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Abstract

Abstract here

1 Introduction

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- 1. justification for our specific format for incremental kinematics, i.e., we want D
- take in incremental displacements, want D and Rhat
- need to justify this
- if you have a corotational rate, it *should* be a Jaumann rate
- 2. computation of D and Rhat
- 3. full accounting of tangent modulus
- 4. traction and pressure BC terms as well
- 5. systematic exposition of accuracy, comparison to code A
- 6. show importance of including all of the terms required for tangent stiffness as it pertains to convergence
- turn off selected terms in tangent stiffness, for example dRhat/duhat

make comment about fatigue - lots of cycles

1.1 Explanation of References

Hughes and Winget have proposed one of the earliest (weakly) objective incremental algorithms in [9] which relies upon the Jaumann rate of stress. Therein, they introduced the notion of "incremental objectivity." Subsequently, Rubinstein and Atluri provided a more rigorous mathematical investigation into the conditions of objectivity for incremental algorithms in [17]. Flanagan and Taylor later proposed an algorithm in [5] based upon the Green-Naghdi co-rotational rate, which considers an evolution of the material state in its "unrotated" configuration.

In contrast with previous works where both the stretching and rotation increment are computed approximately, Roy et. al. have suggested in [15] that the polar decomposition be computed via the Cayley-Hamilton theorem for use in incrementally objective algorithms to improve accuracy.

Rashid introduced the notion of "strong" objectivity in the context of incrementally objective algorithms in [13]. A strongly objective algorithm was then proposed, though it utilized approximate expressions for the stretching and rotation tensors appearing therein. Nonetheless, significant improvements in accuracy were demonstrated by Rashid and Thorne in [14], particularly for cyclic shearing deformations.

Guo has developed relatively simple expressions for the rates of stretch and rotation tensors in [6], which may be easily generalized in order to express the derivatives of these quantities with respect to other tensors of interest. Hoger and Carlson followed up on these developments in [8], where they developed an alternative set of expressions for these same quantities. Carlson and Hoger would later develop yet more general expressions for the derivatives of tensor-valued functions with respect to other tensors in [2], though these are quite convoluted.

Hoger developed an expression for the time rate of logarithmic strain in [7], and Bažant has proposed in [1] an approximate expression for the Hencky (logarithmic) strain and its rate. Jog ultimately arrived at an explicit representation for the logarithm of a tensor and its derivatives in [10] which relies upon the eigendecomposition.

In [3], Danielson has suggested an approach based on successive Newton-Raphson iteration to obtain the polar decomposition of the deformation gradient, for prospective use in various kinematic update algorithms. Alternatively, Scherzinger and Dohrmann have proposed a relatively fast and highly accurate method for determining the eigendecomposition of 3×3 symmetric matricies in [18], which may be used to readily compute many quantities necessary to the incremental stress update procedure.

Fish and Shek have investigated the importance of adopting a consistent linearization of the incrementally objective algorithm of Hughes and Winget in [4], demonstrating very poor solution convergence when an approximate tangent is utilized instead.

Kamojjala et. al. have proposed a series of solid mechanics verification problems in [11], which includes a test for frame indifference (i.e. weak objectivity), though a test for verification of strong objectivity is conspicuously absent.

In [12], Khoei et. al. have developed a specialized incrementally objective algorithm for endochronic constitutive models which uses time sub-increments to integrate the stress rate equations, with the strain increment in each sub-interval obtained via the midpoint rule proposed by Hughes and Winget.

Rubin and Papes discuss the formulation of incrementally objective algorithms for use with elastic-viscoplastic constitutive models in [16], noting a clear advantage of strongly objective algorithms over weakly objective algorithms in that context.

Xiao, Bruhn, and Meyers have argued in [19] and [20] for the use of the so-called "logarithmic" stress rate over other co-rotational rates, citing that such a rate yields work conjugate stress and strain measures. Zhou and Tamma have developed an incrementally objective algorithm based upon the the logarithmic rate in [21], though their formulation utilizes a mid-point approximation scheme to compute the stretch increment. Moreover, little to no discussion is given regarding the computation of a consistent tangent for the proposed algorithm.

