Energy-Conservation Error Due to Use of Green–Naghdi Objective Stress Rate in Commercial Finite-Element Codes and Its Compensation

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The objective stress rates used in most commercial finite element programs are the Jaumann rate of Kirchhoff stress, Jaumann rates of Cauchy stress, or Green–Naghdi rate. The last two were long ago shown not to be associated by work with any finite strain tensor, and the first has often been combined with tangential moduli not associated by work. The error in energy conservation was thought to be negligible, but recently, several papers presented examples of structures with high volume compressibility or a high degree of orthotropy in which the use of commercial software with the Jaumann rate of Cauchy or Kirchhoff stress leads to major errors in energy conservation, on the order of 25–100%. The present paper focuses on the Green–Naghdi rate, which is used in the explicit nonlinear algorithms of commercial software, e.g., in subroutine VUMAT of ABAQUS. This rate can also lead to major violations of energy conservation (or work conjugacy)—not only because of high compressibility or pronounced orthotropy but also because of large material rotations. This fact is first demonstrated analytically. Then an example of a notched steel cylinder made of steel and undergoing compression with the formation of a plastic shear band is simulated numerically by subroutine VUMAT in ABAQUS. It is found that the energy conservation error of the Green–Naghdi rate exceeds 5% or 30% when the specimen shortens by 26% or 38%, respectively. Revisions in commercial software are needed but, even in their absence, correct results can be obtained with the existing software. To this end, the appropriate transformation of tangential moduli, to be implemented in the user's material subroutine, is derived.
[DOI: 10.1115/1.4024411]

1 Introduction

The deformations and stresses in inelastic solids are in finite elements codes analyzed by an incremental updated Lagrangian procedure, in which the material constitutive behavior is in each loading step characterized in the rate form by the constitutive relation

$$\hat{S}_{ij} = C_{ijkl}\dot{e}_{kl} \qquad (1)$$

where repetitions of subscripts imply summation; the subscripts refer to Cartesian coordinates $x_i (i = 1, 2, 3)$; C_{ijkl} = current tangential moduli, which depend on the current stress; $\dot{e}_{ij} = (v_{i,j} + v_{j,i})/2$ = velocity strain = time rate of the small (linearized) strain $e_{ij} = (u_{i,j} + u_{j,i})/2$; $\hat{S}_{ij}$ = objective stress rate (which means a rate that is invariant at coordinate rotations and characterizes the state of the same material element as it deforms).

Many types of stress rates that are objective have been proposed long ago. Some of them have been shown to be associated by work with some finite strain tensor [1], but others are not. The latter ones are, for instance, used by the commercial software ABAQUS. For reasons unclear, it uses different rates in different methods of analysis: (1) the Jaumann rate of Kirchhoff stress (JK rate) for bifurcation analysis, (2) the Jaumann rate of Cauchy stress (JC rate) for implicit (Riks') incremental analysis (in subroutine UMAT), and (3) the Green–Naghdi (G–N) rate [2] for explicit incremental analysis (in subroutine VUMAT). LS-DYNA and ANSYS do the same. The JK rate is work-conjugate to (i.e., is associated by work with) the Hencky (logarithmic) finite strain tensor. The JC rate is not work-conjugate to any finite strain tensor except if the material is incompressible, in which case it becomes identical to JK. The G–N rate is not work-conjugate to any finite strain tensor.

Although these problems with energy conservation (i.e., the first law of thermodynamics) were pointed out already in 1971 [1], they have either been ignored or thought to cause negligible errors. This is in fact mostly true for metals and elastomers, which represented most of the early applications of large strain analysis. Recently, though, it was discovered that significant energy errors arise for rigid foams (polymeric, metallic, and ceramic), honeycomb, certain soils (loess, silt, underconsolidated and organic soils), some rocks (pumice, tuff), light wood, carton osteoporotic bone, and various biologic tissues. These errors afflict the most popular commercial software—ABAQUS (version 6.8), ANSYS (version 12.0), LS-DYNA (included in ANSYS v12.0), and probably others (ATENA, version 4 [3] is one exception, and the open source code OOFEM version 2.1 [4] is another) [5,6].

Regarding the G–N rate, its lack of work-conjugacy was also made clear long ago. Nevertheless it has apparently not yet been studied in detail and the error magnitude has not been appraised. It will be addressed in this paper.

