\partial x_1}\mathbf{I}_3 \\ \frac{\partial \widehat{M}_I}{\partial x_2}\mathbf{I}_3 \\ \frac{\partial \widehat{M}_I}{\partial x_3}\mathbf{I}_3 \end{bmatrix} \ , \qquad [41]$$

are selected so to eliminate the stress parameters $\tilde{\mathbf{p}}$. With the modification: $\int_{\mathcal{B}} \widehat{\mathbf{G}}\, d\mathcal{B} = \mathbf{0}$ we enforce that the (element-wise) constant stress is included in $\tilde{\mathbf{p}}$, which ensures the satisfaction of the patch test (see [ZIT89], Ch. 11).

[1] Stress tensor $\tilde{\mathbf{p}}$ is energy-conjugate to the deformation gradient; Hence from the standard result on energy-conjugate pairs (e.g., see [MAH83]), $\tilde{\mathbf{p}}$ is the first Piola-Kirchhoff stress

The variational equations that follow from [40] are

$$\begin{aligned} \delta\mathbf{a}\cdot\mathbf{r}(\mathbf{u},\mathbf{R},\mathbf{d}) &:= \int_{\mathcal{B}}\{\delta\mathbf{e}(\mathbf{u},\mathbf{R},\mathbf{d})\cdot\mathbf{C}\mathbf{e}(\mathbf{u},\mathbf{R},\mathbf{d})+\delta\boldsymbol{\omega}(\mathbf{u},\mathbf{R},\mathbf{d})\cdot\gamma\boldsymbol{\omega}(\mathbf{u},\mathbf{R},\mathbf{d})\}\,d\mathcal{B} \\ &\quad -\int_{\mathcal{B}}\delta\mathbf{u}\cdot\mathbf{f}\,d\mathcal{B}=0 \\ \delta\boldsymbol{\alpha}\cdot\mathbf{h}(\mathbf{u},\mathbf{R},\mathbf{d}) &:= \int_{\mathcal{B}}\{\delta\mathbf{d}\cdot\boldsymbol{\Lambda}^T\mathbf{C}\mathbf{e}(\mathbf{u},\mathbf{R},\mathbf{d})+\delta\mathbf{d}\cdot\boldsymbol{\Xi}^T\gamma\boldsymbol{\omega}(\mathbf{u},\mathbf{R},\mathbf{d})\}\,d\mathcal{B}=0\ , \end{aligned} \qquad [42]$$

where

$$\begin{aligned} \delta\mathbf{e}(\mathbf{u},\mathbf{R},\mathbf{d}) &= \boldsymbol{\Lambda}(\mathbf{R})\,(\mathbf{y}(\delta\mathbf{u})+[\mathbf{Y}(\mathbf{u})+\mathbf{D}]\,\delta\mathbf{w}) \\ \delta\boldsymbol{\omega}(\mathbf{u},\mathbf{R},\mathbf{d}) &= \boldsymbol{\Xi}(\mathbf{R})\,(\mathbf{y}(\delta\mathbf{u})+[\mathbf{Y}(\mathbf{u})+\mathbf{D}]\,\delta\mathbf{w}) \end{aligned} \qquad [43]$$

and

$$\begin{aligned} \mathbf{Y}(\mathbf{u}) &= \begin{bmatrix}\mathbf{Y}_1(\mathbf{u})\\ \mathbf{Y}_2(\mathbf{u})\\ \mathbf{Y}_3(\mathbf{u})\end{bmatrix}\ ;\ \mathbf{Y}_i\mathbf{b}\equiv\mathbf{y}_i\times\mathbf{b}\ ; \\ \mathbf{D} &= \begin{bmatrix}\mathbf{D}_1\\ \mathbf{D}_2\\ \mathbf{D}_3\end{bmatrix}\ ;\ \mathbf{D}_i\mathbf{b}\equiv\mathbf{D}_i\times\mathbf{b}\ ;\ \forall\mathbf{b}\in\Re^3\ . \end{aligned} \qquad [44]$$

In [42] and [43] we have used $\delta\mathbf{w}$ to denote the axial vector of the matrix of infinitesimal, virtual rotations $\delta\mathbf{W}$ (see [ARG82]) which is given as

$$\delta\mathbf{W}=\delta\mathbf{R}\,\mathbf{R}^T\ ;\ \delta\mathbf{W}\mathbf{b}\equiv\delta\mathbf{w}\times\mathbf{b}\ . \qquad [45]$$