2 Incremental Kinematics

The Jaumann rate of stress for a linear hypoelastic material is characterized by:

$$\overset{\Delta}{\sigma} \equiv \dot{\sigma} + \sigma \cdot W - W \cdot \sigma = C : D$$

where $D = \frac{1}{2}(L + L^{\top})$, $W = \frac{1}{2}(L - L^{\top})$, and $L = \dot{F}F^{-1}$. We would like to know how the stress state changes after applying a prescribed deformation. Our approach is as follows: parameterize the deformation into separate stages of pure stretch and pure rotation. The advantage of this approach is that it allows the terms in the stress rate above to be integrated separately

$$\dot{\sigma} = \begin{cases} C: D & \text{W vanishes for pure stretch} \\ W \cdot \sigma - \sigma \cdot W & \text{D vanishes for pure rotation} \end{cases}$$

Simple analytic solutions exist for each of these ordinary differential equations, provided that D, W are constant (C is also assumed to be constant):

$$\dot{\sigma}(t) = C: D, \ \sigma(0) = \sigma_i \qquad \Longrightarrow \qquad \sigma_{i+\frac{1}{2}} = \sigma_i + C: D\Delta t$$

$$\dot{\sigma}(t) = W \cdot \sigma - \sigma \cdot W, \ \sigma(0) = \sigma_{i + \frac{1}{2}} \qquad \Longrightarrow \qquad \sigma_{i + 1} = \exp(W\Delta t) \ \sigma_{i + \frac{1}{2}} \ \exp(W\Delta t)^{\top}$$

Combining these two results gives us our stress update procedure:

$$\sigma_{i+1} = \exp(W\Delta t) \left(\sigma_i + C : D\Delta t\right) \exp(W\Delta t)^{\top}$$

All that remains is to find reasonable approximations for D, W. To that end, we consider the polar decomposition of the incremental deformation gradient, F = R U. After taking a time derivative of F, and substituting into the definition of L, we get:

$$L \equiv D + W = \dot{R} R^{\top} + R \dot{U} U^{-1} R^{\top}$$

When considering the separate stages of pure stretch and pure rotation, this equation reduces to:

$$\begin{cases} D = \dot{U} \ U^{-1} & \text{pure stretch} \\ W = \dot{R} \ R^{\top} & \text{pure rotation} \end{cases}$$

These are constant-coefficient, ordinary differential equations than can be used to determine D and W. The general solution for equations of this form is

$$Y = \dot{X}X^{-1}, \ X(0) = 1 \implies X(\Delta t) = \exp(Y\Delta t)$$

Which, when applied to the pure stretch and pure rotation versions of the problem gives us our definitions of D, W:

$$D = \frac{1}{\Delta t} \log(U), \qquad W = \frac{1}{\Delta t} \log(R)$$

Substituting these back into our stress update procedure gives

$$\sigma_{i+1} = R\left(\sigma_i + C : \log(U)\right) R^{\top}$$

- 2.1 Description
- 2.2 Implementation Approaches
- 2.2.1 Hughes-Winget
- 2.2.2 Rashid

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3 Finite Element Residual and Tangent Stiffness

This section discusses the greater context of solid mechanics, and the corresponding finite element system of equations in the presence of finite deformations. According to the developments of the previous section, a strongly objective kinematic algorithm and its implementation are proposed in this setting.

For a continuum body which occupies an open domain $\Omega_0 \subset \mathbb{R}^d$ in its undeformed configuration, the weak form equations of equilibrium may be expressed as

$$R_i \equiv \int_{\Omega_0} P_{ij}\phi_{,j} d\Omega_0 + \int_{\Gamma_0} p_i \phi d\Gamma_0 = 0 \quad \forall i, \phi \in H_0^1(\Omega_0), \tag{1}$$

where \mathbf{P} represents the first Piola-Kirchhoff stress tensor, and \mathbf{p} is the Piola traction vector. This representation is amenable to a total Lagrangian approach.

Discuss the need for a consistent linearization of the residual for use in a non-linear Newton solver.

Perhaps without even referring to finite elements, discuss the computations that are needed at the quadrature-point level.

Explain the steps needed for the evaluation of the residual contribution (at a quadrature point), and correspondingly for the evaluation of the tangent contribution:

Elaborate on how to compute exact derivatives of the relevant quantities

include all the derivatives

a complete, full implementation, with code snippet

potentially Sam working on an improved (more novel) implementation of what Mark did

3.1 Generalized Material Update

In a continuum body Ω_0 , a given material point $\mathbf{X} \in \Omega_0$ is endowed with a "material state" $S_k(\mathbf{X})$ at time t_k . In the context of Lagrangian solid mechanics, the material state $S_k = \{\boldsymbol{\sigma}_k, q_{*k}\}$ consists of the Cauchy stress tensor $\boldsymbol{\sigma}_k$, and any (possibly tensorial) internal state variables q_{*k} associated with the material model.