Another problem with energy conservation was shown to be caused by the use of tangential moduli not associated by work, particularly by combining the Jaumann rate of Kirchhoff stress with a constant shear modulus in small-strain shear buckling

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Contributed by the Applied Mechanics of ASME for publication in the JOURNAL OF APPLIED MECHANICS. Manuscript received January 21, 2013; final manuscript received March 29, 2013; accepted manuscript posted May 7, 2013; published online September 16, 2013. Editor: Yonggang Huang.

[6–9]. Such combination causes serious energy errors for materials with very strong orthotropy; for example for fiber-reinforced polymers, homogenized foam-composite sandwich plates, wood and some biologic tissues, or for constitutive models of isotropic materials in which damage is represented by smearing of parallel cracks.

2 Review of Energy-Consistent (or Work-Conjugate) Objective Stress Rates

While the usual way to derive the objective stress rates has been based on tensorial coordinate transformations, the variational energy approach [1] is preferable because it also ensures energy consistency with the finite strain tensor (while it is also much shorter and simpler). Consider incremental finite strain tensors ε_{ij} relative to the initial (stressed) state at the beginning of the load step, using the initial (Lagrangian) coordinates $x_i (i = 1, 2, 3)$ of material points. A broad class of equally admissible finite strain measures is represented by the Doyle–Ericksen tensors whose second-order approximation is

$$\varepsilon_{ij}^{(m)} = e_{ij} + \frac{1}{2} u_{k,i} u_{k,j} - \frac{1}{2}(2-m) e_{ki} e_{kj} \tag{2}$$

where u_i are the material point displacements, $e_{ij} = (u_{i,j} + u_{j,i})/2 =$ small (linearized) strain tensor, and subscripts preceded by a comma denote partial derivatives. The case $m = 2$ gives the Green–Lagrangian strain tensor, $m = 1$ gives the Biot strain tensor, $m = 0$ gives the Hencky (logarithmic) strain tensor, $m = -2$ gives the Almansi–Lagrangian strain tensor. The work δW done at small deformations of a material element of unit initial volume, starting from an initial state under initial Cauchy (or true) stress S_{ij}^0, can be expressed in two equivalent ways:

$$\delta W = (S_{ij}^0 + \tau_{ij}) \delta u_{i,j} \tag{3}$$

$$\delta W = (S_{ij}^0 + \sigma_{ij}^{(m)}) \delta \varepsilon_{ij}^{(m)} \tag{4}$$

where $\delta\varepsilon_{ij}^{(m)} =$ arbitrary variation of incremental finite strain tensor $\varepsilon_{ij}^{(m)}$, and $\sigma_{ij}^{(m)} =$ small stress increment that is symmetric and objective (an incremental second Piola–Kirchhoff stress); and $\tau_{ij} =$ a nonsymmetric small Lagrangian (or first Piola–Kirchhoff) stress increment. Since the first-order work $S_{ij}^0 \delta u_{ij}$ is canceled in the virtual work equation of equilibrium by the work of loads, only the second-order work is of interest.

The two work expressions in Eqs. (3) and (4) must be equal. Impose this equality and substitute $S_{ij}\delta u_{i,j} = S_{ij}\delta e_{ij} = S_{ij}\dot{e}_{ij}\Delta t$ (by virtue of symmetry of S_{ij}), $\sigma_{ij}^{(m)}\delta\varepsilon_{ij}^{(m)} \approx \sigma_{ij}^{(m)}\dot{e}_{ij}\Delta t$ (which suffices for second-order work accuracy in $u_{i,j}$), $S_{ij}\delta\varepsilon_{ij}^{(m)} = S_{pq}(\partial\varepsilon_{pq}^{(m)}/\partial u_{i,j}) v_{i,j}\Delta t$ and $\sigma_{ij}^{(m)} = \hat{S}_{ij}^{(m)}\Delta t$ (where $v_{i,j}\Delta t = \delta u_{i,j}$ and $v_i = \dot{u}_i$). Then introduce the variational condition that the resulting equation must be valid for any $\delta u_{i,j}$. Upon taking the limit $\Delta t \to 0$ This yields the fundamental work-conjugacy relation [1,10]

$$\hat{S}_{ij}^{(m)} = \dot{T}_{ij} - S_{pq} \frac{\partial^2 (\varepsilon_{pq}^{(m)} - e_{pq})}{\partial t \partial u_{i,j}} \tag{5}$$

