

Nonlinear anisotropic hyperelastic arterial wall material models into ANSYS

USER MANUAL & THEORY - v0.1

Nicolas Mesnier*

June 15, 2011

Abstract

This document aims to serve as *user manual* to use and implement anisotropic hyperelastic material models to describe the arterial wall behaviour. Embedded into the classical geometric formulation of continuum mechanics, we provide an explicit derivation of three constitutive models. Their implementation into a user material routine written in modern Fortran is also presented and the Fortran code listing for the user material routine `usermat3d()` is given.

*Permanent e-mail: nicolas.mesnier@gmail.com

Contents

1	Introduction	3
2	Installation	3
2.1	Installation	3
2.2	Recompilation	4
2.2.1	Installation des compilateurs	4
2.2.2	La re-compilation	5
2.2.3	Le premier bug	5
2.2.4	Le cadeau de la v12	6
3	User manual	6
3.1	Linking <code>usermat()</code>	6
3.2	Elements restrictions	7
3.3	ADPL specifications	7
3.3.1	Model 1 - Holzapfel et al. (2000)	7
3.3.2	Model 2 - Baek et al. (2007)	8
3.3.3	Model 3 - Holzapfel et al. (2005)	8
4	Theory and implementation	9
4.1	Theoretical background	9
4.1.1	Variational formulation	9
4.1.2	Corotational kinematics	10
4.1.3	Corotational tangent stiffness	11
4.2	Explicit tangent stiffness	11
4.2.1	Holzapfel (2000) <code>sedf</code>	11
4.2.2	Holzapfel (2005) <code>sedf</code>	12
4.3	Implementation	14
4.3.1	Element orientation and material anisotropy	14
4.3.2	Voigt notation	14
A	Ansys <code>usermat3d()</code> subroutine	16

1 Introduction

Since the arteries may be regarded as a fibre-reinforced composite, we are interested in the numerical implementation of specific anisotropic hyperelastic behaviour laws into ANSYS. In order to describe the anisotropic elastic stress response of arteries, we decided to use the strain energy density function proposed by Holzapfel et al. [2, 3] and Baek et al. [1]. Consequently, the following anisotropic hyperelastic material models are currently implemented:

1. Anisotropic two conjugated fibres family of Holzapfel et al. [2],
2. Anisotropic four fibres family of Baek et al. [1], in which two fibres family are conjugated,
3. Anisotropic two conjugated fibres family of Holzapfel et al. [3].

For that purpose, we first present the way to use these material models with ANSYS. In a second step, we recall some specificity of the finite element method and particularly the way to define a user material (in ANSYS). A special attention is provided on the material tangent, naturally given in the spatial configuration and which need to be recast in the corotated frame. For such purpose, we recall the algorithm for determination of the corotated frame rotation via the polar decomposition of the deformation gradient, as well as the conversion of the stress, material tangent and change of basis operations to Voigt notation. After while we derived the material models and finally we give the Fortran code listing for the user material routine `usermat3d()`.

2 Installation

Dans cette partie, nous avons regroupé les informations permettant d'utiliser ANSYS en version personnalisée sur une distribution linux 32 bits de base debian, comme ubuntu. Les petits détails pas toujours évidents à régler pour y parvenir sont ici mentionnés.

2.1 Installation

Pour utiliser ANSYS, il faut installer la version 32 bits linux. Immédiatement après, il est nécessaire d'installer les librairies `mesa` et `libmotif3`

```
sudo apt-get install libglu1-mesa  
sudo apt-get install libmotif3
```

et de créer quelques liens symboliques dans le répertoire `/usr/lib` du genre

```
sudo ln -s /usr/lib/libGLU.so.1.*.* /usr/lib/libGLU.so  
sudo ln -s /usr/lib/libXm.so.3.*.* /usr/lib/libXm.so  
sudo ln -s /usr/lib/libXi.so.6.*.* /usr/lib/libXi.so  
sudo ln -s /usr/lib/libXext.so.6.*.* /usr/lib/libXext.so  
sudo ln -s /usr/lib/libXmu.so.*.* /usr/lib/libXmu.so  
sudo ln -s /usr/lib/libXp.so.6.*.* /usr/lib/libXp.so  
sudo ln -s /usr/lib/libXt.so.6.*.* /usr/lib/libXt.so  
sudo ln -s /usr/lib/libX11.so.6.*.* /usr/lib/libX11.so
```

associés aux paquets dépendants de motif, notamment libxi6, libxext6, libxmu6, libxp6, libxt6, libx11-6. Ensuite, il est nécessaire de faire pointer la librairie OpenGL vers celle de votre carte graphique. En ce qui concerne mes machines, c'est du nvidia et j'ai créé le lien

```
sudo ln -s /usr/lib/nvidia-current/libGL.so /usr/lib/libGL.so
```

Avec tout ça, vous lancer ansys en mode graphique avec la commande

```
/usr/local/ansys_inc/vXX0/ansys/bin/launcherXX0
```

où vous prendrez soin de remplacer les "XX" par votre version d'ANSYS.

2.2 Recompilation

Pour pouvoir recompiler ANSYS, par exemple pour utiliser son propre modèle de comportement, il est nécessaire d'avoir installé les compilateurs intel cpp V9.1 et intel fortran V9.1 (tel que certifié par Ansys).

2.2.1 Installation des compilateurs

J'ai téléchargé sur le site intel

<http://software.intel.com/en-us/articles/intel-compilers/>
les versions:

- intel cpp 32 bits version 9.1.047,
- intel fortran 32 bits version 9.1.043.

Une fois les archives disponibles, avant de procéder à l'installation des compilateurs, il est nécessaire d'installer les paquets

```
sudo apt-get install alien g++-multilib libstdc++5 build-essential
```

et de faire quelques modifications banales du genre remplacer le lien de sh vers dash, visible par

```
moi@mon-pc:~$ls -l /bin/sh
lrwxrwxrwx 1 root root 9 date heure /bin/sh -> /bin/dash
```

vers bash selon

```
sudo rm /bin/sh
sudo ln -s /bin/bash /bin/sh
```

Après quoi, il est nécessaire de décompresser l'archive de chacun des compilateurs et de créer un *.deb adapté à l'installation sur base debian à partir du *.rpm (RedHat) fourni par intel. Pour le compilateur fortran, il faut exécuter la séquence

```
tar xvzf l_fc_c_9.1.043_ia32.tar.gz
cd l_fc_c_9.1.043_ia32/data
sudo alien -cv intel-ifort91043-9.1.043-1.i386.rpm
sudo dpkg -i intel-ifort91043-9.1.043-1_i386.deb
```

et de façon équivalente pour le compilateur cpp

```

tar xvzf l_cc_c_9.1.047_ia32.tar.gz
cd l_cc_c_9.1.047_ia32/data
sudo alien -cv intel-icc91047-9.1.047-1.i386.rpm
sudo dpkg -i ntel-icc91047-9.1.047-1.i386.deb

```

Bien que les deux compilateurs soient maintenant installés, les fichiers se réfèrent à <INSTALLDIR> et non à /opt/intel/... comme il faudrait. Il est donc nécessaire d'aller remplacer toutes les occurrences pour les deux compilateurs. Comme nous ne sommes pas (encore) fous, on lance une simple commande `sed` en root:

```

sudo sed -i 's/&lt;INSTALLDIR&gt;/\>/opt\intel\fc\9.1.043/g' \
          /opt/intel/fc/9.1.043/bin/ifortvars.sh
sudo sed -i 's/&lt;INSTALLDIR&gt;/\>/opt\intel\cc\9.1.047/g' \
          /opt/intel/cc/9.1.047/bin/iccvars.sh

```

Maintenant, il ne reste plus qu'à copier les fichiers de licence gracieusement offerts par intel pour toute utilisation non-commerciale

```

cp quelque_part/NCOM_L_CMP_FOR*.lic /opt/intel/fc/9.1.043/licenses/.
cp quelque_part/NCOM_L_CMP_CPP*.lic /opt/intel/cc/9.1.047/licenses/.

```

et d'ajouter deux lignes au fichier `~/.bashrc` pour être certain que le shell hérite bien des variables des compilateurs intel:

```

cd ~
echo "source /opt/intel/fc/9.1.043/bin/ifortvars.sh" 1>>.bashrc
echo "source /opt/intel/cc/9.1.047/bin/iccvars.sh" 1>>.bashrc

```

2.2.2 La re-compilation

Les fichiers sources qu'ANSYS vous autorise à recompiler sont dans le répertoire `/usr/local/ansys_inc/vXX0/ansys/customize`. Je vous encourage vivement à copier ce répertoire et le mettre dans un autre répertoire, par exemple celui de vos fichiers sources de simulation. Pour ma part, j'en ai profité pour le renommer `ansys-custom`. Les *User Programmable Features* d'ANSYS résident dans le sous-répertoire `user`. Pour mes travaux, je me suis amusé à éditer le code fortran `ansys-custom/user/usermat3d.F` associé à la définition de modèles de comportement mécanique. Ainsi, une fois que vous avez codé ce que vous souhaitez, vous recompilez ANSYS avec

```
./ansys-custom/user/ANSCUSTOM
```

et tapez deux fois y pour créer un exécutable distribuable qui portera le doux nom de `ansys-custom/user/ansyscust.eXX0`, "XX" étant toujours associé à votre version.

2.2.3 Le premier bug

Un des premiers éléments auxquels vous êtes confronté après avoir installé les compilateurs et essayé votre première compilation est le message d'erreur:

```

/usr/ansys_inc/vxx0/ansys/lib/linia32/libansys.so:
undefined reference to 'glPolygonOffsetEXT'

```

où vous prendrez soin de remplacer les "xx" par la version d'ANSYS. Le palliatif qui a fonctionné est de créer un *wrapper*¹ vers la bonne fonction sous la forme

```
#include <GL/gl.h>

void glPolygonOffsetEXT(float factor, float bias) {
    glPolygonOffset(factor, bias);
}
```

que vous enregistrez par exemple sous le nom `wrapper.c` et que vous compilez ensuite sous forme de librairie:

```
gcc -fPIC -shared -o wrapper.so wrapper.c
```

Partant de ce point, il est nécessaire d'inclure l'appel à cette librairie lors de la compilation. En créant un répertoire `doc` avec le source et la librairie `wrapper.so` dans votre répertoire `ansys-custom`, il vous faut éditer le fichier `user/ANSCUSTOM` et ajouter la ligne

```
-L ./doc -lwrapper \
```

au niveau de l'appel aux librairies graphiques `lopnsx11=...` dans la commande relative aux systèmes linux 32 bits.

