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General constitutive updating for finite strain formulations based on assumed strains and the Jacobian

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ABSTRACT

Compatibility between element technology featuring assumed (finite)-strains based on least-squares and current constitutive formulations employed in elastic and inelastic contexts is a demanding task. Local frames are required for anisotropic and cohesive laws, some assumed-strain element technologies do not explicitly provide the deformation gradient, and total Lagrangian approaches are often inadequate for advanced plasticity models. Kirchhoff stress-based $\boldsymbol{F}_e\,\boldsymbol{F}_p$ decompositions are also not convenient for ductile damage models. In addition, if rotational degrees-of-freedom are used, as is the case in beams and shells, the adoption of a fixed undeformed configuration causes implementation brittleness. An additional aspect to consider is remeshing by element partitioning, which precludes the storage of constitutive tensors in local frames, invalidating the stored quantities. Based on seven algorithmic requirements and the corresponding design solutions, we introduce a general constitutive updating algorithm based on the strain and the Jacobian provided by the element. This allows the use of virtually any constitutive law with any finite-strain element formulation while satisfying the seven requirements. In addition, Newton-Raphson convergence properties are extraordinary, at the cost of precision in the strain rate estimation. As a prototype element implementation, we present a stable hexahedron based on least-squares strains. A BFGS secant estimation is employed for the weight in the least-squares so that softening constitutive laws can be adopted without stability issues at the element level.

1. Introduction

Our recent element partition algorithm [5] introduced an additional requirement to the constitutive updating which is the storage in a common frame of the relevant constitutive tensors. This requirement and the use of continuum formulations that can include as particular case cohesive elements [7] are here addressed. The new approach is based on the reference configuration Jacobian and the relative Green-Lagrange strain. The reference configuration frame is now indirectly obtained from the Jacobian, as is the rotation tensor and the deformation gradient.

In addition, high performance element technology for low-order discretizations (the so-called high-coarse mesh performance elements) is often based on assumed strains [13] and can become unstable when the constitutive models involve strain softening. EAS formulations [34–36] have known stability problems which are seriously aggravated by constitutive softening.

Assumed-strain and enhanced strain elements can be formulated in terms of the deformation gradient [34] or, in alternative, the Green-Lagrange strain [1,17]. Of course from the latter it is impossible in general to obtain the former, since the rotation tensor is missing from the assumed strain tensor. Hence, although polar-decomposition is possible from a non-assumed strain version, this is incompatible with the Green-Lagrange strain. Betsch and Stein state this in clear and direct terms: *"Assumed strain elements usually provide the Green-Lagrangian strain tensor (or equivalently the right Cauchy-Green tensor) whereas the deformation gradient is not given. On the other hand, previously published constitutive algorithms based on the multiplicative decomposition of the deformation gradient into elastic and plastic parts usually require the deformation gradient as input,…"* [14].

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Constitutive constraints (such as incompressibility, plane stress and zero normal stress in shells) are also dependent on specific element formulations, see Refs. [8,10,11]. Unless a unified approach is developed, calculations become very intricate without approximations. Besides the inevitable duplication of effort, these incompatibilities are error-prone and produce code maintenance difficulties. To unify the frame determination problem and the polar decomposition (which is necessary in purely assumed-strain elements) we use Löwdin [27] frames. These provide a moving orthogonal local frame-of-reference. By multiplication of two frames (with a transpose), a rotation tensor (in essence an estimate of the polar-decomposition rotation which is not available) is obtained. Therefore, continuum and structural finite-strain elements are accounted with our algorithm. We use a semi-implicit approach: rotation tensors are integrated explicitly and quadratic strains are integrated implicitly. This allows (at the cost of some measured loss of accuracy) the use of a comparatively small number of steps for intricate nonlinear problems. As few as 2 load steps can be used for the Simo 3D tension test.

This work is organized as follows: Section 2 presents the seven requirements, the relative kinematic decomposition and the constitutive updating, including an upper bound on the error in the estimation of the strain rate. The full Algorithm is described in detail. Section 3 shows the prototype element (a least-squares assumed-strain hexahedron) and Section 4 presents the numerical examples. Finally, Section 5 presents the conclusions.