where $\dot{T}_{ij} = \partial T_{ij}/\partial t = \partial \tau_{ij}/\partial t = \dot{S}_{ij} - S_{ik} v_{j,k} + S_{ij} v_{k,k} = \lim_{\delta t \to 0} \pi_{ij}/\delta t$, $T_{ij} = S_{ij}^0 + \tau_{ij}$, and $\dot{S}_{ij} = \partial S_{ij}/\partial t =$ material rate of Cauchy stress. Restricting attention to Doyle–Ericksen finite strain tensors with parameter m and evaluating Eq. (5) for general m and for $m = 2$, one gets a general expression for the objective stress rate [1,10]

$$\hat{S}_{ij}^{(m)} = \hat{S}_{ij}^{(2)} + \frac{1}{2}(2-m)(S_{ik}\dot{e}_{kj} + S_{jk}\dot{e}_{ki}) \tag{6}$$

where $\hat{S}_{ij}^{(2)} = \dot{S}_{ij} - S_{kj} v_{i,k} - S_{ki} v_{j,k} + S_{ij} v_{k,k} =$ Truesdell rate. For m $= 2$, Eq. (5) reduces to the Truesdell rate. For $m = 1$ it gives the Biot rate. For $m = 0$, Eq. (5) gives the Jaumann rate of Kirchhoff stress

$$\hat{S}_{ij}^{(0)} = \dot{S}_{ij} - \dot{\omega}_{ik} S_{kj} - S_{ik} \dot{\omega}_{kj} + S_{ij} v_{k,k} \tag{7}$$

This rate is work-conjugate to the Hencky (or logarithmic) strain. The Jaumann (or co-rotational) rate of Cauchy stress, Eq. (13), cannot be obtained from Eq. (5) and, thus, is work-conjugate with no finite strain tensor.

When different m are considered, the tangential stress–strain relation in Eq. (1) may generally be rewritten as $\hat{S}_{ij}^{(m)} = C_{ijkl}^{(m)} \dot{e}_{kl}$ where moduli $C_{ijkl}^{(m)}$ are associated with strain tensor $\varepsilon_{ij}^{(m)}$. They are different for different choices of m and are related as follows [1,10]:

$$C_{ijkl}^{(m)} = C_{ijkl}^{(2)} + (2-m)[S_{ik}\delta_{jl}]_{sym} \tag{8}$$

$$[S_{ik}\delta_{jl}]_{sym} = \frac{1}{4}(S_{ik}\delta_{jl} + S_{jk}\delta_{il} + S_{il}\delta_{jk} + S_{jl}\delta_{ik}) \tag{9}$$

Here $C_{ijkl}^{(2)}$ are the tangential moduli associated with the Green–Lagrangian strain $(m = 2)$, taken as a reference; $S_{ij} =$ current Cauchy stress, and $\delta_{ij} =$ Kronecker δ. Using Eq. (8) in each finite element in each loading step, one can convert a black-box commercial finite element program from one objective stress rate to another. A special case of this relation for $m = 0$ was derived, without reference to energy consistency, in Ref. [11].

3 Review of Green–Naghdi Objective Stress Rate

In rigid-body motion, the current (Eulerian) coordinate vector of a material point is given by $\mathbf{x} = \boldsymbol{R}\mathbf{X} + \mathbf{x}_0$ where $\mathbf{X} =$ initial (Lagrangian) coordinate vector of the material point, $\boldsymbol{R} =$ rotation tensor and $\mathbf{x}_0 =$ coordinate vector of the center of rotation. Since $\boldsymbol{R}^{-1} = \boldsymbol{R}^T$ (where superscript T denotes a transpose), solving this equation gives $\mathbf{X} = \boldsymbol{R}^T(\mathbf{x} - \mathbf{x}_0)$. By differentiation, the current velocity of the material point is $\dot{\mathbf{x}} = \dot{\boldsymbol{R}}\mathbf{X} + \dot{\mathbf{x}}_0 = \boldsymbol{\Omega}(\mathbf{x} - \mathbf{x}_0) + \dot{\mathbf{x}}_0$ where

$$\Omega = \dot{R} \cdot R^T \tag{10}$$

where Ω is the tensor of material rotation velocity. The rotation tensor may be calculated as $\boldsymbol{R} = \boldsymbol{F}\boldsymbol{U}^{-1}$ where $\boldsymbol{F} =$ displacement gradient tensor with components $\boldsymbol{F}_{ij} = u_{i,j}$, $u_i =$ components of displacement vector $\mathbf{u}$ and $\boldsymbol{U} = (\boldsymbol{F}^T \cdot \boldsymbol{F})^{1/2} =$ right stretch tensor.