2.2.4 Le cadeau de la v12

Avec la v12, lorsque vous essayez de compiler vos anciens codes, vous êtes confronté à de nouveaux petits problèmes. Pour ma part, ils ont été résolu en créant simplement des liens symboliques associés aux librairies MPI fournies par ANSYS; explicitement

```
sudo ln -s /usr/local/ansys_inc/v120/ansys/hpmpi/\
    linia32/lib/linux_ia32/libmpio.so.1 /usr/lib/.
sudo ln -s /usr/local/ansys_inc/v120/ansys/hpmpi/\
    linia32/lib/linux_ia32/libmpi.so.1 /usr/lib/.
```

Avec ces liens, tout fonctionne (enfin) correctement.

3 User manual

3.1 Linking usermat()

Pour utiliser votre ANSYS recompilé, vous disposez de deux moyens. Le premier est le mode graphique que vous lancez avec la commande

```
/usr/local/ansys\_inc/vXX0/ansys/bin/launcherXX0
```

et pour lequel vous prenez soin dans le second onglet de préciser l'exécutable que vous souhaitez utiliser avant de lancer la commande `run`. Sur un plan pratique, vous cliquez sur `browse` et allez chercher le fichier exécutable ANSYS

```
quelque_part/ansys-custom/user/ansyscust.eXX0
```

¹Les détails sont disponibles sur <http://www.nvnews.net/vbulletin/archive/index.php/t-68080.html>.

qui vous intéresse. Si vide, ce sera ANSYS par défaut.

Le second moyen, plus pratique pour les gros calculs, est d'appeler ANSYS en batch. Dans ce cas, il suffit d'utiliser la séquence de commandes

```
ansys=/usr/local/ansys_inc/vXX0/ansys/bin/ansysXX0
ansyscust=quelque_part/ansys-custom/user/ansyscust.eXX0
file=your-job-file.inp
"$ansys" -p AA_T_ME -j "job-file" -s read -l en-us
-b <"$file" -custom "$ansyscust" | tee -i 'job-file.out'
```

ici associée à l'exécution du job ANSYS appelé `job-file` et dont les instructions sont données dans le fichier `your-job-file.inp`.

3.2 Elements restrictions

The user material routine, `usermat()`, is an ANSYS user-programmable feature for use with the 18x family elements which allow user to write their own material constitutive equations within. In our specification of the code, it can be used with `plane182`, `plane183`, `solid185` and `solid186`. This subroutine is called at all material integration points of these elements during the solution phase. The input parameters for the `usermat` subroutine is defined by command `tb,user`.

3.3 ADPL specifications

Recall that ADPL is nothing but *ANSYS Parametric Design Language*. This is the classical code used to define a simulation file. Then, when you want to use one of the three material behaviour law of the arterial wall, you need the following specifications:

3.3.1 Model 1 - Holzapfel et al. (2000)

The strain energy density proposed by Holzapfel et al. [2] is given by

$$\psi = \frac{\mu}{2} (\bar{I}_1 - 3) + \frac{\kappa}{2} (J - 1)^2 + \sum_{\alpha=1}^2 \frac{k_1}{2k_2} \left(\exp \left[k_2 (\bar{I}_4^\alpha - 1)^2 \right] - 1 \right). \quad (1)$$

To define such material model with the ADPL, you need to furnish to the `usermat()` routine the following definitions:

```
mat-nb=1           ! material number
tb,user,mat-nb,1,6
tbdta,1,1          ! Holzapfel et al. (2000)
tbdta,2,15.02      ! mu
tbdta,3,1e5         ! k (bulk modulus)
tbdta,4,38.57       ! k1
tbdta,5,85.03       ! k2
tbdta,6,67          ! beta, deg
tb,state,mat-nb,,4 ! state var
```

3.3.2 Model 2 - Baek et al. (2007)

The strain energy density proposed by Baek et al. [1] is given by

$$\begin{aligned}\psi = & \frac{\mu}{2} (\bar{I}_1 - 3) + \frac{\kappa}{2} (J - 1)^2 + \sum_{\alpha=1}^2 \frac{k_1}{2 k_2} \left(\exp \left[k_2 (\bar{I}_4^\alpha - 1)^2 \right] - 1 \right) \\ & + \frac{k_1^\theta}{2 k_2^\theta} \left(\exp \left[k_2^\theta (\bar{I}_4^\theta - 1)^2 \right] - 1 \right) + \frac{k_1^z}{2 k_2^z} \left(\exp \left[k_2^z (\bar{I}_4^z - 1)^2 \right] - 1 \right). \quad (2)\end{aligned}$$

To define such material model with the ADPL, you need to furnish to the `usermat()` routine the following definitions:

```
mat-nb=1           ! material number
tb,user,mat-nb,1,10
tbdta,1,2          ! Baek et al. (2007)
tbdta,2,75.53      ! mu
tbdta,3,1e5         ! k (bulk modulus)
tbdta,4,6.25        ! k1\theta
tbdta,5,0.1370      ! k2\theta
tbdta,6,12.71        ! k1z
tbdta,7,0.0290      ! k2z
tbdta,8,0.016        ! k1\alpha
tbdta,9,1.4390      ! k2\alpha
tbdta,10,58.6000     ! beta, deg
tb,state,mat-nb,,4 ! state var
```

3.3.3 Model 3 - Holzapfel et al. (2005)

The strain energy density proposed by Holzapfel et al. [3] is given by

$$\begin{aligned}\psi = & \frac{\mu}{2} (\bar{I}_1 - 3) + \frac{\kappa}{2} (J - 1)^2 \\ & + \frac{k_1}{k_2} \left[\exp \left(k_2 \left[(1 - \rho) (\bar{I}_1 - 3)^2 + \rho (\bar{I}_4 - 1)^2 \right] \right) - 1 \right]. \quad (3)\end{aligned}$$

To define such material model with the ADPL, you need to furnish to the `usermat()` routine the following definitions:

```
mat-nb=1           ! material number
tb,user,mat-nb,1,7
tbdta,1,3          ! Holzapfel et al. (2005)
tbdta,2,15.02      ! mu
tbdta,3,1e5         ! k (bulk modulus)
tbdta,4,38.57       ! k1
tbdta,5,85.03       ! k2
tbdta,6,0.55        ! rho
tbdta,7,67          ! beta, deg
tb,state,mat-nb,,4 ! state var
```

4 Theory and implementation

In this section we first recall the basis to express spatial quantities into the corotational frame. After while, the basis of the finite element method are recalled so as to have the necessary theoretical background to understand the implementation of a user material into the finite element commercial software ANSYS by using the user subroutine `usermat3d()`.

4.1 Theoretical background

We are interested in an anisotropic strain energy density function (sedf) of the form

$$\psi : (\mathbf{g}, \mathbf{b}, \mathbf{a}_\alpha) \rightarrow \mathbb{R} \quad (4)$$

per unit volume of the material manifold \mathcal{B} , where \mathbf{g} is the spatial (euclidean) metric and \mathbf{b} is introduced as relevant deformation measure. It is defined as the inverse of the convected material metric \mathbf{G} , explicitly

$$\mathbf{b} = (\varphi_* \mathbf{G})^{-1} = F_A^i F_B^j G^{AB} \partial_i \otimes \partial_j , \quad (5)$$

and customary denoted the left Cauchy-Green strain tensor. To model anisotropy due to fibres behaviour, we introduce the family of symmetric second order structural tensor

$$\mathbf{a}_\alpha = \varphi_* (\mathbf{f}_\alpha \otimes \mathbf{f}_\alpha) = F_A^i f_\alpha^A f_\alpha^B F_B^j \partial_i \otimes \partial_j , \quad \alpha = 1, \dots, n \quad (6)$$

in which the unit vector \mathbf{f}_α describe the α -fibre direction on the material manifold \mathcal{B} . Following the theory of invariants and classical decomposition methods, we may rewrite the generic sedf in the form

$$\psi = \psi_{\text{vol}}(J) + \psi_{\text{mat}}(\bar{I}_1) + \sum_{\alpha \in \mathcal{B}} \psi_{\text{fib}}^\alpha(\bar{I}_4^\alpha) \quad (7)$$

with the definition of invariants

$$J = \det \mathbf{F} , \quad \bar{I}_1 = J^{-\frac{2}{3}} g_{ij} b^{ij} , \quad \bar{I}_4^\alpha = J^{-\frac{2}{3}} g_{ij} a_\alpha^{ij} . \quad (8)$$

where we used the abbreviation $\bullet = J^{-\frac{2}{3}} \mathbf{•}$.

4.1.1 Variational formulation

In quasi-static finite elasticity, the classical (covariant) variations $\delta_\xi \psi[\partial\varphi] = d_\varepsilon \psi[\partial(\phi^\varepsilon \circ \varphi)]|_{\varepsilon=0}$, where ϕ^ε is the flow generated by the vector field $\xi = \xi^i \partial_i$, may refer to the Lie-derivative

$$\mathfrak{L}_\xi \psi = \frac{\partial \psi}{\partial \mathbf{g}} : \mathfrak{L}_\xi \mathbf{g} = \boldsymbol{\tau} : \mathbf{d} \quad \text{with } \boldsymbol{\tau} = 2 \partial_{\mathbf{g}} \psi \quad (9)$$

where $\mathbf{d} = \text{sym}(\mathbf{l})$ and with $\mathbf{l} = \nabla_i \xi_j dx^i \otimes dx^j$. Thus, the Lie derivative of the Kirshhoff stress may be expressed as

$$\mathfrak{L}_\xi \boldsymbol{\tau} = \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{g}} : \mathfrak{L}_\xi \mathbf{g} = \mathbf{c} : \mathbf{d} . \quad (10)$$

In the above relation, \mathbf{c} is the tangent stiffness, defined by

$$(\mathbf{c})^{ijkl} = 2 \frac{\partial \tau^{ij}}{\partial g_{kl}}. \quad (11)$$

On an other hand, let us recall that the Lie derivative of the Kirshhoff stress classically reads

$$\mathcal{L}_\xi \boldsymbol{\tau} = d_t \boldsymbol{\tau} - \mathbf{l} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{l}^t. \quad (12)$$

with $\mathbf{l} = \mathbf{d} + \boldsymbol{\omega}$, $\boldsymbol{\omega} = \text{skew}(\mathbf{l})$.

