Data Article

Numerical simulation data and FORTRAN code to compare the stress response of two transversely isotropic hyperelastic models in ABAQUS

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A R T I C L E   I N F O

Article history:
Received 17 November 2021
Revised 19 December 2021
Accepted 17 January 2022
Available online 19 January 2022

Keywords:
Finite element
UMAT subroutine
Hyperelasticity
Anisotropic invariants

A B S T R A C T

We present the numerical simulation data obtained by implementing a user material subroutine (UMAT) in the finite element commercial package ABAQUS. The simulation data correspond to the stress response of two transversely isotropic hyperelastic models on homogeneous and non-homogeneous deformations. First model is proposed in the co-submitted article [1] and depends on both anisotropic invariants ($\bar{I}_4$ and $\bar{I}_5$) to describe the fiber reinforcement. The second model is the Holzapfel-Gaser-Ogden (HGO) model described in [2], that only depends on the anisotropic invariant $\bar{I}_4$. Since the first model is not found in the ABAQUS material library, we present a FORTRAN code for a UMAT subroutine. In addition, we introduce in detail the steps to implement the material models using the attached files in ABAQUS.

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DOI of original article: 10.1016/j.ijnonlinmec.2021.103833
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https://doi.org/10.1016/j.dib.2022.107853
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Specifications Table

| Subject | Engineering |
|---------|-------------|
| Specific subject area | Computational Mechanics, Modelling and Computational Simulation of Anisotropic Hyperelastic Materials. |
| Type of data | Tables and Figures |
| | Excel spreadsheet (.xlsx) |
| | Simulation data: ABAQUS input file (.inp), ABAQUS output file (.odb) |
| | FORTRAN code (.for) |
| Description of data collection | The simulations data and FORTRAN codes were generated in a personal computer |
| Data format | Raw, calculated, and processed output data |
| Data source location | The FORTRAN subroutine code (UMAT) was written by the authors. |
| | The simulation data were obtained by running finite element models together with the UMAT in the commercial package FEA ABAQUS. |
| Data accessibility | Repository name: Mendeley Data |
| | Data identification number: 10.17632/tszvwzkckh.2 |
| | Direct URL to data: https://data.mendeley.com/datasets/tszvwzkckh/2 |
| Related research article | [1] Castillo-Méndez, C. and Ortiz, A., Role of anisotropic invariants in numerically modeling soft biological tissues as transversely isotropic hyperelastic materials: A comparative study. International Journal of Non-Linear Mechanics, 2022. 138: p. 103833. |
| | DOI: https://doi.org/10.1016/j.jnonlinmech.2021.103833. |

Value of the Data

- The data can be found helpful by researchers interested in hyperelastic materials, since they show the consequences of using one or both anisotropic invariants, in the modeling of transversely isotropic hyperelastic materials.
- The simulation data can be used by other researchers to compare the behavior of their models.
- The UMAT subroutine provided can easily be modified to implement another material model of particular interest.
- The subroutine can be used as a base and extended to more complex phenomena such as hyper-viscoelasticity or hyper-elastoplasticity.

1. Data Description

This paper presents the data related to the computational simulation of two anisotropic hyperelastic models shown in Eqs. (1) and (2). These data are used to compare the elastic mechanical response of models that depend on a single anisotropic invariant against those that depend on the two anisotropic invariants. The numerical simulations are carried out in the commercial finite element package ABAQUS. Since the model presented in Eq. (1) is not found in the ABAQUS materials library, its implementation is carried out using a user material subroutine (UMAT). The UMAT is a FORTRAN code that uses ABAQUS to update the Cauchy stress tensor and the tangent stiffness tensor.

This article presents four types of data, found in the attachments, and described below:

a) ABAQUS Input file (.inp). It is an ASCII data file and can be created using a text editor or a graphical preprocessor such as ABAQUS/CAE. This file consists of a series of lines containing ABAQUS options (keyword lines) and data (data lines) [3]. The input file generally contains the data that define the model: geometry (nodes and elements), materials, initial conditions,
kinematic interactions and constraints, loads, and the discretization of the geometry (meshing).

b) ABAQUS Output database file (.odb). This type of file contains the final output data of the simulation (force, displacement, reaction forces). This file is in hexadecimal format and can only be read by the ABAQUS viewer.

c) FORTRAN file (.for). This type of file contains source code in the FORTRAN language and is written in a subroutine form (UMAT) that receives and passes variables to the ABAQUS solver.

d) EXCEL file (.xlsx). This file contains the tables with the stress responses of the models for each case described in [1].