According to the Lagrangian description of motion, a material point initially located at a position $\mathbf{X} \in \Omega_0$ will occupy the spatial position \mathbf{x}_k at some later time t_k , undergoing a total displacement $\mathbf{u}_k = \mathbf{x}_k - \mathbf{X}$. In a computational setting, the analysis is subdivided into discrete time steps $\{t_k\}_{k=0}^N$, and the motion of material points from time t_k to t_{k+1} is described by an incremental displacement field, denoted $\hat{\mathbf{u}} = \mathbf{u}_{k+1} - \mathbf{u}_k$. The deformation associated with this motion may be characterized by an incremental deformation gradient $\hat{\mathbf{F}} = \partial \mathbf{x}_{k+1}/\partial \mathbf{x}_k = \mathbf{1} + \nabla \hat{\mathbf{u}}$. This representation of the deformation taking place in discrete increments is equally suitable for updated or total Lagrangian formulations.

Assuming that the material behaves in a rate-independent manner, a generic material update procedure $f: (S_k, \nabla \hat{\mathbf{u}}) \mapsto S_{k+1}$ should yield the updated material state S_{k+1} at time t_{k+1} as a function of the material state S_k at time t_k , and the incremental displacement gradient $\nabla \hat{\mathbf{u}}$. The updated stress may then be used to evaluate residual force contributions. If a tangent stiffness matrix must be constructed, the material

update procedure must also evaluate the tangent derivatives of the Cauchy stress with respect to the input deformation (i.e. $\partial \sigma_{k+1}/\partial \nabla \hat{\mathbf{u}}$).

Within this generalized framework, the displacement gradient may be optionally modified prior to being passed into the material update procedure, in such a fashion as to accommodate mixed or enhanced degrees of freedom (should these be present), or to apply a strain projection methodology (e.g. an F-bar approach).

3.2 Hypoelastic Material Update

For a hypoelastic material, the constitutive model is expressed in rate form:

$$\overset{\circ}{\boldsymbol{\sigma}} = \mathbb{C} : \mathbf{D},\tag{2}$$

where $\mathring{\boldsymbol{\sigma}}$ denotes a particular co-rotational rate of the Cauchy stress (e.g. the Jaumann stress rate), and \mathbb{C} depends upon the material state.

Most numerical implementations for rate-independent material models of this type consider an increment of strain $\Delta \varepsilon$ as the driving input variable, which is used to evolve the material state via a constitutive update procedure (denoted as C), such that

$$S_{k+1} = C(S_k, \Delta \varepsilon). \tag{3}$$

Additionally, a tangent material modulus $\partial \sigma_{k+1}/\partial \Delta \varepsilon$ may be requested if stiffness contributions are needed.

The foregoing constitutive update procedure is sufficient for problems involving small deformations. In the presence of finite deformations, however, an additional procedure R must be defined to allow for rotation of the material state, i.e.

$$S_{k+1} = R(S_k, \mathbf{R}),\tag{4}$$

such that $\sigma_{k+1} = \mathbf{R} \sigma_k \mathbf{R}^T$, and where the material's internal state variables q_{*k} are rotated according to their tensorial character (e.g. $\mathbf{q}_{k+1} = \mathbf{R} \mathbf{q}_k$ if \mathbf{q}_k is a vector-valued quantity). If an evaluation of stiffness terms is required, $\partial \sigma_{k+1}/\partial \mathbf{R}$ must be computed, as well.

Given an input deformation $\nabla \hat{\mathbf{u}}$, it is therefore of interest to compute corresponding strain and rotation increments ($\Delta \boldsymbol{\varepsilon}$ and $\hat{\mathbf{R}}$, respectively) which may be used to update the material state in a step-wise sequence via

$$S_{k+1} = R(C(S_k, \Delta \varepsilon), \hat{\mathbf{R}}), \tag{5}$$

or alternatively,

$$S_{k+1} = C(R(S_k, \hat{\mathbf{R}}), \Delta \varepsilon). \tag{6}$$

This necessitates the specification of a "kinematic splitting" algorithm K of the form

$$\left\{\Delta \boldsymbol{\varepsilon}, \, \hat{\mathbf{R}}\right\} = K(\nabla \hat{\mathbf{u}}),\tag{7}$$

which should also be capable of supplying kinematic tangent terms (i.e. $\partial \Delta \varepsilon / \partial \nabla \hat{\mathbf{u}}$ and $\partial \hat{\mathbf{R}} / \partial \nabla \hat{\mathbf{u}}$).