4.1.2 Corotational kinematics

Let us introduce the transformation $\boldsymbol{\varphi}$ that maps material points \mathbf{X} in the material configuration \mathcal{B}_0 onto a position $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t)$ in the spatial configuration \mathcal{B}_t . The corresponding deformation gradient $\mathbf{F} = \partial_{\mathbf{X}} \boldsymbol{\varphi}(\mathbf{X}, t)$,

$$\mathbf{F} = \partial_A \varphi^i \partial_i \otimes dX^A, \quad (13)$$

with Jacobian $J = \det \mathbf{F} > 0$, denotes the tangent map from the material tangent space $T\mathcal{B}_0$ to the spatial tangent space $T\mathcal{B}_t$. As each $GL(3, \mathbb{R})$ -tensor, it may be recasted into a unique polar decomposition

$$\mathbf{F} = R_a^i U_A^a \partial_i \otimes dX^A \quad (14)$$

where $\mathbf{U} = U_A^a \partial_a \otimes dX^A$ is the stretch tensor. Thus, given a deformation gradient, the frame rotation \mathbf{R} is determined from the closed-form solution of the inverse stretch,

$$\mathbf{U}^{-1} = \frac{1}{III_U} (\mathbf{C} - I_U \mathbf{U} + II_U \mathbf{I}) \quad (15)$$

where I_U , II_U and III_U are the principal invariants of \mathbf{U} . Since the eigenvalues of \mathbf{U} are the square root of the eigenvalues of $\mathbf{C} = \boldsymbol{\varphi}^* \mathbf{g}$ given by the roots of the characteristic polynomial

$$P(\lambda) = -\lambda^3 + \lambda^2 I_1 - \lambda I_2 + I_3 \quad (16)$$

where the principal invariants are

$$I_1 = \text{tr}(\mathbf{C}), \quad I_2 = \frac{1}{2} (I_1^2 - \text{tr}(\mathbf{C}^2)), \quad I_3 = \det(\mathbf{C}). \quad (17)$$

Since $\{C_{AB}\}$ is a symmetric, positive-definite, rank 3 matrix, Eq.(16) has 3 positive real roots given by

$$\lambda_i = \frac{I_1}{3} + \frac{2}{3} \sqrt{I_1^2 - 2I_2} \cos \left(\frac{\beta + 2\pi(i-1)}{3} \right), \quad (18)$$

$$\text{with } \beta = \arccos \left(\frac{2I_1^3 - 9I_1 I_2 + 27I_3}{2\sqrt{(I_1^2 - 2I_2)^3}} \right). \quad (19)$$

This formulation is implemented by means of the `polarRU()` subroutine. For further details, the reader may refers to Simo and Hughes [4, box 7.1 page 743].

4.1.3 Corotational tangent stiffness

Now introducing the corotated Kirhoff stress $\hat{\boldsymbol{\tau}}$, that is explicitly the pull-back of the Kirshhoff stress into the corotated frame

$$\hat{\boldsymbol{\tau}} = \mathbf{R}^*(\boldsymbol{\tau}) = R_i^{-a} \tau^{ij} R_j^{-b} \partial_a \otimes \partial_b \quad (20)$$

$\mathbf{R} = \mathbf{F} \cdot \mathbf{U}^{-1}$ being the rotation of the corotated frame, it is straightforward to see that the push-forward of the Lie derivative of the corotated Kirhoff stress is equivalent to the Lie derivative of the Kirhoff stress, augmented by convective terms. That is explicitly in components,

$$\mathbf{R}_*(\mathfrak{L}_\xi \hat{\boldsymbol{\tau}}) = \mathfrak{L}_\xi \boldsymbol{\tau} + \mathbf{d} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{d} = J\mathcal{C} : \mathbf{d}. \quad (21)$$

In the above relation, \mathcal{C} is the Jaumann tangent stiffness, defined with minor symmetries by

$$(\mathcal{C})^{ijkl} = \frac{1}{J} (\mathbf{c})^{ijkl} + \frac{1}{2J} (g^{ik} \tau^{jl} + \tau^{ik} g^{jl} + g^{il} \tau^{jk} + \tau^{il} g^{jk}). \quad (22)$$

Finally, one obtains the corotated fourth order tangent operator $\hat{\mathcal{C}}$ needed to be calculated at each iteration and at each integration point by simple pull-back in the corotated frame of all its components; explicitly

$$(\hat{\mathcal{C}})^{abcd} = R_i^{-a} R_j^{-b} (\mathcal{C})^{ijkl} R_k^{-c} R_l^{-d}. \quad (23)$$

Then, since we customary used isoparametric finite elements, we must rewrite all these equation into full Cartesian coordinates, i.e. $G_{AB} = \delta_{AB}$ and $g_{ij} = \delta_{ij}$.

4.2 Explicit tangent stiffness

In this section we give the explicit tangent stiffness related to the chosen material models. Since Baek et al. [1] is a simple four fibres extension of Holzapfel et al. [2] model, we just concentrated our efforts on Holzapfel et al. [2] and Holzapfel et al. [3] models.

In what follow, we use the classical derivations of the invariants in terms of the spatial metric

$$\frac{\partial J}{g_{ij}} = \frac{J}{2} g^{ij}, \quad \frac{\partial \bar{I}_1}{g_{ij}} = \bar{b}^{ij} - \frac{\bar{I}_1}{3} g^{ij}, \quad \frac{\partial \bar{I}_4^\alpha}{g_{ij}} = \bar{a}_\alpha^{ij} - \frac{\bar{I}_4^\alpha}{3} g^{ij}, \quad (24)$$

and the useful definition of (minus) the fourth rank identity tensor, computed from the well-known relationship

$$\frac{\partial g^{ij}}{g_{kl}} = -\frac{1}{2} (g^{ik} g^{jl} + g^{il} g^{jk}). \quad (25)$$

4.2.1 Holzapfel (2000) sedf

The strain energy density proposed by Holzapfel et al. [2] is given by

$$\psi = \psi_{\text{vol}}(J) + \psi_{\text{mat}}(\bar{I}_1) + \sum_{\alpha \in \mathcal{B}} \psi_{\text{fib}}^\alpha(\bar{I}_4^\alpha) \quad (26)$$

with the three parts having explicit forms

$$\psi_{\text{vol}} = \frac{\kappa}{2} (J - 1)^2 , \quad (27a)$$

$$\psi_{\text{mat}} = \frac{\mu}{2} (\bar{I}_1 - 3) , \quad (27b)$$

$$\psi_{\text{fib}}^{\alpha} = \frac{k_1^{\alpha}}{2 k_2^{\alpha}} \left(\exp \left[k_2^{\alpha} (\bar{I}_4^{\alpha} - 1)^2 \right] - 1 \right) . \quad (27c)$$

Thus, the elastic stress response is governed by the three contributions

$$\tau_{\text{vol}}^{ij} = \kappa J (J - 1) g^{ij} , \quad (28a)$$

$$\tau_{\text{mat}}^{ij} = \mu (\text{dev } \bar{\mathbf{b}})^{ij} , \quad (28b)$$

$$\tau_{\text{fib}}^{ij} = \sum_{\alpha \in \mathcal{B}} 2 (\psi_{\text{fib}}^{\alpha})_{,\alpha} (\text{dev } \bar{\mathbf{a}})^{ij} . \quad (28c)$$

where

$$(\text{dev } \bar{\mathbf{b}})^{ij} = \bar{b}^{ij} - \frac{\bar{I}_1}{3} g^{ij} , \quad (29)$$

$$(\text{dev } \bar{\mathbf{a}})^{ij} = \bar{a}^{ij} - \frac{\bar{I}_4}{3} g^{ij} , \quad (30)$$

$$(\psi_{\text{fib}}^{\alpha})_{,\alpha} = k_1^{\alpha} (\bar{I}_4^{\alpha} - 1) \exp \left[k_2^{\alpha} (\bar{I}_4^{\alpha} - 1)^2 \right] . \quad (31)$$

Thus, using the decoupled representation of the Kirshhoff stress tensor, its derivatives straightforward leads to the relations for the volumic and isotropic deviatoric parts:

$$(\mathbf{c}_{\text{vol}})^{ijkl} = \kappa J [(2J - 1) g^{ij} g^{kl} - (J - 1) (g^{ik} g^{jl} + g^{il} g^{jk})] , \quad (32a)$$

$$(\mathbf{c}_{\text{mat}})^{ijkl} = \frac{2}{3} \mu \left[\frac{\bar{I}_1}{2} (g^{ik} g^{jl} + g^{il} g^{jk}) + \frac{\bar{I}_1}{3} g^{ij} g^{kl} - (g^{ij} \bar{b}^{kl} + \bar{b}^{ij} g^{kl}) \right] . \quad (32b)$$

Finally, for the anisotropic deviatoric part, we used both derivation on J and \mathbf{a} and obtained

$$\begin{aligned} (\mathbf{c}_{\text{fib}})^{ijkl} &= \sum_{\alpha \in \mathcal{B}} \left\{ 4 (\psi_{\text{fib}}^{\alpha})_{,\alpha} (\text{dev } \bar{\mathbf{a}})^{ij} (\text{dev } \bar{\mathbf{a}})^{kl} \right. \\ &\quad \left. + \frac{4}{3} (\psi_{\text{fib}}^{\alpha})_{,\alpha} \left[\frac{\bar{I}_4^{\alpha}}{2} (g^{ik} g^{jl} + g^{il} g^{jk}) + \frac{\bar{I}_4^{\alpha}}{3} g^{ij} g^{kl} - (g^{ij} \bar{a}_{\alpha}^{kl} + \bar{a}_{\alpha}^{ij} g^{kl}) \right] \right\} \end{aligned} \quad (33)$$

where

$$(\psi_{\text{fib}}^{\alpha})_{,\alpha} = k_1^{\alpha} \left(1 + 2 k_2^{\alpha} (\bar{I}_4^{\alpha} - 1)^2 \right) \exp \left[k_2^{\alpha} (\bar{I}_4^{\alpha} - 1)^2 \right] . \quad (34)$$