Virtual displacements $\delta\mathbf{u}$ and virtual rotations $\delta\mathbf{w}$ are interpolated in the isoparametric manner (e.g. see [ZIT89], Ch. 7) with

$$\begin{aligned} \delta\mathbf{u} &= \textstyle\sum_{I=1}^{8} N_I\,\delta\mathbf{u}_I \\ &= \mathbf{N}\,\delta\mathbf{u}^e \\ \delta\mathbf{w} &= \textstyle\sum_{I=1}^{8} N_I\,\delta\mathbf{w}_I \\ &= \mathbf{N}\,\delta\mathbf{w}^e\ . \end{aligned} \qquad [46]$$

Grouping the last two together, we can write

$$\delta\mathbf{a}=\sum_{I=1}^{8} N_I\,\delta\mathbf{a}_I\ . \qquad [47]$$

Making use of the following matrix notation for the stress tensor

$$\mathbf{p}=\boldsymbol{\Lambda}^T\mathbf{C}\mathbf{e}(\mathbf{u},\mathbf{R},\mathbf{d})+\boldsymbol{\Xi}^T\gamma\boldsymbol{\omega}(\mathbf{u},\mathbf{R},\mathbf{d})\ , \qquad [48]$$

the variational equations [42] lead to a set of equations which can be written as

$$\begin{aligned} \mathbf{r}(\mathbf{u},\mathbf{R},\mathbf{d}) &:= \int_{\mathcal{B}}\widehat{\mathbf{B}}^T\mathbf{p}\,d\mathcal{B}-\int_{\mathcal{B}}\mathbf{N}^T\mathbf{f}\,d\mathcal{B}=0 \\ \mathbf{h}(\mathbf{u},\mathbf{R},\mathbf{d}) &:= \int_{\mathcal{B}}\widehat{\mathbf{G}}^T\mathbf{p}\,d\mathcal{B}=0\ , \end{aligned} \qquad [49]$$

where

$$\begin{aligned} &\widehat{\mathbf{B}}=[\mathbf{B},\widehat{\mathbf{Y}}]\ ;\ \mathbf{B}=[\mathbf{B}_1,\mathbf{B}_2,...,\mathbf{B}_8]\ ;\ \widehat{\mathbf{Y}}=[\widehat{\mathbf{Y}}_1,\widehat{\mathbf{Y}}_2,...,\widehat{\mathbf{Y}}_8]\ ; \\ &\mathbf{B}_I=\begin{bmatrix}\frac{\partial N_I}{\partial x_1}\mathbf{I}_3\\ \frac{\partial N_I}{\partial x_2}\mathbf{I}_3\\ \frac{\partial N_I}{\partial x_3}\mathbf{I}_3\end{bmatrix}\ ;\ \widehat{\mathbf{Y}}_I=[N_I[\mathbf{Y}(\mathbf{u})+\mathbf{D}]]\ . \end{aligned} \qquad [50]$$

One possibility to solve the nonlinear system in [49] is to linearize the complete system, as presented in [IBF93] for a two-dimensional case. However, for the three-dimensional case under consideration this entails a large secondary storage pool for the element arrays related to the incompatible modes. In order to reduce the secondary storage requirements, we resort to the operator split method (see [CHM78]): first the solution of [49] is obtained for incompatible mode parameters $\boldsymbol{\alpha}$, while keeping the values of $\mathbf{u}$ and $\mathbf{R}$ "frozen", which is then followed by the solution for $\mathbf{u}$ and $\mathbf{R}$ for the previously found value of $\boldsymbol{\alpha}$ fixed[2].

The first sweep for computing $\boldsymbol{\alpha}$ follows from the linearized form of $[49]_2$ (for fixed values of displacement parameters) as

$$\mathbf{H}\,\Delta\tilde{\boldsymbol{\alpha}} = \mathbf{h} \implies \tilde{\boldsymbol{\alpha}} = \boldsymbol{\alpha} - \mathbf{H}^{-1}\mathbf{h} \ , \qquad [51]$$

where

$$\mathbf{H} = \int_{\mathcal{B}} \widehat{\mathbf{G}}^T[\boldsymbol{\Lambda}^T\mathbf{C}\boldsymbol{\Lambda} + \boldsymbol{\Xi}^T\gamma\boldsymbol{\Xi}]\widehat{\mathbf{G}}\, d\mathcal{B} \ . \qquad [52]$$

Note that [51] is a set of linear equations in incompatible mode parameters $\boldsymbol{\alpha}$; Hence a single update in $[51]_2$ is sufficient to obtain the final values of the incompatible mode interpolation parameters, denoted as $\tilde{\boldsymbol{\alpha}}$.