Tensor $\boldsymbol{\Omega}$ must be distinguished from the spin tensor $\dot{\boldsymbol{\omega}}$, whose components in Cartesian coordinates x_i $(i = 1, 2, 3)$ are

$$\dot{\omega}_{ij} = \frac{1}{2}(v_{i,j} - v_{j,i}) \tag{11}$$

in which $\mathbf{v} = \dot{\mathbf{u}} = \partial\mathbf{u}/\partial t$ $(t =$ time), with components $\mathbf{v}_i = \dot{\mathbf{u}}_i = \partial\mathbf{u}_i/\partial t$, denotes the velocity of material point.

The Green–Naghdi objective stress rate is defined as [2]

$$\hat{S}_{ij}^{GN} = \dot{S}_{ij} - \Omega_{ik} S_{kj} - S_{ik} \Omega_{jk} \tag{12}$$

(note that this expression is symmetric, as it must, when subscripts i and j are interchanged). The Green–Naghdi rate is similar to the Jaumann rate of Cauchy stress, defined as

$$\hat{S}_{ij}^{JC} = \dot{S}_{ij} - \dot{\omega}_{ik} S_{kj} - S_{ik} \dot{\omega}_{jk} \tag{13}$$

The Jaumann rate of Kirchhoff stress, which is defined as

$$\hat{S}_{ij}^{(0)} = \dot{S}_{ij} - \dot{\omega}_{ik} S_{kj} - S_{ik} \dot{\omega}_{jk} + S_{ij} v_{k,k} \tag{14}$$

differs from the Jaumann rate of Cauchy stress only by the volumetric term $S_{ij} v_{k,k}$

For the present analysis, it is important that $\hat{S}_{ij}^0$ ensues from Eq. (5) for $m = 0$ and, thus, is work-conjugate to the Hencky (or logarithmic) finite strain tensor. This tensor is given by Eq. (2) for $m = 0$ and, up to the second-order small terms, is expressed as

$$\varepsilon_{ij}^{(0)} = e_{ij} + \frac{1}{2} u_{k,i} u_{k,j} - e_{ki} e_{kj} \tag{15}$$

4 Energy Error of Green–Naghdi Objective Stress Rate

The first-order work of stress, which decides equilibrium, bifurcations, and stability, may be written as $S_{ij}\varepsilon_{ij}^{(0)}$. Subtracting this from Eq. (4), we get for the second-order work during time increment Δt per unit volume of a homogeneously stressed material the expression

$$\delta^2 \mathcal{W} = \Delta t(\hat{S}_{ij}^{(0)} \varepsilon_{ij}^{(0)}) + S_{ij}(\varepsilon_{ij}^{(0)} - e_{ij}) \tag{16}$$

where $\varepsilon_{ij}^{(0)} = \Delta\varepsilon_{ij}^{(0)}$ and $e_{ij} = \Delta e_{ij}$ because the deformations are measured from the state at the beginning of the time step Δt. If the Green–Naghdi rate is used, the computer program implies the following second-order work:

$$\delta^2 \mathcal{W}^{\mathcal{GN}} = \Delta t(\hat{S}_{ij}^{GN} \varepsilon_{ij}^{(0)}) + S_{ij}(\varepsilon_{ij}^{(0)} - e_{ij}) \tag{17}$$

in which we have no choice but to use $\varepsilon_{ij}^{(0)}$ because there is no finite strain tensor ε_{ij}^{GN} that would be conjugate to $\hat{S}_{ij}^{GN}$. Anyway, if a finite strain tensor different from $\varepsilon_{ij}^{(0)}$ were used, it would be necessary to calculate $\hat{S}_{ij}^{GN}$ in Eq. (17) from a transformed constitutive law. The Jaumann rate is appropriate because, aside from volumetric strain, it differs from the Green–Naghdi rate only by rotations. Any other objective stress rate differs also by nonvolumetric strains.