4.2.2 Holzapfel (2005) sedf

The strain energy density proposed by Holzapfel et al. [3] is given by

$$\psi = \psi_{\text{vol}} (J) + \psi_{\text{mat}} (\bar{I}_1) + \psi_{\text{fib}} (\bar{I}_1, \bar{I}_4) \quad (35)$$

with the three parts having explicit forms

$$\psi_{\text{vol}} = \frac{\kappa}{2} (J - 1)^2 , \quad (36a)$$

$$\psi_{\text{mat}} = \frac{\mu}{2} (\bar{I}_1 - 3) , \quad (36b)$$

$$\psi_{\text{fib}} = \frac{k_1}{k_2} \left[\exp \left(k_2 \left[(1 - \rho) (\bar{I}_1 - 3)^2 + \rho (\bar{I}_4 - 1)^2 \right] \right) - 1 \right] . \quad (36c)$$

Thus, the elastic stress response is governed by the three contributions

$$\tau_{\text{vol}}^{ij} = \kappa J (J - 1) g^{ij} , \quad (37a)$$

$$\tau_{\text{mat}}^{ij} = \mu (\text{dev } \bar{\mathbf{b}})^{ij} , \quad (37b)$$

$$\tau_{\text{fib}}^{ij} = \left\{ (\psi_{\text{fib}})_{,\bar{I}_1} (\text{dev } \bar{\mathbf{b}})^{ij} + (\psi_{\text{fib}})_{,\bar{I}_4} (\text{dev } \bar{\mathbf{a}})^{ij} \right\} . \quad (37c)$$

where

$$(\text{dev } \bar{\mathbf{b}})^{ij} = \bar{b}^{ij} - \frac{\bar{I}_1}{3} g^{ij} , \quad (38a)$$

$$(\text{dev } \bar{\mathbf{a}})^{ij} = \bar{a}^{ij} - \frac{\bar{I}_4}{3} g^{ij} , \quad (38b)$$

$$(\psi_{\text{fib}})_{,\bar{I}_1} = (1 - \rho) (\bar{I}_1 - 3) \mathcal{F} , \quad (38c)$$

$$(\psi_{\text{fib}})_{,\bar{I}_4} = \rho (\bar{I}_4 - 1) \mathcal{F} , \quad (38d)$$

$$\mathcal{F} = 4 k_1 \exp \left(k_2 \left[(1 - \rho) (\bar{I}_1 - 3)^2 + \rho (\bar{I}_4 - 1)^2 \right] \right) . \quad (38e)$$

Thus, using the decoupled representation of the Kirshhoff stress tensor, its derivatives straightforward leads to the relations for the volumic and isotropic deviatoric parts:

$$(\mathbf{c}_{\text{vol}})^{ijkl} = \kappa J [(2J - 1) g^{ij} g^{kl} - (J - 1) (g^{ik} g^{jl} + g^{il} g^{jk})] , \quad (39a)$$

$$(\mathbf{c}_{\text{mat}})^{ijkl} = \frac{2}{3} \mu \left[\frac{\bar{I}_1}{2} (g^{ik} g^{jl} + g^{il} g^{jk}) + \frac{\bar{I}_1}{3} g^{ij} g^{kl} - (g^{ij} \bar{b}^{kl} + \bar{b}^{ij} g^{kl}) \right] . \quad (39b)$$

Finally, for the anisotropic deviatoric part, we used both derivation on J and \mathbf{a} and obtained

$$\begin{aligned} (\mathbf{c}_{\text{fib}})^{ijkl} &= (\psi_{\text{fib}})_{,\bar{I}_1 \bar{I}_1} (\text{dev } \bar{\mathbf{b}})^{ij} (\text{dev } \bar{\mathbf{b}})^{kl} + (\psi_{\text{fib}})_{,\bar{I}_4 \bar{I}_4} (\text{dev } \bar{\mathbf{a}})^{ij} (\text{dev } \bar{\mathbf{a}})^{kl} \\ &\quad + (\psi_{\text{fib}})_{,\bar{I}_1 \bar{I}_4} [(\text{dev } \bar{\mathbf{b}})^{ij} (\text{dev } \bar{\mathbf{a}})^{kl} + (\text{dev } \bar{\mathbf{a}})^{ij} (\text{dev } \bar{\mathbf{b}})^{kl}] \\ &\quad - \frac{2}{3} (\psi_{\text{fib}})_{,\bar{I}_1} (g^{ij} \bar{b}^{kl} + \bar{b}^{ij} g^{kl}) - \frac{2}{3} (\psi_{\text{fib}})_{,\bar{I}_4} (g^{ij} \bar{a}^{kl} + \bar{a}^{ij} g^{kl}) \\ &\quad + \left[\frac{\bar{I}_1}{3} (\psi_{\text{fib}})_{,\bar{I}_1} + \frac{\bar{I}_4}{3} (\psi_{\text{fib}})_{,\bar{I}_4} \right] \times \left[(g^{ik} g^{jl} + g^{il} g^{jk}) + \frac{2}{3} g^{ij} g^{kl} \right] \end{aligned} \quad (40)$$

where

$$(\psi_{\text{fib}})_{,\bar{I}_1 \bar{I}_1} = 2 (1 - \rho) \left[1 + 2 k_2 (1 - \rho) (\bar{I}_1 - 3)^2 \right] \mathcal{F} , \quad (41a)$$

$$(\psi_{\text{fib}})_{,\bar{I}_1 \bar{I}_4} = 2 \rho (1 - \rho) (\bar{I}_1 - 3) (\bar{I}_4 - 1) \mathcal{F} , \quad (41b)$$

$$(\psi_{\text{fib}})_{,\bar{I}_4 \bar{I}_4} = 2 \rho \left[1 + 2 k_2 \rho (\bar{I}_4 - 1)^2 \right] \mathcal{F} . \quad (41c)$$

4.3 Implementation

4.3.1 Element orientation and material anisotropy

In this section, we present the approach used to determine the anisotropic directions. To determine the initial element orientation \mathbf{f}_0 , we assume a “sufficiently good mesh” so as to base its determination on elements orientation, i.e. on the element sides. For 2-dimensional elements, such as `plane 182` or `plane 183` [see Fig.(1)], the fibre direction is determined through the simple relation

$$\mathbf{f}_0 = \frac{(\mathbf{X}_i - \mathbf{X}_j) + (\mathbf{X}_l - \mathbf{X}_k)}{\|(\mathbf{X}_i - \mathbf{X}_j) + (\mathbf{X}_l - \mathbf{X}_k)\|}, \quad (42)$$

where the subset identified the corresponding node. Similarly, for 3-dimensional elements, such as `solid 185` or `solid 186` [see Fig.(1)], the fibre direction is determined via

$$\mathbf{f}_0 = \frac{(\mathbf{X}_i - \mathbf{X}_j) + (\mathbf{X}_l - \mathbf{X}_k) + (\mathbf{X}_m - \mathbf{X}_n) + (\mathbf{X}_p - \mathbf{X}_o)}{\|(\mathbf{X}_i - \mathbf{X}_j) + (\mathbf{X}_l - \mathbf{X}_k) + (\mathbf{X}_m - \mathbf{X}_n) + (\mathbf{X}_p - \mathbf{X}_o)\|}. \quad (43)$$

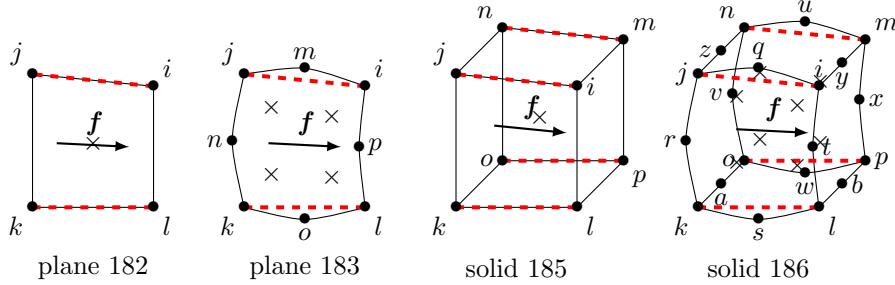


Figure 1: Illustration of determination of ANSYS elements orientation based on the median of highlighted red sides.

Notice that since ANSYS worked with updated coordinates, we first have to get the current node position as well as its current corresponding displacement so as to determine the initial position with

$$\mathbf{X}_i = \mathbf{x}_i - \mathbf{u}_i. \quad (44)$$

Then, once \mathbf{f}_0 is determined, we can compute the local anisotropic directions \mathbf{f}_0^α , which then has to be pushed-forward into the spatial direction with

$$\mathbf{f}^\alpha = \mathbf{F} \cdot \mathbf{f}_0^\alpha, \quad (45)$$

from which we construct the structural tensor

$$\bar{\mathbf{a}}^\alpha = J^{-\frac{2}{3}} \mathbf{f}^\alpha \otimes \mathbf{f}^\alpha. \quad (46)$$

4.3.2 Voigt notation

Let us first recall that using the symmetry properties of second order tensor, we may introduce the Voigt notation by converting pairs of indices to a single

index via $\{11\ 22\ 33\ 12\ 23\ 31\} = \{11\ 22\ 33\ 21\ 32\ 13\} \Rightarrow \{1\ 2\ 3\ 4\ 5\ 6\}$ such that the Jaumann rate of the Cauchy stress may reads in Voigt notation

$$\{\dot{\sigma}\} = [\mathcal{C}] \cdot \{\dot{\mathbf{d}}\} \quad (47)$$

with $\{\dot{\mathbf{d}}\}$ the Voigt notation of the rate of deformation tensor $\mathbf{d} = \text{sym}(\nabla_x \varphi)$, explicitly defined by

$$\{\dot{\mathbf{d}}\} = \{d_{11} \ d_{22} \ d_{33} \ 2d_{12} \ 2d_{23} \ 2d_{13}\}^T. \quad (48)$$