In the second sweep we linearize the system in [49], for the fixed values of $\tilde{\boldsymbol{\alpha}}$. If we denote incremental increase in displacements $\Delta\mathbf{u}$ and rotations $\Delta\mathbf{w}$, i.e. $\Delta\mathbf{a}^T =< \Delta\mathbf{u}^T, \Delta\mathbf{w}^T >$, we can write the linearized form of [49] as

$$\begin{aligned} \mathbf{K}\,\Delta\mathbf{a} + \mathbf{F}^T\,\Delta\tilde{\boldsymbol{\alpha}} &= -\mathbf{r} \\ \mathbf{F}\,\Delta\mathbf{a} + \mathbf{H}\,\Delta\tilde{\boldsymbol{\alpha}} &= \mathbf{0} \end{aligned} \qquad [53]$$

where $\mathbf{H}$ and $\tilde{\alpha}$ are the same as in [51]. In [53] above, $\mathbf{K}$ takes the form

$$\mathbf{K} = \int_{\mathcal{B}} \widehat{\mathbf{B}}^T[\boldsymbol{\Lambda}^T\mathbf{C}\boldsymbol{\Lambda} + \boldsymbol{\Xi}^T\gamma\boldsymbol{\Xi}]\widehat{\mathbf{B}}\, d\mathcal{B} + \int_{\mathcal{B}} \begin{bmatrix} \mathbf{0} & \mathbf{B}^T\mathbf{P}^T\mathbf{N} \\ \mathbf{N}^T\mathbf{P}\mathbf{B} & \mathbf{N}^T\mathbf{E}\mathbf{N} \end{bmatrix} d\mathcal{B} \ , \qquad [54]$$

where

$$\begin{aligned} &\mathbf{P} = [\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3] \ ; \ \mathbf{P}_i\mathbf{b} = \mathbf{p}_i \times \mathbf{b} \ ; \ \mathbf{p}^T = \langle \mathbf{p}_1^T\mathbf{p}_2^T\mathbf{p}_3^T \rangle \\ &\mathbf{E} = \textstyle\sum_{i=1}^3[\mathbf{p}_i \otimes (\mathbf{y}_i(\mathbf{u}) + \mathbf{d}_i) - (\mathbf{p}_i \cdot (\mathbf{y}_i(\mathbf{u}) + \mathbf{d}_i))\mathbf{I}_3] \ . \end{aligned} \qquad [55]$$

Similarly, we have

$$\mathbf{F} = \int_{\mathcal{B}} \widehat{\mathbf{G}}^T[\boldsymbol{\Lambda}^T\mathbf{C}\boldsymbol{\Lambda} + \boldsymbol{\Xi}^T\gamma\boldsymbol{\Xi}]\widehat{\mathbf{B}}\, d\mathcal{B} + \int_{\mathcal{B}} \widehat{\mathbf{B}}^T\mathbf{P}^T\mathbf{N}\, d\mathcal{B} \ , \qquad [56]$$

It is important to note that parameters $\Delta\tilde{\boldsymbol{\alpha}}$ are already known, since they are computed in [51]; Hence, eliminating $\Delta\tilde{\boldsymbol{\alpha}}$ via static condensation (e.g., see [WIL74]) we obtain the final form of the element stiffness matrix.

For clarity, the complete procedure is summarized in Table 1 below.

[2] The same concepts are commonly used in the computational plasticity; See, for example, [IBR94] for a more detailed discussion

Table 1. Operator split solution procedure

- Given: $\mathbf{u}^{(i)}$, $\mathbf{R}^{(i)} \equiv \{q_0^{(i)}; \mathbf{q}^{(i)}\}$ and $\boldsymbol{\alpha}^{(i)}$
- Update incompatible mode parameters

$$\boldsymbol{\alpha}^{(i+1)} = \boldsymbol{\alpha}^{(i)} - \mathbf{H}^{(i)}\mathbf{h}^{(i)}$$

- Store: $\boldsymbol{\alpha}^{(i+1)}$
- Compute displacement and rotation increments $\Delta\mathbf{a}^{(i)} = (\Delta\mathbf{u}^{(i)}, \Delta\mathbf{w}^{(i)})$

$$[\mathbf{K}^{(i)} - \mathbf{F}^{(i)T}\mathbf{H}^{(i)-1}\mathbf{F}^{(i)}]\,\Delta\mathbf{a}^{(i)} = -\mathbf{r}^{(i)}$$