The data organization (in the attached file) is shown in Fig. 1.

The folder named “homogeneous deformation” contains the input files (.inp) for the homogeneous deformation cases described in [1]. The files are described in Table 1.

The folder named “non-homogeneous simulations” contains input files (.inp) for non-homogeneous deformation cases described in [1]. The files are described in Table 2.

The folders named “HD Proposed Model ODB” and “HD HGO Model ODB” contain the odb files corresponding to the homogeneous deformation cases for the models described in Eqs. (1) and (2), respectively. The files are presented in Table 3.

The folders named “NHD Proposed Model ODB” and “NHD HGO Model ODB” contain the odb files corresponding to non-homogeneous deformation cases for models (1) and (2), respectively, see Table 4.

The folder named “FORTRAN file” contains the FORTRAN codes in the form of a material subroutine for modeling the Eqs. (1) and (2) in ABAQUS. Table 5 describes the files.

The folder “EXCEL file” contains the file “Stress.xlsx” with the stress vs. strain data in table form for the cases analyzed in [1].

Fig. 2 shows the steps that must be followed to perform the simulation in ABAQUS with the provided files. These steps are detailed in section 2.3.

The symbols used and their respective meanings are shown in Table 6.
Table 1  
Description for the input files corresponding to homogeneous deformation.

| Filename       | File Description                                                                 |
|----------------|-----------------------------------------------------------------------------------|
| Shear_30.inp   | Input file corresponding to the simple shear case with the direction of the fibers at an angle of \( \theta = 30^\circ \) with the \( E_1 \) axis. |
| Shear_45.inp   | Input file corresponding to the simple shear case with the direction of the fibers at an angle of \( \theta = 45^\circ \) with the \( E_1 \) axis. |
| Shear_60.inp   | Input file corresponding to the simple shear case with the direction of the fibers at an angle of \( \theta = 60^\circ \) with the \( E_1 \) axis. |
| Shear_L.inp    | Input file corresponding to the simple shear with the fibers in the longitudinal (parallel) direction to the \( E_1 \) axis. |
| Shear_P.inp    | Input file corresponding to the simple shear with the fibers in the perpendicular direction to the \( E_1 \) axis. |
| Traction_Biax.inp | Input file corresponding to the biaxial traction.                                |
| Traction_Uniaxial.inp | Input file corresponding to the uniaxial traction in the fiber direction.      |

Table 2  
Description for the input files corresponding to non-homogeneous deformation.

| Filename          | File Description                                                                 |
|-------------------|-----------------------------------------------------------------------------------|
| Shear0_NHD.inp    | Input file corresponding to the non-homogeneous shear case with the direction of the fibers at an angle of \( \theta = 30^\circ \) with the \( E_1 \) axis. |
| Shear45_NHD.inp   | Input file corresponding to the non-homogeneous shear case with the direction of the fibers at an angle of \( \theta = 45^\circ \) with the \( E_1 \) axis. |
| Shear90_NHD.inp   | Input file corresponding to the non-homogeneous shear case with the direction of the fibers at an angle of \( \theta = 90^\circ \) with the \( E_1 \) axis. |
| Traction0_NHD.inp | Input file corresponding to the non-homogeneous traction case with the direction of the fibers at an angle of \( \theta = 30^\circ \) with the \( E_1 \) axis. |
| Traction45_NHD.inp| Input file corresponding to the non-homogeneous traction case with the direction of the fibers at an angle of \( \theta = 60^\circ \) with the \( E_1 \) axis. |
| Traction90_NHD.inp| Input file corresponding to the non-homogeneous traction case with the direction of the fibers at an angle of \( \theta = 90^\circ \) with the \( E_1 \) axis. |