Accordingly, the fourth order Jaumann tangent stiffness may be recast in the following form

$$[\mathcal{C}] = \begin{bmatrix} \mathcal{C}_{1111} & \mathcal{C}_{1122} & \mathcal{C}_{1133} & \mathcal{C}_{1112} & \mathcal{C}_{1123} & \mathcal{C}_{1113} \\ \infty & \mathcal{C}_{2222} & \mathcal{C}_{2233} & \mathcal{C}_{2212} & \mathcal{C}_{2223} & \mathcal{C}_{2213} \\ \infty & \infty & \mathcal{C}_{3333} & \mathcal{C}_{3312} & \mathcal{C}_{3323} & \mathcal{C}_{3313} \\ \infty & \infty & \infty & \mathcal{C}_{1212} & \mathcal{C}_{1223} & \mathcal{C}_{1213} \\ \infty & \infty & \infty & \infty & \mathcal{C}_{2323} & \mathcal{C}_{2313} \\ \infty & \infty & \infty & \infty & \infty & \mathcal{C}_{1313} \end{bmatrix}, \quad (49)$$

where the symbol ∞ stands for symmetric terms. Notice that the stress in the tangent stiffness are

$$[\mathcal{C}] - \frac{1}{J} [\mathbf{c}] = \frac{1}{2} \begin{bmatrix} 4\sigma_1 & 0 & 0 & 2\sigma_4 & 0 & 2\sigma_6 \\ \infty & 4\sigma_2 & 0 & 2\sigma_4 & 2\sigma_5 & 0 \\ \infty & \infty & 4\sigma_3 & 0 & 2\sigma_5 & 2\sigma_6 \\ \infty & \infty & \infty & \sigma_1 + \sigma_2 & \sigma_6 & \sigma_5 \\ \infty & \infty & \infty & \infty & \sigma_2 + \sigma_3 & \sigma_4 \\ \infty & \infty & \infty & \infty & \infty & \sigma_1 + \sigma_3 \end{bmatrix}. \quad (50)$$

Thus, once the Cauchy stress $\{\sigma\}$ and the Jaumann tangent stiffness $[\mathcal{C}]$ are determined, they need to be expressed into the corotated frame. Denoting $[\mathbf{Q}]$ the change of basis matrix, it is defined from the orthogonal rotation tensor $\mathbf{R}^{-1} \equiv \mathbf{R}^T$ by

$$[\mathbf{Q}] = \begin{bmatrix} [\mathbf{Q}_{11}] & [\mathbf{Q}_{12}] \\ [\mathbf{Q}_{21}] & [\mathbf{Q}_{22}] \end{bmatrix}. \quad (51)$$

with

$$[\mathbf{Q}_{11}] = \begin{bmatrix} R_{11}^2 & R_{21}^2 & R_{31}^2 \\ R_{12}^2 & R_{22}^2 & R_{32}^2 \\ R_{13}^2 & R_{23}^2 & R_{33}^2 \end{bmatrix}, \quad (52)$$

$$[\mathbf{Q}_{12}] = 2 \begin{bmatrix} R_{11}R_{21} & R_{21}R_{31} & R_{11}R_{31} \\ R_{12}R_{22} & R_{22}R_{32} & R_{12}R_{32} \\ R_{13}R_{23} & R_{23}R_{33} & R_{13}R_{33} \end{bmatrix}, \quad (53)$$

$$[\mathbf{Q}_{21}] = \begin{bmatrix} R_{11}R_{12} & R_{21}R_{22} & R_{31}R_{32} \\ R_{12}R_{13} & R_{22}R_{23} & R_{32}R_{33} \\ R_{13}R_{11} & R_{23}R_{21} & R_{33}R_{31} \end{bmatrix}, \quad (54)$$

$$[\mathbf{Q}_{22}] = \begin{bmatrix} R_{11}R_{22} + R_{21}R_{12} & R_{21}R_{32} + R_{31}R_{22} & R_{11}R_{32} + R_{31}R_{12} \\ R_{12}R_{23} + R_{22}R_{13} & R_{22}R_{33} + R_{32}R_{23} & R_{12}R_{33} + R_{32}R_{13} \\ R_{13}R_{21} + R_{23}R_{11} & R_{23}R_{31} + R_{33}R_{21} & R_{13}R_{31} + R_{33}R_{11} \end{bmatrix}. \quad (55)$$

Thus, we may obtain the corotated Cauchy stress and Jaumann tangent stiffness with the relations

$$\{\hat{\sigma}\} = [\mathbf{Q}] \cdot \{\sigma\}, \quad (56)$$

$$[\hat{\mathcal{C}}] = [\mathbf{Q}] \cdot [\mathcal{C}] \cdot [\mathbf{Q}]^T. \quad (57)$$

This formulation is implemented by means of the `trans_matrix_6()` subroutine. This is all what is needed to implement a behaviour law into ANSYS by means of the user subroutine `usermat3d()`.

References

- [1] Baek, S., Gleason, R., Rajagopal, K., Humphrey, J., 2007. Theory of small on large: Potential utility in computations of fluid–solid interactions in arteries. Computer Methods in Applied Mechanics and Engineering 196 (31-32), 3070–3078.
- [2] Holzapfel, G., Gasser, T., Ogden, R., 2000. A New Constitutive Framework for Arterial Wall Mechanics and a Comparative Study of Material Models. Journal of Elasticity 61 (1), 1–48.
- [3] Holzapfel, G. A., Sommer, G., Gasser, C. T., Regitnig, P., Nov 2005. Determination of layer-specific mechanical properties of human coronary arteries with nonatherosclerotic intimal thickening and related constitutive modeling. Am J Physiol Heart Circ Physiol 289 (5), H2048–H2058.
- [4] Simo, J., Hughes, T., 2000. Computational inelasticity. Springer.

A Ansys usermat3d() subroutine

```
*****
*** anisotropic hyperelastic models ***
author:      Nicolas Mesnier
creation:   06/02/2010
last modified: 07/03/2011
```

Models:

- 1 - Holzapfel 2000 hyperelastic anisotropic compressible law [1]
- 2 - model 1 with two additional fibre family [2]
- 3 - Holzapfel 2005 hyperelastic anisotropic compressible law [3]

References :

- [1] Holzapfel et al, J Elasticity 61 (2000)
- [2] Baek et al, Comp Meth Appl Mech Eng 196 (2007)
- [3] Holzapfel et al, AJP 289 (2005)

```
*****
*deck,usermat3d parallel user nmesnier
  subroutine usermat3d(matId, elemId,kDomIntPt, kLayer, kSectPt,
&                      ldstep,isubst,keycut,
&                      nDirect,nShear,ncomp,nStatev,nProp,
&                      Time,dTime,Temp,dTemp,
&                      stress,uStatev,dsdePl,sedEl,sedPl,epseq,
&                      Strain,dStrain, epsPl, prop, coords,
&                      var0, F0, F1,
&                      tsstif, epsZZ,
&                      var1, var2, var3, var4, var5,
&                      var6, var7, var8)
!-----  

  IMPLICIT NONE
  integer,parameter :: RK=KIND(1.D0)           ! real kind
! external procedures
  external polarRU                           ! polar decomposition subroutine
  external trans_matrix_6                     ! 6D voigt rotation matrix subroutine
  external elmgmt                            ! ANSYS fct, getting element nodes
  external ndgxyz                            ! ANSYS fct, get node position
  external dspget                             ! ANSYS fct, get node solution
! input arguments
  integer, intent(IN) :: matID               ! material ID number
  integer, intent(IN) :: elemID              ! element ID number
  integer, intent(IN) :: kDomIntPt          ! integration point
  integer, intent(IN) :: kLayer               ! layer number
  integer, intent(IN) :: kSectPt             ! section number
  integer, intent(IN) :: ldstep               ! load step number
  integer, intent(IN) :: isubst               ! substep number
  integer, intent(IN) :: ncomp                ! no. stress components
  integer, intent(IN) :: nDirect              ! no. direct stress components
  integer, intent(IN) :: nShear               ! no. shear stress components
  integer, intent(IN) :: nStatev              ! size of state variable array
  integer, intent(IN) :: nProp                 ! size of property array
  real(RK),intent(IN) :: Time                ! time at begining of increment
  real(RK),intent(IN) :: dTime               ! time increment
  real(RK),intent(IN) :: Temp                ! temperature at begining of increment
  real(RK),intent(IN) :: dTemp               ! temperature increment
  real(RK),intent(IN) :: Strain(ncomp)       ! strain at begining of inc
  real(RK),intent(IN) :: dStrain(ncomp)      ! strain increment
  real(RK),intent(IN) :: epsPl(ncomp)        ! woRK space
  real(RK),intent(IN) :: prop(nProp)         ! mat props, user input
  real(RK),intent(IN) :: coords(3)           ! coordinates of material point
  real(RK),intent(IN) :: F1(3,3)              ! deformation gradient at t+dt
  real(RK),intent(IN) :: F0(3,3)              ! deformation gradient at t
  real(RK),intent(IN) :: var0(*),var1,var2,var3,var4 !place holder
  real(RK),intent(IN) :: var5,var6,var7,var8 !place holder
! input output arguments
  real(RK),intent(INOUT) :: sedEl            ! stored (elastic) energy
  real(RK),intent(INOUT) :: sedPl            ! dissipated (plastic) energy
  real(RK),intent(INOUT) :: epseq             ! equivalent plastic strain
  real(RK),intent(INOUT) :: epsZZ            ! plane stress thickness strain
  real(RK),intent(INOUT) :: stress(ncomp)    ! stress
  real(RK),intent(INOUT) :: uStatev(nStatev) !state variables
! output arguments
  integer, intent(OUT) :: keycut             ! time step reduction
  real(RK),intent(OUT) :: dsdePl(ncomp,ncomp) !tangent stiffness
  real(RK),intent(OUT) :: tsstif(2)           ! transverse shear stiffness
```

```

!-----+
integer :: i,j,k,l
real(RK), parameter :: pi = 3.14159265358979324_RK
real(RK) :: mu,bm,K1(4),K2(4),beta,rho      ! material parameters
real(RK) :: model                           ! material model
!-----+
real(RK) :: detF,detF23                      ! Jacobian and factor
real(RK) :: Bbar(6)                           ! isochoric left cauchy green
!-----+
integer :: elmget,ndgxyz,dspget              ! ANSYS fct
integer :: tmp,Item(2),ElemData(10)
integer :: nodes(8)                          ! node vector, depends of elements
real(RK) :: Disp(2)                           ! node displacement
real(RK) :: ActnodePos(3)                   ! current position of a node
real(RK) :: nodesPos(4,2)                   ! 2D nodes positions
real(RK) :: uElemOrientVec(2)               ! unormed element orientation
real(RK) :: normElemOrient                 ! norm of uElemOrientVec
real(RK) :: ElemOrientVec(2)                ! element orientation
real(RK) :: fib(4,3),spafib(4,3)            ! orthoradial, longitudinal and crossed material and
spatial fibers
real(RK) :: A(4,6)                           ! spatial structural tensor
!-----+
real(RK) :: I1bar                           ! first invariant
real(RK) :: I4bar(4)                         ! fourth invariants
!-----+
real(RK) :: I1bar3                          ! I1/3
real(RK) :: dw1(4),dw2(4)                   ! first and second sedf derivatives w.r.t. I4bar(i)
real(RK) :: expf(4)                          ! fiber exponential factor
real(RK) :: dw2f(4)                          ! fiber factor for second derivatives
real(RK) :: C1,C2                            ! constants
!-----+
real(RK) :: sigma(6)                        ! cauchy stress
real(RK) :: M(6,6)                           ! material jacobian
real(RK) :: stressfull(6)                   ! full 3D stress
real(RK) :: dsddePlfull(6,6)                ! full 3D tangent stiffness
real(RK) :: R(3,3), Q(6,6)                  ! rotations
real(RK) :: U(3,3)                           ! stretch
!-----+
real(RK) :: EVR(3)                          ! E_R vector
real(RK) :: EVT(3)                           ! E_Theta vector
real(RK) :: normspaevt                      ! norm e_theta vector
real(RK) :: spaevt(2)                        ! spatial element orientation
*****+
! *** kinematics
!-----+
! Jacobian
detF = F1(1,1) * (F1(2,2)*F1(3,3) - F1(2,3)*F1(3,2))
& + F1(1,2) * (F1(2,3)*F1(3,1) - F1(2,1)*F1(3,3))
& + F1(1,3) * (F1(2,1)*F1(3,2) - F1(2,2)*F1(3,1))
! time step reduction condition
if(detF<=0._RK)then
  keycut=1
  return
else
  detF23 = detF**(-2._RK/3._RK)
endif
! isochoric left Cauchy Green
Bbar(1)=(F1(1,1)*F1(1,1)+F1(1,2)*F1(1,2)+F1(1,3)*F1(1,3))*detF23 ! Bbar(1,1)
Bbar(2)=(F1(2,1)*F1(2,1)+F1(2,2)*F1(2,2)+F1(2,3)*F1(2,3))*detF23 ! Bbar(2,2)
Bbar(3)=(F1(3,1)*F1(3,1)+F1(3,2)*F1(3,2)+F1(3,3)*F1(3,3))*detF23 ! Bbar(3,3)
Bbar(4)=(F1(2,1)*F1(1,1)+F1(2,2)*F1(1,2)+F1(2,3)*F1(1,3))*detF23 ! Bbar(2,1)
Bbar(5)=(F1(3,1)*F1(2,1)+F1(3,2)*F1(2,2)+F1(3,3)*F1(2,3))*detF23 ! Bbar(3,2)
Bbar(6)=(F1(3,1)*F1(1,1)+F1(3,2)*F1(1,2)+F1(3,3)*F1(1,3))*detF23 ! Bbar(3,1)
!-----+
! *** get elements orientation
if (Time.lt.1._RK) then
!-----+
  tmp = elmget(elemId,ElemData,nodes)          ! get element nodes
  Item(:) = (/1,2/)
! get node position
do i=1,4
  tmp = ndgxyz(nodes(i),ActnodePos)
  tmp = dspget(nodes(i),2,Item,Disp)