- Update displacements

$$\mathbf{u}^{(i+1)} = \mathbf{u}^{(i)} + \Delta\mathbf{u}^{(i)}$$

- Update rotations (quaternion representation, see [ARG82])

$$\begin{aligned}
&\Delta w^{(i)} = (\Delta\mathbf{w}^{(i)} \cdot \Delta\mathbf{w}^{(i)})^{1/2} \\
&q_{w0}^{(i)} = cos(\Delta w^{(i)}/2) \ ; \ \mathbf{q}_w^{(i)} = \left(sin(\Delta w^{(i)}/2)/\Delta w^{(i)}\right)\mathbf{w}^{(i)} \\
&q_0^{(i+1)} = q_{w0}^{(i)}q_0^{(i)} - \mathbf{q}_w^{(i)} \cdot \mathbf{q}^{(i)} \ ; \ \mathbf{q}^{(i+1)} = q_{w0}^{(i)}\mathbf{q}^{(i)} + q_0^{(i)}\mathbf{q}_w^{(i)} + \mathbf{q}_w^{(i)} \times \mathbf{q}^{(i)} \\
&\mathbf{R}^{(i+1)} = (2q_0^{(i+1)2} - 1)\mathbf{I}_3 + 2q_0^{(i+1)}[\mathbf{q}^{(i+1)} \times \mathbf{I}_3] + 2\mathbf{q}^{(i+1)} \otimes \mathbf{q}^{(i+1)}
\end{aligned}$$

- Store: $\{q_0^{(i+1)}; \mathbf{q}^{(i+1)}\}$

5. Alternative rotation parameterization

The derivation given in the preceding is based on the parameterization of the finite rotations via an orthogonal matrix. An important advantage of such a parameterization is its intrinsic nature and typically the simplest forms of the resulting expressions. However, this sort of parameterization has few disadvantages as well. First, even with the number of parameters being reduced significantly with the quaternion representation of the orthogonal matrix of finite rotations, costly secondary storage manipulations are necessary for handling the rotation update (see Table 1). Second, the tangent stiffness matrix is in general non-symmetric (see eqs [55]), which doubles the computational effort in equation solving. One can say that the second disadvantage is particularly worrisome having in mind that the equation solving is anyhow a cost-dominant phase in the solution procedure of a three-dimensional problem.

Therefore, in this section we propose an alternative parameterization of finite rotations via so-called rotation vector (see [IFK95]), for which both deficiencies alluded to in the above can be removed. According to the Euler theorem for finite rotations there exist a vector $\boldsymbol{\theta}$ which is not affected by the rotation, so that $\boldsymbol{\theta} = \mathbf{R}\boldsymbol{\theta}$. If $\boldsymbol{\theta}$ is considered as the axial vector of a skew-symmetric matrix Θ, i.e. if $\Theta\mathbf{b} = \boldsymbol{\theta} \times \mathbf{b}$; $\forall \mathbf{b} \in \Re^3$, we can compute the corresponding orthogonal matrix of finite rotations via so-called Rodrigues formula

$$\mathbf{R} = cos\theta\,\mathbf{I} + \frac{sin\theta}{\theta}\Theta + \frac{1-cos\theta}{\theta^2}\boldsymbol{\theta}\otimes\boldsymbol{\theta} \equiv exp[\Theta] \ , \qquad [57]$$

where $\theta = (\boldsymbol{\theta}\cdot\boldsymbol{\theta})^{1/2}$ is the rotation vector magnitude. By using the well-known vector identity $\Theta(\Theta\mathbf{b}) = [\boldsymbol{\theta}\otimes\boldsymbol{\theta} - \theta^2\mathbf{I}]\mathbf{b}$ from [57] we can recover an alternative form of the Rodrigues formula which was used in [ARG82].

It is important to note that the expression in [57] is singularity-free for any magnitude of the rotation vector, hence $\boldsymbol{\theta}$ can also be used to parameterize the finite rotation. In this case with $\boldsymbol{\theta}$ being an element of a vector space, the admissible variations $\delta\boldsymbol{\theta}$ belong to the same space. One can establish a relationship between these admissible variations and the virtual rotations $\delta\mathbf{W}$ by making use of [57] and the following expression (see [IFK95])

$$exp[\Theta + t\,\delta\Theta] = exp[t\,\delta\mathbf{W}]exp[\Theta] \ . \qquad [58]$$

Linearized form of [58] then leads to the corresponding relation of the axial vectors

$$\begin{aligned} \delta\mathbf{w} &= \mathbf{S}(\boldsymbol{\theta})\,\delta\boldsymbol{\theta}, \\ \mathbf{S}(\boldsymbol{\theta}) &= \tfrac{sin\theta}{\theta}\mathbf{I} + \tfrac{1-cos\theta}{\theta^2}\Theta + \tfrac{\theta-sin\theta}{\theta^3}\boldsymbol{\theta}\otimes\boldsymbol{\theta} \ . \end{aligned} \qquad [59]$$

A detailed derivation of the relationship in [59] is given in [IFK95]. We note that the matrices $\mathbf{R}$ and $\mathbf{S}$ are linear combinations of the same matrices. Moreover, they share the same eigenvectors, which can be used to prove a number of interesting results (see [IFK95]).

