Inconsistency of \texttt{uhyper} and \texttt{umat} in ABAQUS for compressible hyperelastic materials

Herbert Baaser\textsuperscript{1} and Robert J. Martin\textsuperscript{2} and Patrizio Neff\textsuperscript{3}

September 1, 2017

\textit{Dedicated to Zdenek Bažant}

\textbf{Abstract}

We demonstrate an error in the implementation of the popular commercial Finite-Element-System ABAQUS by an explicit and simple example. This error has previously been brought to attention by Bažant et al. who, in a series of papers, pointed out that the \texttt{umat} user interface subroutine returns erroneous results for nonlinear elastic models of highly compressible materials.

In this paper, we compare the \texttt{uhyper} and \texttt{umat} results for quasi-incompressible (rubber-like) as well as for highly compressible (foam-like) materials, showing the inconsistencies in the compressible case. We also implement a correction suggested by Bažant to demonstrate its capability to re-establish the correct results.

\textbf{Mathematics Subject Classification:} 74B20, 74S05

\textbf{Key words:} Abaqus, finite element methods, hyperelasticity, finite strain, Jaumann rate, compressible material, Cauchy stress, tangential stiffness

\textbf{Contents}

1 Introduction 2
   1.1 Stress rates and time integration .......................................................... 3

2 Three ways of implementing hyperelasticity in ABAQUS 4
   2.1 Bažant’s proposed modification of the tangent modulus .......................... 5

3 Examples of numerical results for different implementations 5
   3.1 Quasi-incompressible material behaviour ............................................. 6
   3.2 Compressible material behaviour ......................................................... 6

4 Conclusion 7

5 References 8

\\n\\n\textsuperscript{1}Mechanical Engineering, University of Applied Sciences Bingen, Germany, h.baaser@th-bingen.de
\textsuperscript{2}Lehrstuhl für Nichtlineare Analysis und Modellierung, Fakultät für Mathematik, Universität Duisburg–Essen, Thea-Leymann Str. 9, 45127 Essen, Germany, robert.martin@uni-due.de
\textsuperscript{3}Head of Lehrstuhl für Nichtlineare Analysis und Modellierung, Fakultät für Mathematik, Universität Duisburg–Essen, Thea-Leymann Str. 9, 45127 Essen, Germany, patrizio.neff@uni-due.de
1 Introduction

The most basic problem in nonlinear hyperelasticity is to find a sufficiently regular function (or deformation) \( \varphi : \Omega \rightarrow \mathbb{R}^n \) on a connected region \( \Omega \subset \mathbb{R}^n \) (the elastic body) solving the equilibrium equations

\[
\begin{aligned}
\text{Div} \, S_1(\nabla \varphi(x)) &= 0, \\
S_1(F) &= \frac{\partial W(F)}{\partial F},
\end{aligned}
\]  

(1.1)
i.e. the Euler-Lagrange equations corresponding to the energy functional

\[
\varphi \mapsto \int_{\Omega} W(\nabla \varphi(x)) \, dx,
\]

under appropriate boundary conditions. Here, \( S_1 \) denotes the first Piola-Kirchhoff stress tensor, \( F = \nabla \varphi \) is the deformation gradient and \( W : \text{GL}^+(n) \rightarrow \mathbb{R}^n \) is a given elastic energy potential on the set \( \text{GL}^+(n) \) of invertible matrices with positive determinant.

In particular, a hyperelastic material model, i.e. the stress response function, is completely determined by the choice of an energy function \( W \); note that

\[
\sigma = S_1 \cdot (\text{Cof} F)^{-1} = \frac{\partial W(F)}{\partial F} \cdot (\text{Cof} F)^{-1}
\]

for the Cauchy stress tensor \( \sigma \), where \( \text{Cof} F \) denotes the cofactor of \( F \). In the following, we will consider only isotropic materials; in this case, the energy function satisfies the invariance condition \( W(Q_1 F Q_2) = W(F) \) for all \( F \in \text{GL}^+(n) \) and all proper rotations \( Q_1, Q_2 \).