```

```

    nodesPos(i,1:2)=ActnodePos(1:2)-Disp(1:2)
    ActnodePos(1:3) = 0._RK
  end do
! element orientation unormed vector
  uElemOrientVec(:) = (nodesPos(3,1:2)-nodesPos(2,1:2))
  &                  + (nodesPos(4,1:2)-nodesPos(1,1:2))
! element orientation normed version
  normElemOrient = sqrt(uElemOrientVec(1)*uElemOrientVec(1)
  &                  + uElemOrientVec(2)*uElemOrientVec(2))
  ElemOrientVec(1:2) = uElemOrientVec(1:2)/normElemOrient
!
!----- ustatev(1) = ElemOrientVec(1)
!----- ustatev(2) = ElemOrientVec(2)
!
!----- else
!
!----- ElemOrientVec(1) = ustatev(1)
!----- ElemOrientVec(2) = ustatev(2)
!
!----- end if
EVR(1:3) = (/ElemOrientVec(2),-ElemOrientVec(1),0._RK/)
EVT(1:3) = (/ElemOrientVec(1),ElemOrientVec(2),0._RK/)

!*** model choice
!
model = prop(1)
if(model.eq.1._RK)then
***** << model 1
! model 1:      anisotropic hyperelastic two fibre families model
! author:        Nicolas Mesnier
! creation date: 06/02/2010
! last modified: 19/07/2010
!
! The behaviour is described by the holzapfel hyperelastic anisotropic
! compressible law [1]
  W = Wiso + Wvol + Waniso
where each contribution is defined as:
  Wiso = mu /2 * (I1 - 3 )
  Wvol = K / 2 * (J - 1 ) ^2
  Waniso = k1 / (2*k2)* { exp[ k2 * (I4 - 1)^2 ] - 1 }
with the two fiber family:
  fib1 = cos(beta) Et + sin(beta) Ez
  fib2 = cos(beta) Et - sin(beta) Ez
Input material properties:
  mu   : shear modulus
  k    : bulk modulus
  k1   : stress-like
  k2   : dimensionless
  beta : angle in degrees, 0° < beta < 90°
References :
  [1] G.Holzapfel et al, J Elasticity 61 (2000)
*****
!
! *** input material parameters
!
mu    = prop(2)          ! shear modulus
bm    = prop(3)          ! bulk modulus
K1(1) = prop(4)          ! aniso parameter (stress-like)
K2(1) = prop(5)          ! aniso parameter (dimensionless)
K1(2) = prop(4)
K2(2) = prop(5)
beta  = prop(6)*pi/180._RK ! fiber angle (radians)
!
! *** material anisotropy
!
! init fibers
  fib(:,:)= 0._RK
! crossed fibers
  fib(1,1:3) = (/ElemOrientVec(1)*cos(beta),
  &           ElemOrientVec(2)*cos(beta),sin(beta)/)
  fib(2,1:3) = (/ElemOrientVec(1)*cos(beta),
  &           ElemOrientVec(2)*cos(beta),-sin(beta)/)
  fib(3,1:3) = (/ElemOrientVec(1)*cos(beta),
  &           ElemOrientVec(2)*cos(beta),sin(beta)/)

```

```

    fib(4,1:3) = (/ElemOrientVec(1)*cos(beta),
&                      ElemOrientVec(2)*cos(beta),-sin(beta)/)
!-----+
! init fibers
!   fib(:,:) = 0._RK
! orthoradial fiber
!   fib(3,1:2) = (/ElemOrientVec(1),ElemOrientVec(2)/)
! crossed fibers
!   fib(1,1:3) = (/fib(3,1)*cos(beta),fib(3,2)*cos(beta),sin(beta)/)
!   fib(2,1:3) = (/fib(3,1)*cos(beta),fib(3,2)*cos(beta),-sin(beta)/)
! spatial fibers
!   do k=1,4
!     spafib(k,:)= (/
! &           F1(1,1)*fib(k,1)+F1(1,2)*fib(k,2)+F1(1,3)*fib(k,3),
! &           F1(2,1)*fib(k,1)+F1(2,2)*fib(k,2)+F1(2,3)*fib(k,3),
! &           F1(3,1)*fib(k,1)+F1(3,2)*fib(k,2)+F1(3,3)*fib(k,3)/)
!   end do
! spatial anisotropic tensors
!   do k=1,4
!     A(k,:)= (/ detF23*spafib(k,1)*spafib(k,1),
! &           detF23*spafib(k,2)*spafib(k,2),
! &           detF23*spafib(k,3)*spafib(k,3),
! &           detF23*spafib(k,2)*spafib(k,1),
! &           detF23*spafib(k,3)*spafib(k,2),
! &           detF23*spafib(k,3)*spafib(k,1)/)
!   end do
!-----+
! *** invariants
!-----+
! 1st invariant
!   I1bar = (Bbar(1) + Bbar(2) + Bbar(3))
!   I1bar3 = I1bar/3._RK      ! I1bar / 3
! 4th invariants
!   I4bar(:)= (/A(1,1)+A(1,2)+A(1,3),
! &             A(2,1)+A(2,2)+A(2,3),
! &             A(3,1)+A(3,2)+A(3,3),
! &             A(4,1)+A(4,2)+A(4,3)/)
!-----+
! *** anisotropic sedf derivatives
!-----+
!   do k=1,2
! fiber exponential factor
!   expf(k) = exp(K2(k)*(I4bar(k)-1._RK)**2)
! fiber factor for second derivatives
!   dw2f(k) = 1._RK + 2._RK* K2(k)*(I4bar(k)-1._RK)**2
! sedf derivative w.r.t. I4bar(i)
!   dw1(k) = K1(k)*(I4bar(k)-1._RK)*expf(k)
! sedf derivative w.r.t. I4bar(i), I4bar(i)
!   dw2(k) = K1(k)*dw2f(k)*expf(k)
!   end do
!-----+
! *** update sedf
!-----+
!   sedEl = mu*(I1bar-3._RK) + bm*(detF-1._RK)**2
!   do k=1,2
!     sedEl = sedEl + K1(k)/K2(k)*(expf(k)-1._RK)
!   end do
!   sedEl = sedEl/2._RK /detF
!   sedPl = 0._RK
!-----+
! *** cauchy stress in spatial frame
!-----+
! isotropic contributions
!   sigma(1:3) = mu *(Bbar(1:3)-I1bar3)/ detF + bm*(detF-1._RK)
!   sigma(4:6) = mu*(Bbar(4:6)) / detF
! add anisotropic parts
!   do k=1,2
!     sigma(1:3) = sigma(1:3)
!     & + 2._RK*dw1(k)/detF*(A(k,1:3)-I4bar(k)/3._RK)
!     sigma(4:6) = sigma(4:6) + 2._RK*dw1(k)/detF*A(k,4:6)
!   end do
!-----+
! *** Jaumann tangent stiffness in spatial frame