2. Specific kinematics and constitutive updating

2.1. Requirements

The goal of generality in this contribution, namely compatibility between finite-strain constitutive laws and mixed element (in particular plane stress/strain, 3D and shell) formulations, as well as experience in computational nonlinear solid mechanics, led the Authors to introduce the following seven requirements for constitutive updating:

1. Constitutive updating must comply with the geometric requisites of anisotropic constitutive laws (both ab-initio and induced). Specifically, both locally defined and global frames-of-reference must be available [3]. This also applies to *continuum*-based cohesive law formulations, cf [6,7].
2. Constitutive updating must be compatible, by removal of rows in stress and/or strain Voigt forms, with local constitutive constraints such as zero-normal-stress, plane stress and inextensibility [6,8].
3. Constitutive updating must be compatible with both hyperelastic and incremental (or rate-based) constitutive laws, such as inelastic constitutive models [2]. Sensitivity of the stress with respect to strain must be exact and straightforward.
4. Constitutive updating should allow the use of purely assumed-strain elements (e.g. Refs. [1,17]) for which a compatible deformation gradient may not be available or might be computationally costly. This important issue was discussed in the seminal paper by Betsch and Stein [14].
5. Cauchy stresses, or a sufficiently good approximation, must be used so that yield functions are accurately represented. This has been discussed in Ref. [2]. For quasi-incompressible materials the Kirchhoff stress could be used (as in Refs. [33–35]), but many constitutive laws involve significant volume change [9] for which the use of the Kirchhoff stress might be inadequate. This important topic has already been the subject of discussion by Meschke and Liu [30] who used the spectral decomposition of the right stretch tensor.
6. Only relative degrees-of-freedom should be required, which in degenerate shell versions of elements would make use of relative *rotations* [2]. Quaternion parameterization avoid this, but introduce additional housekeeping tasks. A discussion of this theme, including the use of intermediate configurations, is performed in Ref. [16].
7. History variables, such as accumulated strain and stress in configuration Ω_b must use frame 0 so that remeshing by partitioning [5] can be directly performed when local frames change.

These seven requirements are the cause of the following design solutions:

- Requirements 1. and 2. impose the use of a local frame which follows each element motion. Rotation must be compatible with local frame rotations.
- Requirement 2. enforces special significance to the directions of a local frame. For example, in solid-shell variants of 3D elements [4], direction 3 is attributed to the thickness. Although this could be explicitly tailored a the element level, the parent-domain coordinates (here identified by ξ) have traditionally been related to these special directions. In shells, for example, ξ_3 is usually used for the thickness direction, and in beams ξ_3 is used for the longitudinal direction. We therefore make use of this pre-existing convention to adopt the parent-domain Jacobian matrix $\boldsymbol{J}$ as a constitutive quantity.
- Requirement 3. prevents the use of corotational or hypoelastic techniques since they are incompatible with hyperelasticity. It also forces the use of a deformed configuration in which the strain rate is straightforwardly defined. The calculation of stress sensitivity can be performed exactly without the presence of rotation derivatives.
- Requirement 4. enforces a constitutive updating that relies exclusively on the relative Green-Lagrange strain between two configurations Ω_b and Ω_a, here denoted $\boldsymbol{e}_{ab}$, and a frame for configuration Ω_b, which is here established using the orthogonal tensor $\boldsymbol{R}_{0b}$. $\boldsymbol{R}_{0b}$ relates the frame b with a fixed basis in the undeformed configuration.
- Requirement 5. can be addressed by an approximation to the Cauchy stress, here introduced as the relative second Piola-Kirchhoff stress between configurations Ω_b and Ω_a. This relative stress is identified as $\mathbf{S}_{ab}$.
- Requirement 6. enforces the use of step-wise configurations, where the reference configuration corresponds to a converged solution. This allows the use of *relative degrees-of-freedom* between current and converged (or previous) configurations, avoiding rotation condition problems.
- Requirement 7. requires the use of storage of tensors in the initial frame. Since the local frame is defined by $\boldsymbol{R}_{0b}$, transformation back-and-forth between frames 0 and b is necessary for an efficient implementation of partition-based remeshing algorithms, see Ref. [5].

When these design solutions are adopted, we achieve the following: our general constitutive updating must be based on the Jacobian matrix and the relative Green-Lagrange, both provided by the element calculations.

2.2. Frames obtained by SVD of the Jacobians

Unique frames are useful in most elements dealing with finite strain, especially when anisotropic and complex constitutive laws are required. Even with isotropic elements, certain constraints can take advantage of local frames. A *change* in frame-of-reference can be defined by multiplication of two matrices containing the frame basis vectors as columns. This provides the rotation. Consider two configurations[1] Ω_a and Ω_b identified by time instances t_a and t_b such that $t_a \geq t_b$. The initial configuration ($t = 0$) is denoted Ω_0. Let the positions of a given point X in configurations Ω_a and Ω_b be $\boldsymbol{x}_a(\xi, t_a) \in \Omega_a$ and $\boldsymbol{x}_b(\xi, t_b) \in \Omega_b$, respectively. Considering only one *element*, parent-domain coordinates ξ are

[1] We use standard notation in continuum mechanics [39]. Configurations are assumed to possess attached frames.