Since $\hat{S}_{ij}^{(0)}$ possesses a work-conjugate finite strain tensor, Eq. (16) gives the correct expression for work. Therefore, the error of Green–Naghdi rate in energy conservation per step and unit volume of material is

$$\Delta\mathcal{W}_{\text{err}} = \delta^2\mathcal{W}^{\mathcal{GN}} - \delta^2\mathcal{W} = \varepsilon_{ij}^{(0)}(\hat{S}^{GN} - \hat{S}^{(0)})\Delta t \approx e_{ij}(\hat{S}^{GN} - \hat{S}^{(0)})\Delta t \tag{18}$$

where the replacement of $\varepsilon_{ij}^{(0)}$ by e_{ij} is admissible since higher than second-order accuracy is not necessary. Substituting Eqs. (14) and (12) and denoting the objective stress increments $\hat{S}^{(0)}\Delta t = \Delta S^{(0)}$ and $\hat{S}^{GN}\Delta t = \Delta S^{GN}$, we may write the incremental second-order work per step as follows:

$$\Delta\mathcal{W}_{\text{err}} = \Delta\mathcal{W}_{\text{err,rot}} + \Delta\mathcal{W}_{\text{err,compr}} \tag{19}$$

$$\text{where } \Delta\mathcal{W}_{\text{err,rot}} = [(\omega_{ik} - \Delta\Omega_{ik})S_{kj} + S_{ik}(\omega_{jk} - \Delta\Omega_{jk})]e_{ij} \tag{20}$$

$$\Delta\mathcal{W}_{\text{err,compr}} = -S_{ij}e_{ij}e_{kk} = -S_{ij}u_{i,j}u_{k,k} \tag{21}$$

Error $\Delta\mathcal{W}_{\text{err,compr}}$ is the energy error due to compressibility of the material, which is the same as the error of the Jaumann rate of Cauchy stress. Error $\Delta\mathcal{W}_{\text{err,rot}}$ is an additional energy error of the Green–Naghdi rate due to material rotation increments.

Equation (18) further implies that the overall energy error of the Green–Naghdi rate is equal to the area between the load-deflection curves of a structure calculated with the Green–Naghdi rate and with the Jaumann rate of Kirchhoff stress.

5 Nonsymmetry of Tangential Stiffness Tensor of Green–Naghdi Rate

Although the tangential stiffness tensor C_{ijrs}^{GN} associated with the Green–Naghdi rate is not computed in the explicit finite element programs using this rate, it is interesting to examine its difference from the tangential tensor $C_{ijrs}^{(0)}$ associated with the energy-consistent Jaumann rate of Kirchhoff stress. The tangential stiffness tensors are defined by the relations

$$\hat{S}_{ij}^{GN} = C_{ijrs}^{GN} v_{r,s}, \hat{S}_{ij}^{(0)} = C_{ijrs}^{(0)} v_{r,s} \tag{22}$$

According to Eqs. (12) and (14), the difference $\hat{S}_{ij}^{GN} - \hat{S}_{ij}^{(0)}$ may be expressed as follows:

$$\begin{aligned}&\left(C_{ijrs}^{GN} - C_{ijrs}^{(0)}\right)v_{r,s}\\ &\quad = \left(\frac{\partial(\Omega_{ik} - \dot{\omega}_{ik})}{\partial v_{r,s}} S_{jk} + \frac{\partial(\Omega_{jk} - \dot{\omega}_{jk})}{\partial v_{r,s}} S_{ik} + S_{ij}\delta_{kr}\delta_{ks}\right) v_{r,s}\end{aligned} \tag{23}$$

This may be regarded as a variational equation that must hold for any velocity gradient $v_{r,s}$. Therefore,

$$C_{ijrs}^{GN} - C_{ijrs}^{(0)} = \frac{\partial(\Omega_{ik} - \dot{\omega}_{ik})}{\partial v_{r,s}} S_{jk} + \frac{\partial(\Omega_{jk} - \dot{\omega}_{jk})}{\partial v_{r,s}} S_{ik} + S_{ij}\delta_{rs} \tag{24}$$

in which one could further eliminate $\dot{\omega}_{ik}$ and $\dot{\omega}_{jk}$ by noting the relation

$$\frac{\partial\dot{\omega}_{ik}}{\partial v_{r,s}} S_{kj} + \frac{\partial\dot{\omega}_{jk}}{\partial v_{r,s}} S_{ik} = \frac{1}{2}\left(\delta_{is}S_{jr} - \delta_{ir}S_{js} + \delta_{js}S_{ir} - \delta_{jr}S_{is}\right) \tag{25}$$

For the incremental potential (incremental Helmholtz free energy density) to exist, the tangential stiffness must satisfy the requirement of major symmetry, i.e., must not change upon interchanging subscripts *ij* and *rs*. Tensor $C_{ijrs}^{(0)}$ satisfies the requirement of major symmetry. However, the above stiffness tensor difference does not satisfy this requirement.