```

```

! factors
C1 = 2._RK/3._RK*mu/detF
C2 = 3._RK/4._RK*C1
! isotropic deviatoric components
!-----
M(1,1) = C1 * (Bbar(1) + I1bar3)
M(2,2) = C1 * (Bbar(2) + I1bar3)
M(3,3) = C1 * (Bbar(3) + I1bar3)
!-----
M(2,1) =-C1 * (Bbar(1) + Bbar(2) - I1bar3)
M(3,1) =-C1 * (Bbar(1) + Bbar(3) - I1bar3)
M(3,2) =-C1 * (Bbar(2) + Bbar(3) - I1bar3)
!-----
M(4,1) = C1 * Bbar(4) / 2._RK
M(6,1) = C1 * Bbar(6) / 2._RK
M(4,2) = C1 * Bbar(4) / 2._RK
M(5,2) = C1 * Bbar(5) / 2._RK
M(5,3) = C1 * Bbar(5) / 2._RK
M(6,3) = C1 * Bbar(6) / 2._RK
!-----
M(5,1) =-C1 * Bbar(5)
M(6,2) =-C1 * Bbar(6)
M(4,3) =-C1 * Bbar(4)
!-----
M(4,4) = C2 * (Bbar(1) + Bbar(2))
M(5,5) = C2 * (Bbar(2) + Bbar(3))
M(6,6) = C2 * (Bbar(1) + Bbar(3))
!-----
M(5,4) = C2 * Bbar(6)
M(6,4) = C2 * Bbar(5)
M(6,5) = C2 * Bbar(4)
! anisotropic deviatoric components
!-----
do k=1,2
!-----
M(1,1)=M(1,1)+4._RK/detF*(dw2(k)*(A(k,1)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,1)+I4bar(k)/3._RK))
M(2,2)=M(2,2)+4._RK/detF*(dw2(k)*(A(k,2)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,2)+I4bar(k)/3._RK))
M(3,3)=M(3,3)+4._RK/detF*(dw2(k)*(A(k,3)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,3)+I4bar(k)/3._RK))
!-----
M(2,1)=M(2,1)+4._RK/detF*
& dw2(k)*(A(k,2)-I4bar(k)/3._RK)*(A(k,1)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,2)-A(k,1)))
M(3,1)=M(3,1)+4._RK/detF*
& dw2(k)*(A(k,3)-I4bar(k)/3._RK)*(A(k,1)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,3)-A(k,1)))
M(3,2)=M(3,2)+4._RK/detF*
& dw2(k)*(A(k,3)-I4bar(k)/3._RK)*(A(k,2)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,3)-A(k,2)))
!-----
M(4,1)=M(4,1)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,4)
& + dw1(k)/3._RK*A(k,4))
M(6,1)=M(6,1)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,6)
& + dw1(k)/3._RK*A(k,6))
M(4,2)=M(4,2)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,4)
& + dw1(k)/3._RK*A(k,4))
M(5,2)=M(5,2)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,5)
& + dw1(k)/3._RK*A(k,5))
M(5,3)=M(5,3)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,5)
& + dw1(k)/3._RK*A(k,5))
M(6,3)=M(6,3)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,6)
& + dw1(k)/3._RK*A(k,6))
!-----
M(5,1)=M(5,1)+4._RK/detF*(dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,5)
& - dw1(k)/3._RK*A(k,5))
M(6,2)=M(6,2)+4._RK/detF*(dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,6)

```

```

& - dw1(k)/3._RK*A(k,6))
M(4,3)=M(4,3)+4._RK/detF*(dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,4)
& - dw1(k)/3._RK*A(k,4))

!-----
& M(4,4)=M(4,4)+1._RK/detF*(4._RK*dw2(k)*(A(k,4))**2
& + dw1(k)*(A(k,1)+A(k,2)))
M(5,5)=M(5,5)+1._RK/detF*(4._RK*dw2(k)*(A(k,5))**2
& + dw1(k)*(A(k,2)+A(k,3)))
M(6,6)=M(6,6)+1._RK/detF*(4._RK*dw2(k)*(A(k,6))**2
& + dw1(k)*(A(k,1)+A(k,3)))

!-----
M(5,4)=M(5,4)+1._RK/detF*(4._RK*dw2(k)*A(k,4)*A(k,5)
& + dw1(k)*A(k,6))
M(6,4)=M(6,4)+1._RK/detF*(4._RK*dw2(k)*A(k,4)*A(k,6)
& + dw1(k)*A(k,5))
M(6,5)=M(6,5)+1._RK/detF*(4._RK*dw2(k)*A(k,5)*A(k,6)
& + dw1(k)*A(k,4))

end do
*****  

end if
if(model.eq.2._RK)then
***** << model 2
model 2:      anisotropic hyperelastic four fibre families model
author:        Nicolas Mesnier
creation date: 06/02/2010
last modified: 19/07/2010

-----  

The behaviour is described by the holzapfel hyperelastic anisotropic
compressible law [1] with two additional fibre family [2]
W = Wiso + Wvol + Waniso
where each contribution is defined as:
Wiso = mu /2 * ( I1 - 3 )
Wvol = KK /2 * ( J - 1 ) ^2
Waniso(i) = kli / (2*k2i) * { exp[ k2i * (I4i - 1)^2 ] - 1 }
with the four fiber family:
fib1 = Et
fib2 = Ez
fib3 = cos(beta) Et + sin(beta) Ez
fib4 = cos(beta) Et - sin(beta) Ez
Input material properties:
mu    : shear modulus
k     : bulk modulus
kli   : stress-like, k13 = k14
k2i   : dimensionless, k23 = k24
beta  : angle in degrees, 0° < beta < 90°
References :
[1] G.Holzapfel et al, J Elasticity 61 (2000)
[2] Baek et al, Comp Meth Appl Mech Eng 196 (2007)
*****  

-----  

*** input material parameters
-----  

mu    = prop(2)          ! shear modulus
bm    = prop(3)          ! bulk modulus
K1(1) = prop(4)          ! aniso parameter (stress-like)
K2(1) = prop(5)          ! aniso parameter (dimensionless)
K1(2) = prop(6)
K2(2) = prop(7)
K1(3) = prop(8)
K2(3) = prop(9)
K1(4) = prop(8)
K2(4) = prop(9)
beta  = prop(10)*pi/180._RK ! fiber angle (radians)
-----  

*** material anisotropy
-----  

init fibers
fib(:,:) = 0._RK
orthoradial fiber
fib(1,1:2) = (/ElemOrientVec(1),ElemOrientVec(2)/)
longitudinal fiber
fib(2,3) = 1._RK
crossed fibers
fib(3,1:3) = (/fib(1,1)*cos(beta),fib(1,2)*cos(beta),sin(beta)/)

```

```

    fib(4,1:3) = (/fib(1,1)*cos(beta),fib(1,2)*cos(beta),-sin(beta)/)
! spatial fibers
  do k=1,4
    spafib(k,:)= (/
      & F1(1,1)*fib(k,1)+F1(1,2)*fib(k,2)+F1(1,3)*fib(k,3),
      & F1(2,1)*fib(k,1)+F1(2,2)*fib(k,2)+F1(2,3)*fib(k,3),
      & F1(3,1)*fib(k,1)+F1(3,2)*fib(k,2)+F1(3,3)*fib(k,3)/)
  end do
! spatial anisotropic tensors
  do k=1,4
    A(k,:)= (/ detF23*spafib(k,1)*spafib(k,1),
    & detF23*spafib(k,2)*spafib(k,2),
    & detF23*spafib(k,3)*spafib(k,3),
    & detF23*spafib(k,2)*spafib(k,1),
    & detF23*spafib(k,3)*spafib(k,2),
    & detF23*spafib(k,3)*spafib(k,1)/)
  end do
! -----
! *** invariants
! -----
! 1st invariant
  I1bar = (Bbar(1) + Bbar(2) + Bbar(3))
  I1bar3 = I1bar/3._RK      ! I1bar / 3
! 4th invariants
  I4bar(:)= (/A(1,1)+A(1,2)+A(1,3),
  &          A(2,1)+A(2,2)+A(2,3),
  &          A(3,1)+A(3,2)+A(3,3),
  &          A(4,1)+A(4,2)+A(4,3)/)
! -----
! *** anisotropic sedf derivatives
! -----
  do k=1,4
! fiber exponential factor
  expf(k) = exp(K2(k)*(I4bar(k)-1._RK)**2)
! fiber factor for second derivatives
  dw2f(k) = 1._RK + 2._RK* K2(k)*(I4bar(k)-1._RK)**2
! sedf derivative w.r.t. I4bar(i)
  dw1(k) = K1(k)*(I4bar(k)-1._RK)*expf(k)
! sedf derivative w.r.t. I4bar(i), I4bar(i)
  dw2(k) = K1(k)*dw2f(k)*expf(k)
  end do
! -----
! *** update sedf
! -----
  sedEl = mu*(I1bar-3._RK) + bm*(detF-1._RK)**2
  do k=1,4
    sedEl = sedEl + K1(k)/K2(k)*(expf(k)-1._RK)
  end do
  sedEl = sedEl/2._RK /detF
  sedPl = 0._RK
! -----
! *** cauchy stress in spatial frame
! -----
! isotropic contributions
  sigma(1:3) = mu *(Bbar(1:3)-I1bar3)/ detF + bm*(detF-1._RK)
  sigma(4:6) = mu*(Bbar(4:6)) / detF
! add anisotropic parts
  do k=1,4
    sigma(1:3) = sigma(1:3)
    & + 2._RK*dw1(k)/detF*(A(k,1:3)-I4bar(k)/3._RK)
    sigma(4:6) = sigma(4:6) + 2._RK*dw1(k)/detF*A(k,4:6)
  end do
! -----
! *** Jaumann tangent stiffness in spatial frame
! -----
! factors
  C1 = 2._RK/3._RK*mu/detF
  C2 = 3._RK/4._RK*C1
! isotropic deviatoric components
! -----
  M(1,1) = C1 * (Bbar(1) + I1bar3)
  M(2,2) = C1 * (Bbar(2) + I1bar3)
  M(3,3) = C1 * (Bbar(3) + I1bar3)
! -----