Nowadays, the finite element implementation of nonlinear material behaviour is considered a routine matter, with many commercial software packages providing predefined user interfaces assisting in this task. In this paper, we consider the well-established FEM-software Abaqus, which is widely used in research as well as industrial applications. Concerning nonlinear hyperelasticity, Abaqus offers at least two direct ways for the user to specify a stress response. The first is by choosing any of the predefined elastic energies (including, for example, the compressible neo-Hooke or the Mooney-Rivlin model). The other is based on the \texttt{hyper} interface subroutine, which lets the user define a custom isotropic strain energy \( W = W(F) \) of the deformation gradient \( F \). This energy must be provided by the user in the form of a function

\[
W(F) = \hat{W}(I_1(B), I_2(B), I_3(B))
\]

(1.2)
of the principal invariants

\[
\begin{align*}
I_1 &= \text{tr} B, \\
I_2 &= \frac{1}{2}[(\text{tr} B)^2 - \text{tr}(B^2)] = \text{tr} \, \text{Cof} B, \\
I_3 &= \text{det} B
\end{align*}
\]

(1.3)
of the Finger tensor \( B = F \cdot F^T \), cf. [7, 1], where \( \text{tr} \) denotes the trace operator. It is well known that every isotropic and objective strain energy can be represented in terms of the principal invariants of \( B \). In many cases, however, the representation \( \hat{W} \) is not readily available. Oftentimes, the energy \( W \) is stated more naturally in terms of the principal logarithmic stretches \( \lambda_i \), i.e. represented as

\[
W(F) = \Psi(\lambda_1, \lambda_2, \lambda_3)
\]

(1.4)

with a symmetric function \( \Psi \); for example, Ogden–type models [10] or energies in terms of the principal logarithmic stretches [4, 15, 6] can be easily expressed in the form (1.4). In these cases, it is of course still possible to write \( (\lambda_1, \lambda_2, \lambda_3) \) as a function of the principal invariants \( (I_1, I_2, I_3) \) using Cardano’s formulas and thus find the representation \( \hat{W} \). Unfortunately, since the mapping \( (I_1, I_2, I_3) \mapsto (\lambda_1, \lambda_2, \lambda_3) \) is not well-behaved, this method is generally not suitable for working with the predefined Abaqus routines.
In particular, during our previous work [12] with the exponentiated Hencky energy [14] (cf. [13, 11, 17])

\[ W_{\text{eH}}(\mathbf{F}) = \mu e^k \| \text{dev log} \mathbf{V} \|^2 + \frac{\kappa}{2} e^{\hat{k}} [(\log \det \mathbf{V})]^2, \]

(1.5)

where \( \mathbf{V} = \sqrt{\mathbf{B}} \) is the left stretch tensor, \( \log \) denotes the principal matrix logarithm and \( \text{dev log} \mathbf{V} \) denotes its deviatoric part, we realized that expressing \( W_{\text{eH}} \) in terms of the invariants would not be a promising approach for a finite-element implementation within ABAQUS. Instead, we opted for the more general \( \text{umat} \)-environment provided by ABAQUS, which allowed us to work directly with the representation (1.4) of \( W_{\text{eH}} \) in terms of the principal stretches, in accordance with the ABAQUS user manual [1].

Our specific choice of parameters for the exponentiated Hencky model corresponded to an almost incompressible material, and the results computed by ABAQUS did not cause any concern. However, we became aware of several articles of Bažant and coworkers [3, 9] who, while investigating the use of different stress rates within commercial finite element codes (including ABAQUS and ANSYS), discovered a certain error in ABAQUS’s treatment of the problem for highly compressible materials. The computational examples presented by Bažant et al. (including the shear deformation at a skew-notched cylinder [18]) are, however, based on an elasto-plastic approach and therefore not easily understood regarding their impact on pure hyperelasticity.

In this short paper we want to illustrate Bažant’s observation by a very simple boundary value problem involving a purely hyperelastic, highly compressible material. We thereby demonstrate the inconsistency between the predefined material model and the \( \text{uhyper} \) method on the one hand and the corresponding implementation with the \( \text{umat} \) procedure on the other. We also implement Bažant’s suggestion of how to circumvent this problem by modifying the formulas given in the ABAQUS manual and prescribing the correct tangent operator. Our example demonstrates the correctness of this ingenious fix.