Therefore, the tangential stiffness tensor C_{ijrs}^{GN} associated with the Green–Naghdi objective stress rate violates the requirement of major symmetry (except if the material incompressible and $\Omega_{ij} = \dot{\omega}_{ij}$), so an incremental potential does not exist.

It may be noted that symmetry of the stiffness matrix or tensor can legitimately occur because of friction, which is associated with shear. But here the symmetry violation is due exclusively to rotations and volume change, both of which have nothing to do with friction (on the other hand, since Eq. (25) does satisfy major symmetry, the terms with $\dot{\omega}_{ij}$ cause no violation of energy conservation).

The error in energy conservation per step and unit volume of material may be written as

$$\Delta\mathcal{W}_{\text{err}} = v_{i,j}(C_{ijrs}^{GN} - C_{ijrs}^{(0)})v_{r,s} \tag{26}$$

If the tangential moduli correction indicated by Eq. (24) is made in each finite element of each time step, the subroutine such as VUMAT in ABAQUS will deliver energy consistent results corresponding to the Jaumann rate of Kirchhoff stress ($m = 0$). Furthermore, by expressing $C_{ijkl}^{(0)}$ in Eq. (24) in terms of $C_{ijkl}^{(2)}$ according to Eq. (8), one obtains the correct results for the Truesdell rate. This is how the correct results for the following examples have been calculated.

6 Numerical Example of Energy Error in Some Practical Problems

Let us now demonstrate a possible magnitude of the error caused by the wrong definition of the stress rate. As an example, the experiment reported in Ref. [12] may be used. The specimen shown in Fig. 1, made of the 1018 cold-rolled steel, is compressed between two rigid platens, producing a band of large shear strains with large material rotations. The steel is considered to have Young's modulus $E = 200$ GPa, Poisson's ratio $\nu = 0.29$, yield strength $f_y = 350$ MPa, and to follow von Mises plasticity with linear kinematic hardening and hardening modulus $H = 2$ GPa. To

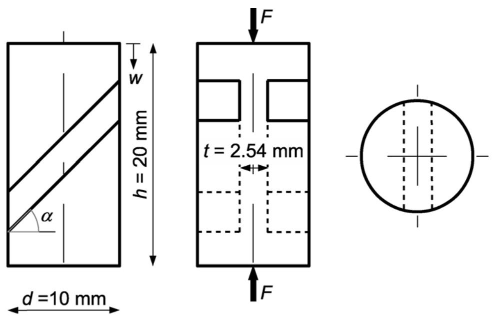

Fig. 1 Elevations and plan view skew-notched cylinder analyzed

simulate different stress rates, the user material subroutine (VUMAT) in the commercial software ABAQUS [13] is employed.

The error in energy conservation is plotted in Fig. 2 as a function of the relative shortening w/d of the specimen. Figure 2(*c*) depicts the evolution of the average total rotation magnitude $|\mathbf{r}^{(n)}|$ among all the finite elements within the notched part. The total rotation is obtained from a series of rotation increments ΔR in the individual loading steps, which are calculated with second-order accuracy from Hughes and Winget's formula [14] (see also Ref. [15])