Table 3  
The filename of the odb files contained in the homogeneous deformation folders.

| Folders            | HD HGO Model ODB                                                                 |
|--------------------|--------------------------------------------------------------------------------|
| HD Proposed Model ODB | HGO_Shear30.odb  
|                    | HGO_Shear_45.odb  
|                    | HGO_Shear_60.odb  
|                    | HGO_Shear_Lodb    
|                    | HGO_Shear_Podb    
|                    | HGO_Shear_Todb    
|                    | HGO_Traction_Biax.odb  
|                    | HGO_Traction_Uniaxial.odb          |
|                    | PM_Shear_30.odb  
|                    | PM_Shear_45.odb  
|                    | PM_Shear_60.odb  
|                    | PM_Shear_Lodb    
|                    | PM_Shear_Podb    
|                    | PM_Shear_Todb    
|                    | PM_Traction_Biax.odb  
|                    | PM_Traction_Uniaxial.odb          |

Table 4  
The filename of the “odb files” contained in the non-homogeneous deformation folders.

| Folders            | NHD HGO Model ODB                                                                 |
|--------------------|--------------------------------------------------------------------------------|
| NHD Proposed Model ODB | PM_Shear0_NHD.odb  
|                     | PM_Shear45_NHD.odb  
|                     | PM_Shear90_NHD.odb  
|                     | PM_Traction0_NHD.odb  
|                     | PM_Traction45_NHD.odb  
|                     | PM_Traction90_NHD.odb  
|                     | HGO_Shear0_NHD.odb  
|                     | HGO_Shear45_NHD.odb  
|                     | HGO_Shear90_NHD.odb  
|                     | HGO_Traction0_NHD.odb  
|                     | HGO_Traction45_NHD.odb  
|                     | HGO_Traction90_NHD.odb  |
Fig. 2. Steps to carry out the simulation in ABAQUS.
Table 5
Description of FORTRAN files.

| Filename                     | File Description                                                                 |
|------------------------------|----------------------------------------------------------------------------------|
| UMAT_AnisoHyper_PM.for       | FORTRAN file containing the UMAT subroutine to implement the Proposed Model, Eq. (1). |
| UMAT_AnisoHyper_HGO.for      | FORTRAN file containing the UMAT subroutine to implement the HGO Model, Eq. (2).  |

Table 6
Nomenclature.

| Symbol  | Meaning                                                                 |
|---------|------------------------------------------------------------------------|
| $\psi$  | Strain energy function                                                 |
| $\overline{\psi}$ | Deviatoric strain energy function                                      |
| $\kappa$ | Bulk modulus                                                          |
| $c_1, c_2, c_3, c_4, c_5$ | Material parameters                                                    |
| $J$     | Determinant of the deformation gradient                                |
| $I_1, I_2$ | Isotropic deviatoric strain invariants                             |
| $I_4, I_5$ | Anisotropic deviatoric strain invariants                          |
| $\sigma_{ij}$ | Cauchy stress tensor                                                |
| $p$     | Hydrostatic pressure                                                  |
| $\delta_{ij}$ | Kronecker Delta                                                |
| $\mathbf{B}_{ij}$ | Deviatoric Left Cauchy-Green deformation tensor                  |
| $C_{ij}$ | Deviatoric Right Cauchy-Green deformation tensor                     |
| $\mathbf{m}$ | Unit vector on the fiber direction in the deformed configuration    |
| $m_0$   | Unit vector on the fiber direction in the reference configuration      |
| $\otimes$ | Tensor product                                                       |
| $(C^{ijkl})_{ijkl}$ | Tangent stiffness tensor                     |
| $F_{ij}$ | Deformation gradient tensor                                          |
| $E_1, E_2, E_3$ | Basis vector                                                             |
| $\psi_1, \psi_2, \psi_3, \psi_5$ | Partial derivative of the term $\psi$ with respect to $I_1, I_2, I_4, I_5$ |