Since the ABAQUS software is ubiquitous in academia and industry alike, we believe that the developers have a certain responsibility towards their users and should fix these issues as soon as possible. A direct interface based on the representation (1.4) of the elastic energy potential in terms of the principal stretches would also be a helpful addition to ABAQUS and would render the use of the \( \text{umat} \) routine unnecessary for many applications in pure hyperelasticity.

1.1 Stress rates and time integration

In Section (1.5.3) of the ABAQUS Theory Guide [1], the Jaumann rate of change of the Kirchhoff stress \( \mathbf{\tau} = J \mathbf{\sigma} \) is given by (cf. [7])

\[ \mathbf{\tau} = \frac{d}{dt}(J \mathbf{\sigma}) := \frac{d}{dt}(J \mathbf{\sigma}) - J(\mathbf{w} \cdot \mathbf{\sigma} - \mathbf{\sigma} \cdot \mathbf{w}), \]

(1.6)

where

\[ \mathbf{w} := \frac{1}{2} (\mathbf{L} - \mathbf{L}^T) \]

(1.7)

is the spin tensor, i.e. the skew-symmetric part of the spatial gradient \( \mathbf{L} := \partial \mathbf{v}/\partial \mathbf{x} = \mathbf{F} \cdot \mathbf{F}^{-1} \) of a particle’s material velocity \( \mathbf{v} \) and \( J = \det \mathbf{F} = \sqrt{I_3} \) denotes the volume ratio corresponding to the deformation gradient \( \mathbf{F} \).

According to the ABAQUS Theory Guide, it is assumed that “the constitutive theory will define \( \frac{d}{dt}(J \mathbf{\sigma}) \), the corotational stress rate per reference volume, in terms of the rate of deformation and past history, so this equation provides a convenient link between that material model and the overall change in ‘true’ (Cauchy) stress (which is the stress measure defined directly from the equilibrium equations),” while “[f]or hyperelastic materials a total formulation is used; hence, the concept of an objective rate is not relevant for the constitutive law.”

Thus the internal handling of constitutive modeling – and especially its time integration scheme – differs between the standardized \( \text{uhyper} \) routine, which is inherently restricted to hyperelastic materials based on strain energy functions, and the more general \( \text{umat} \) interface, even if the latter is applied only to a purely hyperelastic material.

Nevertheless, one would expect that the overall results by such finite element systems for nonlinear, hyperelastic behaviour should be (exactly) the same.
2 Three ways of implementing hyperelasticity in ABAQUS

We consider a very simple hyperelastic, isotropic, compressible model of neo-Hooke type, given by the elastic strain energy

\[ W(F) = c_1(T_1 - 3) + \frac{1}{D_1} (J - 1)^2 = c_1 \left( \left\| \frac{F}{\det F^{1/3}} \right\|^2 - 3 \right) + \frac{1}{D_1} (\det F - 1)^2 \]  

(2.1)

with the shear modulus \( \mu = G = 2c_1 \) and the bulk modulus \( \kappa = K = \frac{2c_1}{J_1} \), where \( J_1 = J^{-2/3} I_1 \) is the scaled first invariant of the Finger tensor \( B = F \cdot F^T \), see (1.3). We implement this material model in ABAQUS in three different ways.

Predefined material model The compressible neo-Hookean model (2.1) is available in ABAQUS internally via *hyperelastic, neo hooke*. The parameters \( c_1 \) and \( D_1 \) can be chosen by the user within the *material description*.

The uhyper subroutine Alternatively, ABAQUS provides the option to add custom hyperelastic models via a user subroutine called uhyper, which allows the user to define the stress response by specifying an arbitrary isotropic strain energy. The energy must be given in the form \( W \), i.e. as a function \( W \) of the invariants \( T_1, T_2 \) and \( J \). Furthermore, the uhyper method requires the user to provide the derivatives of \( W \) up to order three, i.e.

\[ \frac{\partial W}{\partial T_1}, \frac{\partial W}{\partial T_2}, \frac{\partial W}{\partial J}, \frac{\partial^2 W}{\partial T_1^2}, \frac{\partial^2 W}{\partial T_1 \partial T_2}, \frac{\partial^2 W}{\partial J^2}, \frac{\partial W}{\partial J^3}, \ldots \]  

(2.2)

Note that implementing the model (2.1) this way is relatively simple due to the fact that most terms in (2.2) are zero.