Given a set $\{K, C, R\}$ consisting of the aforementioned procedures, a generic hypoelastic meterial update is formulated in algorithm 1 which is valid for rate independent models.

Algorithm 1 Hypoelastic material update procedure for rate independent models

Input: S_k and $\nabla \hat{\mathbf{u}}$

Output: S_{k+1} (optionally $\partial \boldsymbol{\sigma}_{k+1}/\partial \nabla \hat{\mathbf{u}}$)

 $Kinematic\ split:$

1: $\{\Delta \boldsymbol{\varepsilon}, \, \hat{\mathbf{R}}\} = K(\nabla \hat{\mathbf{u}})$ (optionally compute $\partial \Delta \boldsymbol{\varepsilon} / \partial \nabla \hat{\mathbf{u}}$ and $\partial \hat{\mathbf{R}} / \partial \nabla \hat{\mathbf{u}}$)

 $Constitutive\ update:$

2: $S_{k+\frac{1}{2}} = C(S_k, \Delta \varepsilon)$ (optionally compute $\partial \sigma_{k+\frac{1}{2}}/\partial \Delta \varepsilon$)

 $Rotate\ state:$

3: $S_{k+1} = R(S_{k+\frac{1}{2}}, \hat{\mathbf{R}})$ (optionally compute $\partial \boldsymbol{\sigma}_{k+1} / \partial \hat{\mathbf{R}})$

(Optionally) compute an algorithmically consistent tangent:

4:
$$\frac{\partial \sigma_{k+1}}{\partial \nabla \hat{\mathbf{u}}} = \frac{\partial \sigma_{k+1}}{\partial \hat{\mathbf{R}}} : \frac{\partial \hat{\mathbf{R}}}{\partial \nabla \hat{\mathbf{u}}} + R(\frac{\partial \sigma_{k+1/2}}{\partial \Delta \varepsilon} : \frac{\partial \Delta \varepsilon}{\partial \nabla \hat{\mathbf{u}}}, \hat{\mathbf{R}})$$

3.3 Kinematic Splitting Algorithm

The specification of an appropriate kinematic splitting algorithm depends on two primary considerations: the objective stress rate with which the intended algorithm is to maintain consistency, and the desired level of accuracy that the algorithm should achieve.

A material update procedure is called *consistent* with a given objective stress rate if the truncation error $\tau(\Delta t)$ of the algorithm approaches zero in the limit as $\Delta t \to 0$, i.e.

$$\lim_{\Delta t \to 0} \tau(\Delta t) = 0. \tag{8}$$

It suffices to show that

$$\lim_{\Delta t \to 0} \frac{\sigma_{k+1} - \sigma_k}{\Delta t} = \mathring{\sigma} + \mathbf{W} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \mathbf{W}, \tag{9}$$

where $\Delta t = t_{k+1} - t_k$. It can be easily shown that algorithm 1 is consistent with the Jaumann rate, provided an appropriate kinematic splitting algorithm is employed.

Algorithm 2 Strongly objective kinematic splitting algorithm

Input: $\nabla \hat{\mathbf{u}}$

Output: $\Delta \varepsilon$ and $\hat{\mathbf{R}}$ (optionally $\partial \Delta \varepsilon / \partial \nabla \hat{\mathbf{u}}$ and $\partial \hat{\mathbf{R}} / \partial \nabla \hat{\mathbf{u}}$)

 $Compute\ the\ incremental\ Green-Lagrange\ strain:$

1:
$$\hat{\mathbf{E}} = \frac{1}{2}(\hat{\mathbf{C}} - \mathbf{1}) = \frac{1}{2}(\nabla \hat{\mathbf{u}} + \nabla \hat{\mathbf{u}}^T + \nabla \hat{\mathbf{u}}^T \nabla \hat{\mathbf{u}})$$

 $Compute\ the\ eigendecomposition:$

2:
$$\frac{1}{2}\mathbf{Q}(\mathbf{\Lambda}^2 - \mathbf{1})\mathbf{Q}^T = \operatorname{eig}(\hat{\mathbf{E}})$$

 $Compute\ the\ rotation\ increment:$

3:
$$\hat{\mathbf{R}} = (\mathbf{1} + \hat{\mathbf{u}})\mathbf{Q}\mathbf{\Lambda}^{-1}\mathbf{Q}^T$$