2. Experimental Design, Materials and Methods

2.1. Description of the material model

The simulation data were obtained by implementing in ABAQUS two hyperelastic models that are given by

$$
\psi = \frac{1}{2} \kappa (J - 1)^2 + \frac{c_1}{2} (I_1 - 3) \\
+ \frac{c_2}{2c_3} \left\{ \exp \left[ c_3 (I_4 - 1)^2 \right] - 1 \right\} + \frac{c_4}{2c_5} \left\{ \exp \left[ c_5 (I_5 - I_4^2) \right] - 1 \right\},
$$

(1)

$$
\overline{\psi} = \frac{c_1}{2} (I_1 - 3) + \frac{c_2}{2c_3} \left\{ \exp \left[ c_3 (I_4 - 1)^2 \right] - 1 \right\}.
$$

(2)

Eq. (1) is proposed in [1], and Eq. (2) is known as the HGO (Holzapfel-Gasser-Ogden) model described in [2]. These models are implemented by user material. To write the UMAT subroutine is necessary to define the Cauchy stress tensor and the tangent stiffness tensor. For the transversely isotropic case. The Cauchy stress tensor in index notation is given by

$$
\sigma_{ij} = \left[ p - \frac{2}{3J} (I_1 \psi_1 + 2I_2 \psi_2 + I_4 \psi_4 + 2I_5 \psi_5) \right] \delta_{ij} \\
+ 2J^{-1} \left[ (\psi_1 + I_1 \psi_2) \mathbf{B}_{ij} - \psi_2 \mathbf{B}_{ij}^2 + \psi_4 (\mathbf{m} \otimes \mathbf{m})_{ij} + \psi_5 (\mathbf{m} \otimes \mathbf{m} \otimes \mathbf{m} \otimes \mathbf{m})_{ij} \right],
$$

(3)
and the tangent stiffness tensor in index notation is given by

\[
(C^\Delta J)_{ijkl} = E_i F_{ij} F_{kl} \left( \frac{4 \beta^2 \psi}{\partial \psi \partial C_{ij} \partial C_{kl}} \right) + \delta_{ik} \sigma_{jl} + \sigma_{ik} \delta_{jl}.
\] (4)

A detailed deduction of Eqs. (3) and (4) can be consulted in [4].

2.2. Application of the models

The stress response of the models is analyzed in homogeneous and non-homogeneous deformations using the methodology described in the co-submitted article [1].

2.3. Running the simulation in ABAQUS

To run the simulations in ABAQUS must be taken into account that the ABAQUS solver needs to be linked to a FORTRAN compiler. In this article, the INTEL FORTRAN compiler (ifort) contained in the package Intel Parallel Studio XE 2019 is used, in addition ABAQUS 6.14-1 and Visual Studio 2013 as IDE.

a) Open the ABAQUS/CAE application in the “Job module.” Select “create job” in the source tab, select “input file” and select the path of the desired input file, as shown in Fig. 2(a).

b) In the “edit job” window, the “general” tab is selected, and in the “user subroutine file” section, the path of the desired FORTRAN file is placed, creating a “Job” in ABAQUS (see Fig. 2(b)).

c) In the window “Job manager” press the tab "submit" (see Fig. 2(c)). The model will begin to work immediately, and once completed, an output file (.odb) is created.

An alternative manner of running the code is to use the “ABAQUS command” application and enter the command “ABAQUS job = Shear45_NHD user = UMAT_AnisoHyper_PM” (see Fig. 2(d)). The simulation starts immediately after running the command.

2.4. View results

To view the results, it is necessary to open the ABAQUS CAE application, and the odb file must be opened in the “visualization” module. This module contains different tools to visualize, simulate and graph the results that have been defined in the model. For example, stress, strain, displacements, reaction force, see Fig 2(e).

Ethics Statement

This work did not involve human subjects, animal experiments, or data collected from social media platforms.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
CRediT Author Statement

**Carlos Castillo-Méndez:** Conceptualization, Methodology, Software, Validation, Formal analysis, Writing – original draft; **Armando Ortiz:** Resources, Supervision, Writing – review & editing, Project administration.

Acknowledgments

This work was funded by The National Council of Science and Technology (CONACYT) of the United Mexican States by doctoral fellowship for the first author. The authors thank Dr. Rafael Schouwenaars and Dr. Fernando Velazquez-Villegas for their helpful comments on this work.

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