Theumat subroutine As a third option, ABAQUS provides a general user material interface called umat, which enables the user to define their own constitutive models by specifying the Cauchy stress tensor \( \sigma \) (by its six components in the three-dimensional case) and the so-called tangent modulus [1] Section 4.6

\[ C = \frac{1}{J} \frac{\partial \Delta(J \sigma)}{\partial \Delta \varepsilon} \]  

(2.3)

where \( \varepsilon = \log V \) denotes the logarithmic (or true) strain tensor corresponding to the left stretch tensor \( V = \sqrt{B} \), which is given by the polar decomposition \( F = V \cdot R \) of \( F \), and the rotation tensor \( R \).

Again, we use the hyperelastic model (2.1) and implement the Cauchy stress tensor

\[ \sigma(B) = \frac{2}{J} \frac{\partial W}{\partial J} B + \frac{\partial W}{\partial J} I \]  

(2.4)

and its modulus (2.3) within ABAQUS as a user material via the umat interface. The components of the fourth-order tensor \( C \) in (2.3) can be obtained from the variation

\[ \delta \tau = J C : \delta D = J (C_{iso} + C_{vol}) : \delta D \]  

(2.5)

of the Kirchhoff stress \( \tau \), with the additive decomposition of \( C \) into an isochoric part \( C_{iso} \) and a volumetric part \( C_{vol} \) following from the additive structure in (2.1) and (2.4). Here, \( D := \frac{1}{2} (L + L^T) \) is the symmetric part of the spatial gradient \( L \) of the material velocity \( l \), and \( X : Y \) denotes the double contraction of two tensors \( X, Y \). We can determine \( C_{iso} \) and \( C_{vol} \) using the equality

\[ J (C_{iso} + C_{vol}) = 4B \frac{\partial^2 W_{iso}(B)}{\partial B \partial B} B + 4B \frac{\partial^2 W_{vol}(J)}{\partial B \partial B} B, \]

where \( W_{iso} \) and \( W_{vol} \) are the isochoric and volumetric parts of the energy (depending only on \( B = J^{-2/3} B \) and \( J = \sqrt{\det B} \), respectively). We thereby obtain, in accordance with the ABAQUS Theory guide [1],

\[ J C_{ijkl} = \mu \left\{ \frac{1}{2} (\delta_{ik} B_{jl} + B_{ik} \delta_{jl} + \delta_{il} B_{jk} + B_{il} \delta_{jk}) - \frac{2}{3} (\delta_{ij} B_{kl} + B_{ij} \delta_{kl}) + \frac{2}{3} \delta_{ij} \delta_{kl} B_{mm} \right\} + \kappa (2J - 1) \delta_{ij} \delta_{kl}, \]

(2.6)
where $\delta_{ij}$ is the Kronecker symbol for the second-order identity $I$, following the Einstein convention for summation. An equivalent representation is given by Itskov \cite{8}. Using (2.6) as well as (2.4), the neo-Hooke model (2.1) can now be implemented using the umat subroutine.

Remark 2.1. It is mentioned in the ABAQUS Theory Guide \cite{1} that, especially for “almost incompressible” materials, using the umat routine “is suitable for material models that use an incremental formulation (for example, metal plasticity) but is not consistent with a total formulation that is commonly used for hyperelastic materials.” Nevertheless, here we show the dramatic inconsistencies that arise from following the umat based approach for implementing (highly) compressible hyperelastic material behaviour.

In summary, we now have three different implementations of the neo-Hooke model (2.1) within ABAQUS at our disposal: first the integrated material call, then the implementation via the uhyper routine and lastly the umat realization.

2.1 Bažant’s proposed modification of the tangent modulus

In addition to these three implementations, we also consider the modified tangent modulus

$$C_{ijkl}^{\text{mod}} = C_{ijkl} - \sigma_{ij} \delta_{kl},$$

(2.7)

where $C$ is given by (2.6) and $\sigma = \tau/J$ is the Cauchy stress tensor, which was proposed by Bažant \cite{3,9} to compensate for the difference in results produced by ABAQUS for different implementations. In order to compare the numerical results, we implement the model with the umat subroutine again, this time using the modified modulus $C_{ijkl}^{\text{mod}}$ instead of $C$ from (2.6).