 $Compute\ the\ logarithmic\ strain\ increment:$

4:
$$\Delta \varepsilon = \mathbf{Q} \log(\mathbf{\Lambda}) \mathbf{Q}^T$$

4 Examination of Numerical Accuracy

4.1 Uniaxial Compression with Finite Rotation

For the sake of comparison with the strongly objective algorithm proposed in [13], an example problem similar to the one given therein will be considered, consisting of a block of isotropic material which is compressed uniaxially and simultaneously rotated according to the deformation gradient given by

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \begin{bmatrix} \cos \omega t & -\sin \omega t & 0 \\ \sin \omega t & \cos \omega t & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 - \beta t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{10}$$

The material model will be chosen as the isotropic hypoelastic model of grade zero, i.e.

$$\overset{\circ}{\mathbf{T}} = \lambda \mathbf{1} \operatorname{tr}(\mathbf{D}) + 2\mu \mathbf{D},\tag{11}$$

where $\lambda = E\nu/(1+\nu)(1-2\nu)$ and $\mu = E/2(1+\nu)$ are the standard Lamé parameters. Exact solutions for the Cauchy stress components according to the Jaumann rate are easily obtained for this problem:

$$\begin{cases}
T_{11} \\
T_{22} \\
T_{33} \\
T_{23} \\
T_{13} \\
T_{12}
\end{cases} = \begin{cases}
[\lambda + \mu(1 - \cos 2\omega t)] \ln(1 - \beta t) \\
[\lambda + \mu(1 + \cos 2\omega t)] \ln(1 - \beta t) \\
\lambda \ln(1 - \beta t) \\
0 \\
0 \\
-\mu(\sin 2\omega t) \ln(1 - \beta t)
\end{cases}.$$
(12)

Numerical solutions were computed for the values $\omega = \pi$, $\beta = 0.5$, $E = 2.09 \times 10^5$, $\nu = 0.3$, and $t \in [0, 1]$. The results are depicted in figure 1.

Worst-case relative errors between the exact solution ${\bf T}$ and approximate solutions ${\bf T}^h$ were computed via

% error
$$(\mathbf{T}^h) = \sqrt{\frac{\max_t(\mathbf{T}^h - \mathbf{T}) : (\mathbf{T}^h - \mathbf{T})}{\max_t \mathbf{T} : \mathbf{T}}} \times 100\%,$$
 (13)

and tabulated in table 1.

Table 1: Relative errors for the problem of uniaxial compression with finite rotation

		\ /	proposed algorithm
$\%$ error (\mathbf{T}^h)	11.21704	0.01718	0.00014

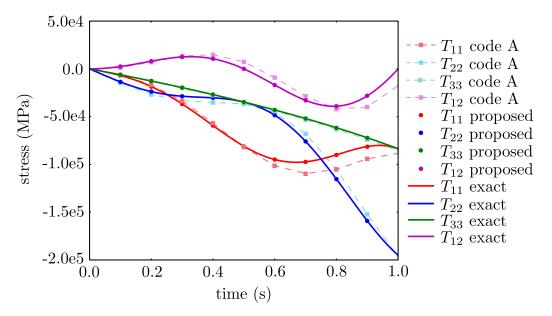


Figure 1: Stress components plotted vs. time for the problem of uniaxial compression with finite rotation.

4.2 Cyclic Shear

In a retrospective examination of solution accuracy, the problem discussed in [14] will be examined within the present context. The problem consists of a block of material which is subjected to a simple, cyclic shearing deformation given by

$$\mathbf{F} = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{L} = \begin{bmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{14}$$

and where

$$\gamma(t) = 2\Gamma\left(\frac{2t}{T} - \left\lfloor \frac{2t}{T} + \frac{1}{2} \right\rfloor\right) (-1)^{\left\lfloor \frac{2t}{T} + \frac{1}{2} \right\rfloor}$$
 (15)

corresponds to the triangle wave with period T and peak amplitude Γ , whose time derivative

$$\dot{\gamma}(t) = \frac{4\Gamma}{T}(-1)^{\left\lfloor \frac{2t}{T} + \frac{1}{2} \right\rfloor} \tag{16}$$

is the square wave with period T. As before, the isotropic hypoelastic model of grade zero will be employed, where $\mu=E/2(1+\nu)$ represents the shear modulus of the material. The exact solution for the Cauchy stress components according to the Jaumann rate is given by the solution to the differential equation:

$$\left\{ \begin{array}{c} \dot{T}_{11} \\ \dot{T}_{22} \\ \dot{T}_{12} \end{array} \right\} = \left[\begin{array}{ccc} 0 & 0 & \dot{\gamma} \\ 0 & 0 & -\dot{\gamma} \\ -\dot{\gamma}/2 & \dot{\gamma}/2 & 0 \end{array} \right] \left\{ \begin{array}{c} T_{11} \\ T_{22} \\ T_{12} \end{array} \right\} + \mu \left\{ \begin{array}{c} 0 \\ 0 \\ \dot{\gamma} \end{array} \right\}, \tag{17}$$