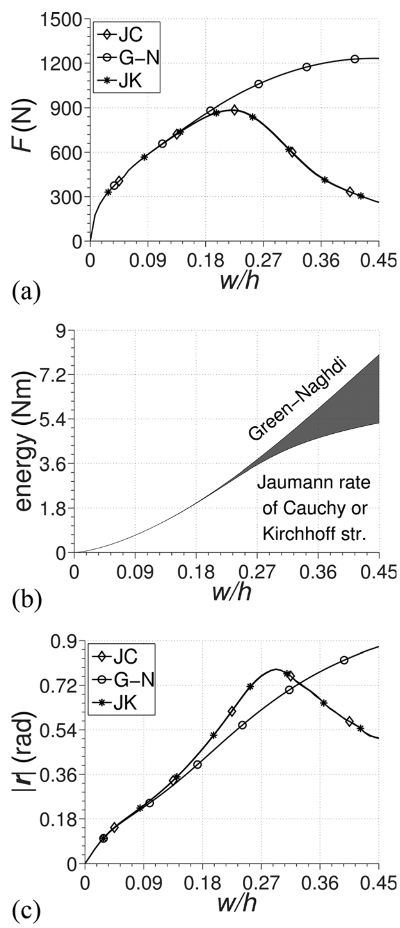

Fig. 2 Comparison of computation results for different stress rates: (*a*) curve of load versus relative displacement *w*/*h* (JC = Jaumann rate of Cauchy stress, JK = Jaumann rate of Kirchhoff stress, G–N = Green–Naghdi stress rate); (*b*) error in energy; (*c*) average magnitudes of rotation vector (in radians) within the notched part, computed from the rotation increments used in the G–N and JK stress rates, plotted as a function of *w*/*h*

$$\Delta \boldsymbol{R} = \left(\boldsymbol{I} - \frac{1}{2}\Delta\boldsymbol{\omega}\right)^{-1}\left(\boldsymbol{I} + \frac{1}{2}\Delta\boldsymbol{\omega}\right) \tag{27}$$

where $\boldsymbol{I}$ stands for the identity matrix (strictly speaking, $\Delta\boldsymbol{\Omega}$ should here be used instead of $\Delta\omega$, but for small enough loading steps the difference is negligible). The rotation in the nth step is calculated recursively as

$$\boldsymbol{R}^{(n)} = \Delta\boldsymbol{R}\boldsymbol{R}^{(n-1)} \tag{28}$$

From the rotation tensor $\boldsymbol{R}^{(n)}$, the rotation vector $\mathbf{r}^{(n)}$ is determined as

$$r_i^{(n)} = -\frac{1}{2}e_{ijk}\boldsymbol{R}_{jk}^{(n)} \tag{29}$$

where e_{ijk} is the permutation symbol (equal to 1 for permutations of 123, -1 for permutations of 132, and 0 when any two subscripts are equal). At the end, the rotation magnitude after n loading steps is evaluated as

$$\left|r^{(n)}\right| = \sqrt{r_i^{(n)} r_i^{(n)}} \tag{30}$$

Equations (27)–(30) are used to evaluate the rotation magnitude for the Jaumann rates [16] of Kirchhoff and of Cauchy stress. For the Green–Naghdi rate $\boldsymbol{\omega}$ is substituted by $\boldsymbol{\Omega}$ in Eq. (27).

Because the volume change of steel during loading is small, the Jaumann rates of the Kirchhoff stress and of the Cauchy stress deliver nearly identical results, graphically almost indistinguishable in Fig. 2(*a*) (overlapping curves). The undeformed and deformed meshes, consisting of the standard ABAQUS first-order tetrahedral element C3D4, are shown in Fig. 3. The same geometry and mesh were used in all the calculations.

7 Categorization of Energy Consistency Violations

Having clarified the error in the Green–Naghdi rate, we can now discern three kinds of energy errors:

(1) error of the *first* kind, which is due to omitting the volumetric term from the Jaumann rate of Cauchy stress and from

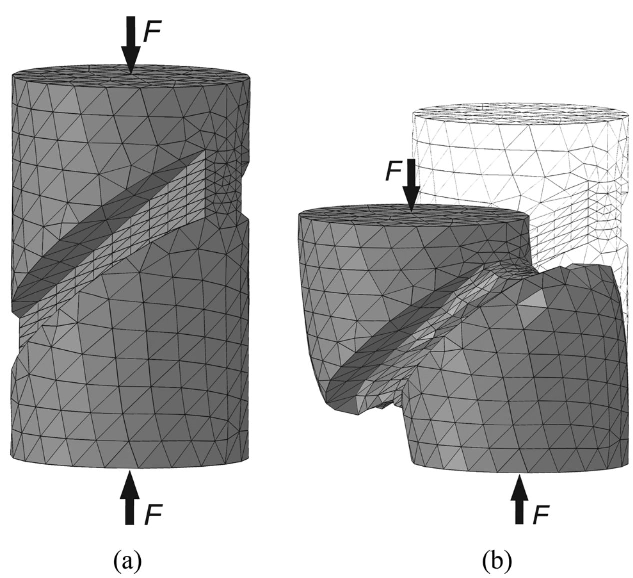

Fig. 3 Axonometric view of (*a*) undeformed and (*b*) deformed meshes used in finite element computations; (*b*) the shown deformation corresponds to Jaumann rate of Cauchy stress, which conserves energy

the Green–Naghdi rate. This error afflicts applications to highly compressible materials (see in detail Ref. [5,10]).