3 Examples of numerical results for different implementations

Using the different ABAQUS implementations of our material model introduced in the previous section, we now consider two boundary value problems in order to highlight the discrepancies between the results.

Figure 1: Axisymmetric model of a “quasi-incompressible” O-ring seal on a rod under pressure.

Figure 2: Radial reaction force during pressure loading of an O-ring seal. All implementations in ABAQUS coincide for the quasi-incompressible hyperelastic response.
3.1 Quasi-incompressible material behaviour

First, we consider the mounting and pressure loading of an O-ring in a realistic sealing application with the axisymmetric geometry shown in Fig. 1. First, the O-ring is mounted in the outer casing by a radial shift of 0.25 mm into the groove. It is then loaded by a pressure of 5.0 MPa (50 bar) from below in order to simulate a sealing situation along the rod within the casing. The material is assumed to be quasi-incompressible; the chosen material parameters are shown in Tab. 1.

Fig. 2 shows the numerical result for the radial reaction force on the rod during the pressure loading step for the three different material model implementations. As expected, the three different responses show exactly the same behaviour since, due to the quasi-incompressibility, \( J \approx 1 \) and thus \( \sigma \approx \tau \).

| \( r_i \) | \( d \) | \( \mu = G \) | \( \kappa = K = 2/D_1 \) |
|----------|----------|-------------|------------------|
| 28 mm    | 2 mm     | 1.0 MPa     | 2000 MPa         |

Table 1: Geometry and material parameters (O-ring example).

3.2 Compressible material behaviour

Next, we reconsider the numerical example from [12] of a mostly bounded block of hyperelastic material being compressed by a flat, unilateral displacement as shown in Fig. 3. Again, we use our neo-Hookean model (2.1); the material parameters used here are shown in Tab. 2. Note that, in order to test the behavior of the different implementations for a highly compressible material, we choose a very low bulk modulus of \( \kappa = 0.78 \) MPa.

| \( a \) | \( t \) | \( \mu \) | \( \kappa \) |
|--------|--------|--------|--------|
| 20 mm  | 5 mm   | 1.0 MPa| 0.78 MPa|

Table 2: Geometry and material parameters (footing example).
Figure 4: Reaction force – footing example: comparison of neo-Hooke implementations via \texttt{uhyper}, \texttt{umat} and Abaqus’ internal material model. The squares show the result for the modified \texttt{umat} implementation proposed by Bažant, which exactly agrees with the \texttt{uhyper} response for compressible hyperelasticity. In contrast, the internal neo-Hooke implementation (with *hyperelastic, neo hooke) results in a much stiffer response for the low bulk modulus $\kappa = 0.78$ MPa.

As depicted in Fig. 4, completely different stress responses occur for the different considered implementations. Using the neo-Hooke energy predefined by Abaqus, the material behavior is quite stiff – apparently due to the assumption of incompressibility and the non-observance of the very low $\kappa$ value – while using the \texttt{uhyper} routine with \eqref{eq:2.1} induces the least stiff stress response. Implementing \eqref{eq:2.1} using the \texttt{umat} subroutine without additional modifications (i.e. as required by the Abaqus Theory Guide) yields an intermediary stiffness. However, if the \texttt{umat} method is applied using the modified tangent modulus \eqref{eq:2.7} proposed by Bažant, the stress response is identical to the one induced by the \texttt{uhyper} routine. This latter behavior is also in agreement with independent calculations based on the FEM software DAEdalon \cite{2}.