With the finite element interpolations of the rotation parameters $\boldsymbol{\theta}$ given as

$$\begin{aligned} \boldsymbol{\theta} &= \textstyle\sum_{I=1}^{8} N_I\,\boldsymbol{\theta}_I \\ &= \mathbf{N}\,\boldsymbol{\theta}^e \ , \end{aligned} \qquad [60]$$

for the given values of the nodal rotation parameters $\boldsymbol{\theta}^e$, we can directly compute $\boldsymbol{\theta}$ in [60] and hence the orthogonal matrix $\mathbf{R}$ in [57] at any point in the solid element (e.g., a Gauss integration point). Hence, in sharp contrast with the quaternion parameters, no secondary storage manipulations are needed.

The admissible variations of rotation parameters are also interpolated with the type of interpolations in [60] with

$$\begin{aligned} \delta\boldsymbol{\theta} &= \textstyle\sum_{I=1}^{8} N_I\,\delta\boldsymbol{\theta}_I \\ &= \mathbf{N}\,\delta\boldsymbol{\theta}^e \ , \end{aligned} \qquad [61]$$

which replaces the interpolations in [46]. The new form of the nonlinear algebraic equations in $[49]_1$ can be written as

$$\mathbf{r}(\mathbf{u},\boldsymbol{\theta},\mathbf{d}) := \int_{\mathcal{B}} \tilde{\mathbf{B}}^T\mathbf{p}\,d\mathcal{B} - \int_{\mathcal{B}} \mathbf{N}^T\mathbf{f}\,d\mathcal{B} = \mathbf{0} \ , \qquad [62]$$

where

$$\tilde{\mathbf{B}} = [\mathbf{B}, \tilde{\mathbf{Y}}] \; ; \; \mathbf{B} = [\mathbf{B}_1, \mathbf{B}_2, ..., \mathbf{B}_8] \; ; \; \tilde{\mathbf{Y}} = [\tilde{\mathbf{Y}}_1, \tilde{\mathbf{Y}}_2, ..., \tilde{\mathbf{Y}}_8] \; ;$$
$$\mathbf{B}_I = \begin{bmatrix} \frac{\partial N_I}{\partial x_1}\mathbf{I}_3 \\ \frac{\partial N_I}{\partial x_2}\mathbf{I}_3 \\ \frac{\partial N_I}{\partial x_3}\mathbf{I}_3 \end{bmatrix} \; ; \; \tilde{\mathbf{Y}}_I = N_I \begin{bmatrix} [\mathbf{Y}_1(\mathbf{u}) + \mathbf{D}_1]\mathbf{S} \\ [\mathbf{Y}_2(\mathbf{u}) + \mathbf{D}_2]\mathbf{S} \\ [\mathbf{Y}_3(\mathbf{u}) + \mathbf{D}_3]\mathbf{S} \end{bmatrix} . \qquad [63]$$

The form of the residual $\mathbf{h}$ in $[49]_2$, due to incompatible modes, remains unaffected by this reparameterization of finite rotations. The operator split procedure still applies as given in [51] to [53], except that the tangent stiffness now takes a different form from the one given in [54]. We now have

$$\mathbf{K} = \int_{\mathcal{B}} \tilde{\mathbf{B}}^T[\mathbf{\Lambda}^T\mathbf{C}\mathbf{\Lambda} + \mathbf{\Xi}^T\gamma\mathbf{\Xi}]\tilde{\mathbf{B}}\, d\mathcal{B} + \int_{\mathcal{B}} \begin{bmatrix} 0 & \mathbf{B}^T\tilde{\mathbf{P}}^T\mathbf{N} \\ \mathbf{N}^T\tilde{\mathbf{P}}\mathbf{B} & \mathbf{N}^T\tilde{\mathbf{A}}\mathbf{N} \end{bmatrix} d\mathcal{B} \, , \qquad [64]$$

where

$$\tilde{\mathbf{P}} = \mathbf{S}^T[\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3] \qquad [65]$$