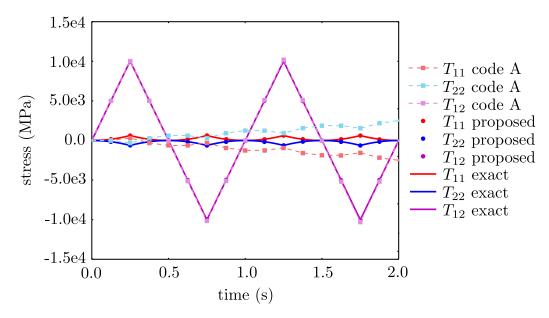


Figure 2: Stress components plotted vs. time for the problem of cyclic shear.

Table 2: Relative errors for the problem of cyclic shear

$$\%$$
 error (\mathbf{T}^h) 24.94638 Rashid (1993) proposed algorithm 0.00227 0.00205

which yields

$$\left\{ \begin{array}{l} T_{11} \\ T_{22} \\ T_{33} \\ T_{23} \\ T_{13} \\ T_{12} \end{array} \right\} = \left\{ \begin{array}{l} \mu(1 - \cos\gamma(t)) \\ \mu(\cos\gamma(t) - 1) \\ 0 \\ 0 \\ 0 \\ \mu\sin\gamma(t) \end{array} \right\}. \tag{18}$$

Numerical solutions were computed for the values $\Gamma=0.5, E=2.09\times 10^5, \nu=0.3, T=1.0,$ and $t\in[0,2],$ yielding 2 complete cycles of deformation. The results are depicted in figure 2.

Worst-case relative errors between the exact solution \mathbf{T} and approximate solutions \mathbf{T}^h were computed via equation 13 and tabulated in table 2.

4.3 Twisting Prism

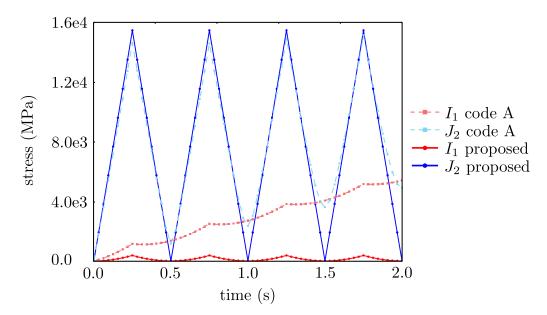


Figure 3: Stress measures plotted vs. time for the twisting prism problem, where I_1 is the first invariant of the Cauchy stress tensor, and J_2 is the second invariant of the deviatoric stress tensor

5 Performance Evaluation of Nonlinear Solution Convergence

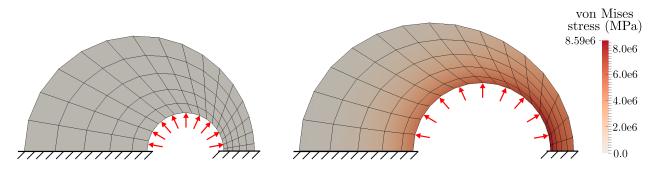


Figure 4: Pressurized eccentric cylinder modeled with half-symmetry.

Table 3: Number of Newton-Raphson iterations per time step for the eccentric cylinder problem

Step	Hughes-Winget	Rashid (1993)	Proposed Algorithm
1	3	3	3
2	2	2	2
3	2	2	2
4	2	2	2
5	2	2	2
6	2	3	2
7	2	3	2
8	2	3	2
9	3	4	3
10	4	27	4

Table 4: Number of Newton-Raphson iterations using an inconsistent linearization

Step	Consistent	Rotation Off	Pressure Off	Rotation & Pressure Off
1	3	5	6	6
2	2	5	7	8
3	2	6	9	10
4	2	6	11	13
5	2	8	14	16
6	2	10	18	20
7	2	14	25	24
8	2	22	42	31
9	3	40	123	41
10	4	771	>1000	784

6 Conclusions

7 Appendix

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