4 Conclusion

Our results confirm that the discrepancy between the different implementations of hyperelastic models in Abaqus repeatedly mentioned by Bažant has considerable consequences for the solution of FE-problems, especially for highly compressible materials. We also demonstrate that Bažant’s proposed modification of the tangent modulus can easily be implemented and is able to completely remedy this inconsistency.
5 References

[1] *ABAQUS/Standard User’s Manual*. Providence, RI, USA: Simulia, 2016.
[2] H. Baaser. *Development and Application of the Finite Element Method based on MATLAB*. Springer, 2010.
[3] Z. Bažant, M. Gattu, and J. Vorel. “Work conjugacy error in commercial finite-element codes: its magnitude and how to compensate for it”. *Proceedings of the Royal Society* 468 (2012), pp. 3047–3058.
[4] G.F. Becker. “The finite elastic stress-strain function”. *American Journal of Science* 46 (1893). newly typeset version available at [https://www.uni-due.de/imperia/md/content/mathematik/ag_neff/becker_latex_new1893.pdf](https://www.uni-due.de/imperia/md/content/mathematik/ag_neff/becker_latex_new1893.pdf), pp. 337–356.
[5] A. Bertram. *Elasticity and Plasticity of Large Deformations: An Introduction*. Springer Berlin Heidelberg, 2008.
[6] H. Hencky. “Welche Umstände bedingen die Verfestigung bei der bildsamen Verformung von festen isotropen Körpern?” *Zeitschrift für Physik* 55 (1929). available at [www.uni-due.de/imperia/md/content/mathematik/ag_neff/hencky1929.pdf](www.uni-due.de/imperia/md/content/mathematik/ag_neff/hencky1929.pdf), pp. 145–155.
[7] G. Holzapfel. *Nonlinear Solid Mechanics*. Wiley, 2000.
[8] M. Itskov. *Tensor Algebra and Tensor Analysis for Engineers: With Applications to Continuum Mechanics*. 2nd ed. Springer, 2009.
[9] W. Ji, A. Waas, and Z. Bažant. “On the importance of work-conjugacy and objective stress rates in finite deformation incremental finite element analysis”. *Journal of Applied Mechanics* 80.4 (2013), pp. 041024–041024.
[10] C. Miehe. “Aspects of the formulation and finite element implementation of large strain isotropic elasticity”. *International Journal for Numerical Methods in Engineering* 37 (1994), pp. 1981–2004.
[11] G. Montella, S. Govindjee, and P. Neff. “The exponentiated Hencky strain energy in modeling tire derived material for moderately large deformations”. *Journal of Engineering Materials and Technology* 138.3 (2016), pp. 031008–1–031008–12.
[12] B. Nedjar, H. Baaser, R.J. Martin, and P. Neff. “A finite element implementation of the isotropic exponentiated Hencky-logarithmic model and simulation of the eversion of elastic tubes”. to appear in *Computational Mechanics* (2017). available at arXiv:1705.08381.
[13] P. Neff, B. Eidel, and R.J. Martin. “Geometry of logarithmic strain measures in solid mechanics”. *Archive for Rational Mechanics and Analysis* 222.2 (2016). available at arXiv:1505.02203, pp. 507–572. doi: [10.1007/s00205-016-1007-x](https://doi.org/10.1007/s00205-016-1007-x).
[14] P. Neff, I.-D. Ghiba, and J. Lankeit. “The exponentiated Hencky-logarithmic strain energy. Part I: Constitutive issues and rank-one convexity”. *Journal of Elasticity* 121.2 (2015), pp. 143–234. doi: [10.1007/s10659-015-9524-7](https://doi.org/10.1007/s10659-015-9524-7).
[15] P. Neff, I. Münch, and R.J. Martin. “Rediscovering G.F. Becker’s early axiomatic deduction of a multiaxial nonlinear stress–strain relation based on logarithmic strain”. *Mathematics and Mechanics of Solids* 21.7 (2016), pp. 856–911. doi: [10.1177/1081286514542296](https://doi.org/10.1177/1081286514542296).
[16] R.W. Ogden. *Non-Linear Elastic Deformations*. 1st ed. Mathematics and its Applications. Chichester: Ellis Horwood, 1983.
[17] J. Schröder, M. von Hoegen, and P. Neff. “The exponentiated Hencky energy: Anisotropic extension and biomechanical applications”. to appear in *Computational Mechanics* (2016). available at arXiv:1702.00394.
[18] J. Vorel and Z. Bažant. “Review of energy conservation errors in finite element softwares caused by using energy–inconsistent objective stress rates”. *Advances in Engineering Software* 72 (2014), pp. 3–7.