and

$$\tilde{\mathbf{A}} = \mathbf{S}^T\mathbf{E}\mathbf{S} + \mathbf{M}(\tilde{\mathbf{v}}) \; ; \; \tilde{\mathbf{v}} = \sum_{i=1}^{3} \mathbf{p}_i \times (\mathbf{y}_i(\mathbf{u}) + \mathbf{d}_i) \, , \qquad [66]$$

with

$$\mathbf{M}(\tilde{\mathbf{v}}) = c_1\,[\tilde{\mathbf{v}} \otimes \boldsymbol{\theta}] \; + \; c_2\,[\tilde{\mathbf{v}} \times \boldsymbol{\theta} \otimes \boldsymbol{\theta}] \; + \; c_3(\boldsymbol{\theta} \cdot \delta\boldsymbol{\theta})\,[\boldsymbol{\theta} \otimes \boldsymbol{\theta}]$$
$$+ \; c_4\,[\tilde{\mathbf{v}} \times \mathbf{I}] \; + \; c_5\,[(\tilde{\mathbf{v}} \cdot \boldsymbol{\theta})\mathbf{I} + [\boldsymbol{\theta} \otimes \tilde{\mathbf{v}}]] \; ; \qquad [67]$$
$$c_1 = \frac{\theta\cos\theta - \sin\theta}{\theta^3} \, , \; c_2 = \frac{\theta\sin\theta + 2\cos\theta - 2}{\theta^4} \, ,$$
$$c_3 = \frac{3\sin\theta - 2\theta - \theta\cos\theta}{\theta^5} \, , \; c_4 = \frac{1 - \cos\theta}{\theta^2} \, , \; c_5 = \frac{\theta - \sin\theta}{\theta^3} \, .$$

As opposed to matrix $\mathbf{E}$ in [54] and [55], matrix $\tilde{\mathbf{A}}$ in [65] and [66] is a symmetric matrix, which renders the element stiffness matrix symmetric as well. Thus when solving the linearized system one can take advantage of symmetry and reduce the computational effort rather significantly.

For clarity, the new form of the operator split procedure is summarized in Table 2 below.

Table 2. Operator split solution procedure

- Given: $\mathbf{u}^{(i)}$, $\boldsymbol{\theta}^{(i)}$
- Update incompatible mode parameters

$$\boldsymbol{\alpha}^{(i+1)} = \boldsymbol{\alpha}^{(i)} - \mathbf{H}^{(i)}\,\mathbf{h}^{(i)}$$

- Store: $\boldsymbol{\alpha}^{(i+1)}$
- Compute displacement and rotation increments $\Delta\mathbf{a}^{(i)} = (\Delta\mathbf{u}^{(i)}, \Delta\boldsymbol{\theta}^{(i)})$

$$[\mathbf{K}^{(i)} - \mathbf{F}^{(i)T}\mathbf{H}^{(i)-1}\mathbf{F}^{(i)}]\,\Delta\mathbf{a}^{(i)} = -\mathbf{r}^{(i)}$$

- Update displacements

$$\mathbf{u}^{(i+1)} = \mathbf{u}^{(i)} + \Delta \mathbf{u}^{(i)}$$

- Update rotations

$$\theta^{(i+1)} = \theta^{(i)} + \Delta \theta^{(i)}$$

6. Numerical examples

6.1. Patch test

To check the element consistency we first performed the patch test (e.g., see [ZIT89], Ch. 11) for a mesh of 7 irregular solid elements that fit together into a cube of unit volume. See Figure 1.

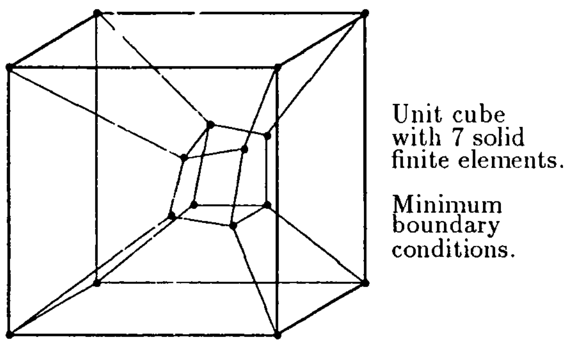

Figure 1. Unit cube for the patch test

Large displacement analysis is carried out. The cube is fixed with a minimum number of constraints which prevent the occurrence of rigid body modes. It is exposed to a homogeneous stress state, obtained by the four concentrated forces each equal to $f_1 = 250$, applied at the free end of the cube. For the given values of Young's modulus $E = 1000$ and Poisson's ratio $\nu = 0.1$, the cube undergoes the large longitudinal displacements $u_1 = 1$, and lateral contractions $u_2 = u_3 = 0.1$. The convergence is obtained with one iteration.