(2) error of the *second* kind, which is due to an inappropriate measure of material rotation used in the Green–Naghdi rate, as explained here.

(3) error of the *third* kind, which is due to using a stress rate that is work-conjugate to a wrong finite strain tensor, i.e., a tensor that is not associated with the tangential moduli used. This energy error is endemic for highly orthotropic homogenized soft-in-shear columns, plates, and shells at small strain, analyzed by the Jaumann rate of Kirchhoff stress with a constant tangential shear modulus. In that case, the energy conservation under axial compression permits the use of the Truesdell rate only ($m=2$). E.g., when the Jaumann rate of Cauchy stress is used for a soft matrix such as polymer or foam reinforced by unidirectional fibers and compressed in the linear small-strain range, the bifurcation load can have a 100% error unless the shear modulus of the matrix is varied as a function of the fiber stress so as to make the result equivalent to that for the Truesdell rate. This error (occurring in ABAQUS, ANSYS, LS-DYNA, etc., though not in ATENA and OOFEM) can be avoided if the user makes the transformation of the shear modulus in subroutine UMAT or iterates this transformation in the bifurcation subroutine. This error was presaged almost seven decades ago by Haringx's discovery of a shear buckling formula that can give a critical load grossly deviating from Engesser's. In the opposite case of compression normal to the strong orthotropy direction, as in bridge or seismic isolation bearings, an energy error is avoided only by conversion to the Lie derivative corresponding to $m=-2$ or by an equivalent variation of the tangential moduli (see Ref. [7]; in more detail Ref. [8]; in general also Refs. [1,10].

The Jaumann rate of Kirchhoff stress, used in bifurcation analysis of ABAQUS, suffers only from the error of the third kind, which. for example, means that it gives wrong critical loads for columns, plates, and shells very soft in shear. The Jaumann rate of Cauchy stress is worse since it suffers from both the first and third kinds of error. The Green–Naghdi rate is the worst since it suffers from all the three kinds of error.

8 Concluding Comments

In view of the present and recent demonstrations of the magnitude or energy errors, revisions should be made in the most popular commercial software. There is no advantage that would outweigh the energy error of the Green–Naghdi rate nor the Jaumann rate of Cauchy stress. Minimally, these two rate should be replaced by the Jaumann rate of Kirchhoff stress, which conserves energy. Optimally, though, all commercial programs that do not use the Truesdell rate should switch to it. This rate, which is associated by work with Green's Lagrangian strain tensor, eliminates all the three kinds of errors (except for the case of transversely compressed highly orthotropic structures such as bridge and seismic isolation bearings, for which a transformation to $m=-2$ is inevitable).

Until (or unless) these corrections are made, the manuals of commercial software should at least warn that, in the instances of high compressibility or high orthotropy or large rotations, the user must not use the black-box subroutines but can work with the user's material subroutines and implement in them a simple conversion to the Truesdell rate and Green's Lagrangian strain tensor, based on boxed Eqs. (24) and (8).

Apart from their energy errors, the Green–Naghdi rate and both Jaumann rates correspond to the Hencky (logarithmic) finite strain tensor, which is (next to Biot strain tensor) the most intuitive and convenient for formulating the constitutive relations (e.g., it has the advantage of tension-compression symmetry). Association with the Hencky strain is a practical advantage of the Jaumann rate of Kirchhoff stress and is probably the reason why, in the 1970s, the three aforementioned rates were widely adopted. For this reason, the constitutive laws may (except for cases of very strong orthotropy) continue to be formulated in terms of the Hencky strain and, incrementally, in terms of the associated Jaumann rate of Kirchhoff stress. However, it is not difficult to make a conversion to Truesdell rate and the Green's Lagrangian finite strain measure before the finite element analysis is begun.

Acknowledgment

Financial support under Grant N00014-11-1-0155 from the Office of Naval Research to Northwestern University, monitored by Dr. Roshdy Barsoum, is gratefully acknowledged. The second author wishes to express his thanks for being supported under this grant during his one-year Visiting Scholar appointment at Northwestern University. Thanks are also due to the Grant Agency of Czech Republic for additional funding in Prague under research project GAČR P105/12/P353.

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