6.2. Large displacement analysis of 45-degree bend

The second example presents large displacement analysis of a 45-degree bend subjected to vertical forces applied at the free-end. See Figure 2. The bend is modeled by 16 8-node solid elements presented herein. This example is adopted from the work of Bathe [BAB79], where a reference solution is obtained by 16 20-node isoparametric solid elements.

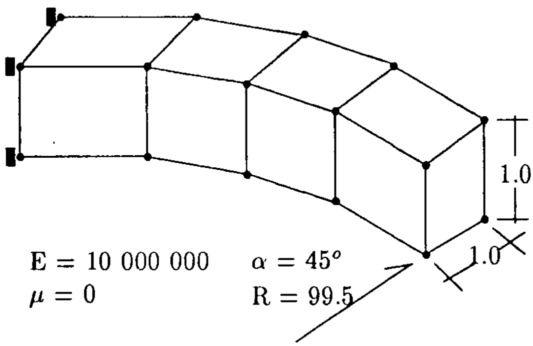

Figure 2. Cantilever 45-degree bend

The analysis is performed for the total value of free-end forces equal to $f_3 = 600$. Total loading is applied in six equal load steps. In each step, the solution exhibits the quadratic convergence rate for both parameterization of finite rotations. See results shown in Table 3 for the last load step

Table 3. Convergence rates for the 45-degree bend

Iter.	Orthogonal matrix		Rotation vector	
No.	Residual norm	Energy norm	Residual norm	Energy norm
0	5.000×10^1	3.509×10^2	5.000×10^1	3.509×10^2
1	6.299×10^5	1.605×10^4	6.296×10^5	1.607×10^4
2	6.585×10^1	4.274×10^0	6.603×10^1	4.306×10^0
3	7.562×10^3	2.381×10^0	7.617×10^3	2.419×10^0
4	6.385×10^{-2}	3.899×10^{-6}	5.016×10^{-2}	2.668×10^{-6}
5	7.155×10^{-3}	2.282×10^{-12}	7.463×10^{-3}	3.978×10^{-12}
6	5.735×10^{-7}	2.076×10^{-20}	4.716×10^{-7}	3.054×10^{-20}

The results obtained for the free-end displacement components (for the point in the center of the cross-section) are presented in Table 4, along with the results obtained in [BAB79].

Table 4. Free-end displacements for 45-degree bend

Model	u_1	u_2	u_3
Present	13.642	-23.299	53.206
Bathe and Bolourchi	13.4	-23.5	53.4

6.3. Cork-screw motion of a T-shape cantilever

In the final example we consider a T-shape cantilever. The chosen material properties are: Young's modulus $E = 2 \times 10^4$ and Poisson's ratio $\nu = 0$. The cantilever is modeled with 21 brick elements (21 unit cubes), 10 for the rib and 11 for the flange, and the total number of nodes is 88. See Figure 3.

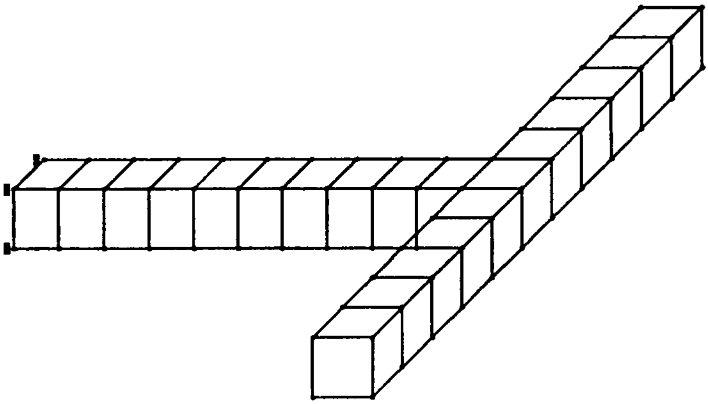

Figure 3. FE model for a T-shape cantilever

The nonlinear analysis, which we performed, mimics the motion of a cork-screw: we first twisted the rib of the T-shape through the angle of 2π by applying the torsional moment $m_t = 1080$, and then bent the flange ends, each through the angle of π, by applying the bending moments $m_b = 960$. This nonlinear analysis is performed in 4 load steps. Deformed shapes obtained in each step are shown in Figure 4.

7. Closing remarks

One can say that, in general, both a sound theoretical foundations and the fine details of numerical implementation need to be addressed in constructing an optimal solid element for finite deformation analysis. We hope that this work has presented both.

A sound variational formulation draws on the fundamental work of Fraeijs de Veubeke, but than departs from it crucially in proposing a regularized form of the variational principle which facilitates the finite element implementation. On the finite element implementation side, we set to produce a new 8-node solid finite element with 6 degrees of freedom per node and an enhanced performance. The key role in achieving that objective is played by the modified method of incompatible modes.

On the computational efficiency side, we have shown how exploiting the idea of the operator split methodology, the implementation of the modified method of incompatible modes can be rendered very efficient (with a single iteration to recover the incompatible mode parameters), and the secondary storage requirements reduced. We have also shown how the efficiency can be further reinforced by adopting a vector-like parameterization of finite rotations.

In this work we have discussed the elastic deformations only; However, the proposed formulation is very well suited for extension to a more general case of inelastic deformations. Finally, the presence of the element rotational degrees of freedom could prove advantageous in the nonlinear analysis of thick plates and shells.

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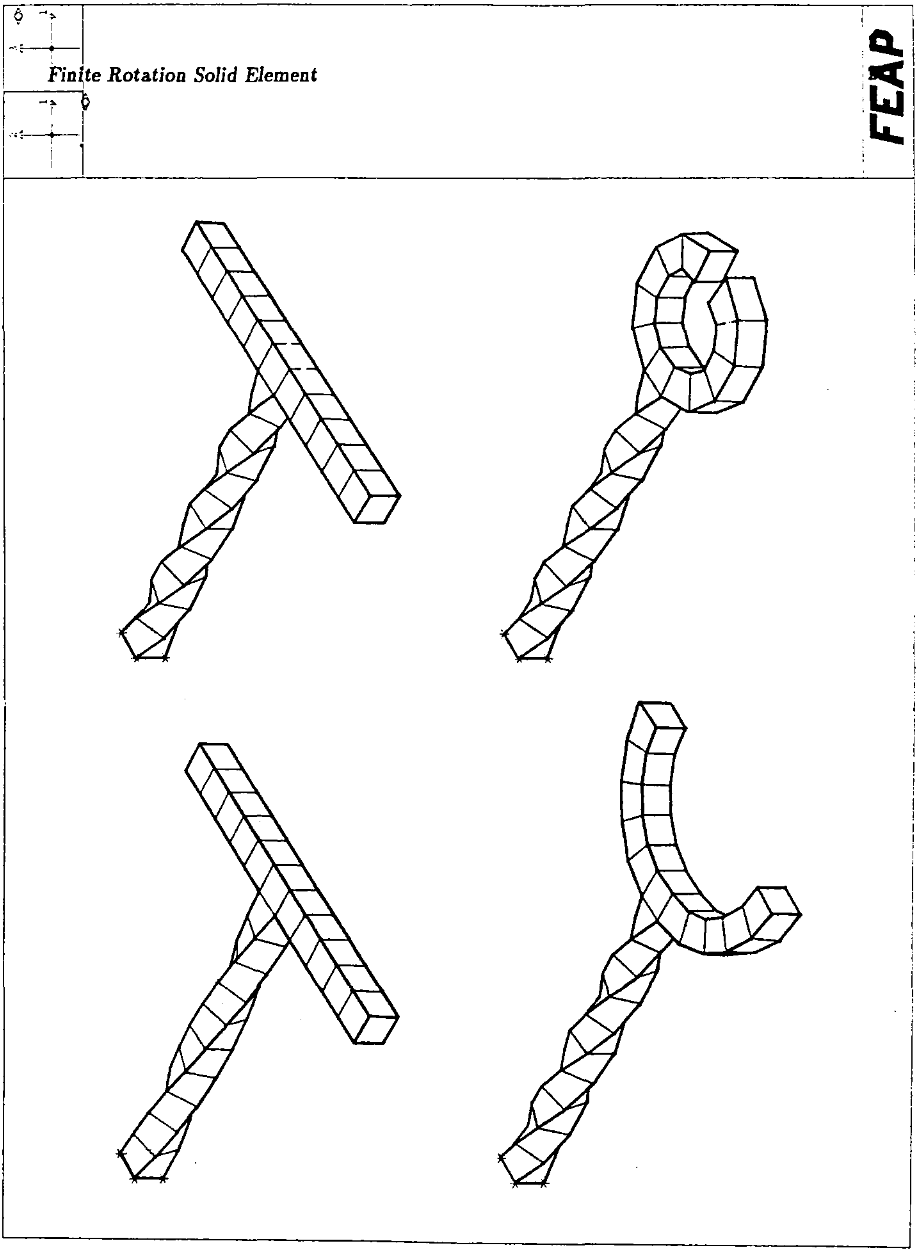

Figure 4. Deformed shapes of the T-shape cantilever

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