```

```

M(2,1) =-C1 * (Bbar(1) + Bbar(2) - I1bar3)
M(3,1) =-C1 * (Bbar(1) + Bbar(3) - I1bar3)
M(3,2) =-C1 * (Bbar(2) + Bbar(3) - I1bar3)
!-----
M(4,1) = C1 * Bbar(4) / 2._RK
M(6,1) = C1 * Bbar(6) / 2._RK
M(4,2) = C1 * Bbar(4) / 2._RK
M(5,2) = C1 * Bbar(5) / 2._RK
M(5,3) = C1 * Bbar(5) / 2._RK
M(6,3) = C1 * Bbar(6) / 2._RK
!-----
M(5,1) =-C1 * Bbar(5)
M(6,2) =-C1 * Bbar(6)
M(4,3) =-C1 * Bbar(4)
!-----
M(4,4) = C2 * (Bbar(1) + Bbar(2))
M(5,5) = C2 * (Bbar(2) + Bbar(3))
M(6,6) = C2 * (Bbar(1) + Bbar(3))
!-----
M(5,4) = C2 * Bbar(6)
M(6,4) = C2 * Bbar(5)
M(6,5) = C2 * Bbar(4)
! anisotropic deviatoric components
!-----
do k=1,4
!-----
M(1,1)=M(1,1)+4._RK/detF*(dw2(k)*(A(k,1)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,1)+I4bar(k)/3._RK))
M(2,2)=M(2,2)+4._RK/detF*(dw2(k)*(A(k,2)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,2)+I4bar(k)/3._RK))
M(3,3)=M(3,3)+4._RK/detF*(dw2(k)*(A(k,3)-I4bar(k)/3._RK)**2
& + dw1(k)/3._RK*(A(k,3)+I4bar(k)/3._RK))
!-----
M(2,1)=M(2,1)+4._RK/detF*
& dw2(k)*(A(k,2)-I4bar(k)/3._RK)*(A(k,1)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,2)-A(k,1)))
M(3,1)=M(3,1)+4._RK/detF*
& dw2(k)*(A(k,3)-I4bar(k)/3._RK)*(A(k,1)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,3)-A(k,1)))
M(3,2)=M(3,2)+4._RK/detF*
& dw2(k)*(A(k,3)-I4bar(k)/3._RK)*(A(k,2)-I4bar(k)/3._RK)
& + dw1(k)/3._RK*(I4bar(k)/3._RK-A(k,3)-A(k,2)))
!-----
M(4,1)=M(4,1)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,4)
& + dw1(k)/3._RK*A(k,4))
M(6,1)=M(6,1)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,6)
& + dw1(k)/3._RK*A(k,6))
M(4,2)=M(4,2)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,4)
& + dw1(k)/3._RK*A(k,4))
M(5,2)=M(5,2)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,5)
& + dw1(k)/3._RK*A(k,5))
M(5,3)=M(5,3)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,5)
& + dw1(k)/3._RK*A(k,5))
M(6,3)=M(6,3)+2._RK/detF*
& 2._RK*dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,6)
& + dw1(k)/3._RK*A(k,6))
!-----
M(5,1)=M(5,1)+4._RK/detF*(dw2(k)*(A(k,1)-I4bar(k)/3._RK)*A(k,5)
& - dw1(k)/3._RK*A(k,5))
M(6,2)=M(6,2)+4._RK/detF*(dw2(k)*(A(k,2)-I4bar(k)/3._RK)*A(k,6)
& - dw1(k)/3._RK*A(k,6))
M(4,3)=M(4,3)+4._RK/detF*(dw2(k)*(A(k,3)-I4bar(k)/3._RK)*A(k,4)
& - dw1(k)/3._RK*A(k,4))
!-----
M(4,4)=M(4,4)+1._RK/detF*(4._RK*dw2(k)*(A(k,4))**2
& + dw1(k)*(A(k,1)+A(k,2)))
M(5,5)=M(5,5)+1._RK/detF*(4._RK*dw2(k)*(A(k,5))**2
& + dw1(k)*(A(k,2)+A(k,3)))
M(6,6)=M(6,6)+1._RK/detF*(4._RK*dw2(k)*(A(k,6))**2

```

```

& + dw1(k)*(A(k,1)+A(k,3)))
!-----  

& M(5,4)=M(5,4)+1._RK/detF*(4._RK*dw2(k)*A(k,4)*A(k,5)  

& + dw1(k)*A(k,6))  

M(6,4)=M(6,4)+1._RK/detF*(4._RK*dw2(k)*A(k,4)*A(k,6)  

& + dw1(k)*A(k,5))  

M(6,5)=M(6,5)+1._RK/detF*(4._RK*dw2(k)*A(k,5)*A(k,6)  

& + dw1(k)*A(k,4))
end do  

!*****  

end if  

if(model.eq.3._RK)then  

!***** << model 3  

! model 3:      anisotropic hyperelastic two fibre families model  

! author:        Nicolas Mesnier  

! creation date: 03/05/2010  

! last modified: 20/07/2010  

!-----  

The behaviour is described by the holzapfel hyperelastic anisotropic  

compressible law [3] with two additional fibre family [2]  

W = Wiso + Wvol + Waniso  

where each contribution is defined as:  

Wiso = mu /2 * ( I1 - 3 )  

Wvol = KK /2 * ( J - 1 ) ^2  

Waniso = k1/k2*{ exp[ k2 *{(1-rho)*(I1-3)^2+rho*(I4-1)^2}] -1}  

with the two fiber family:  

fib1 = cos(beta) Et + sin(beta) Ez  

fib2 = cos(beta) Et - sin(beta) Ez  

Input material properties:  

mu   : shear modulus  

k    : bulk modulus  

k1   : stress-like  

k2   : dimensionless  

rho  : dimensionless, 0 < rho < 1  

beta : angle in degrees, 0° < beta < 90°  

References :  

[3] Holzapfel et al, AJP 289 (2005)
*****  

! *** input material parameters  

!-----  

mu    = prop(2)          ! shear modulus  

bm    = prop(3)          ! bulk modulus  

K1(1) = prop(4)          ! aniso parameter (stress-like)  

K2(1) = prop(5)          ! aniso parameter (dimensionless)  

rho   = prop(6)          ! aniso proportion (dimensionless)  

beta  = prop(7)*pi/180._RK ! fiber angle (radians)  

!-----  

! *** material anisotropy  

!-----  

! init fibers  

fib(:,:)= 0._RK  

! crossed fiber  

fib(1,1:3) = (/ElemOrientVec(1)*cos(beta),  

&           ElemOrientVec(2)*cos(beta),  

&           sin(beta)/)
fib(2,1:3) = (/ElemOrientVec(1)*cos(beta),  

&           ElemOrientVec(2)*cos(beta),  

&           -sin(beta)/)
! spatial fibers
do k=1,2
  spafib(k,:)= (/  

&     F1(1,1)*fib(k,1)+F1(1,2)*fib(k,2)+F1(1,3)*fib(k,3),  

&     F1(2,1)*fib(k,1)+F1(2,2)*fib(k,2)+F1(2,3)*fib(k,3),  

&     F1(3,1)*fib(k,1)+F1(3,2)*fib(k,2)+F1(3,3)*fib(k,3)/)
end do
! spatial anisotropic tensors
do k=1,2
  A(k,:)= (/ detF23*spafib(k,1)*spafib(k,1),
&           detF23*spafib(k,2)*spafib(k,2),
&           detF23*spafib(k,3)*spafib(k,3),
&           detF23*spafib(k,2)*spafib(k,1),
&           detF23*spafib(k,3)*spafib(k,2),
&           detF23*spafib(k,3)*spafib(k,1)/)

```

```

end do
A(3,1:6) = (A(1,1:6)+A(2,1:6))/2._RK
A(1,1:6) = A(3,1:6)

! *** invariants
!
! 1st invariant
I1bar = (Bbar(1) + Bbar(2) + Bbar(3))
I1bar3 = I1bar/3._RK      ! I1bar / 3
!
! 4th invariants
I4bar(1) = A(1,1)+A(1,2)+A(1,3)

! *** anisotropic sedf derivatives
!
! fiber exponential factor
expf(1) = 4._RK*K1(1)*
&           exp(K2(1)*((1._RK-rho)*(I1bar-3._RK)**2
&           +rho*(I4bar(1)-1._RK)**2))
!
! fiber factor for second derivatives
dw2f(1) = 1._RK+2._RK* K2(1)*(1._RK-rho)*(I1bar-3._RK)**2
dw2f(2) = 1._RK+2._RK* K2(1)*rho*(I4bar(1)-1._RK)**2
!
! sedf derivative w.r.t. I1bar and I4bar
dw1(1) = (1._RK-rho)*(I1bar-3._RK)*expf(1)/detF
dw1(2) = rho*(I4bar(1)-1._RK)*expf(1)/detF
!
! sedf derivative w.r.t. I1barI1bar, I4barI4bar, I1barI4bar
dw2(1) = 2._RK*(1._RK-rho)*dw2f(1)*expf(1)/detF
dw2(2) = 2._RK*rho*dw2f(2)*expf(1)/detF
dw2(3) = 4._RK*rho*(1._RK-rho)*K2(1)
&           *(I1bar-3._RK)*(I4bar(1)-1._RK)*expf(1)/detF

! *** update sedf
!
sedEl = mu*(I1bar-3._RK) + bm*(detF-1._RK)**2
&           + 2._RK*K1(1)/K2(1)*
&           (exp(K2(1)*((1._RK-rho)*(I1bar-3._RK)**2
&           +rho*(I4bar(1)-1._RK)**2))-1._RK)
sedEl = sedEl/2._RK /detF
sedPl = 0._RK

! *** cauchy stress in spatial frame
!
sigma(1:3) = (mu/detF+dw1(1)) *(Bbar(1:3)-I1bar3)
&           + dw1(2)*(A(1,1:3)-I4bar(1)/3._RK)
&           + bm*(detF-1._RK)
sigma(4:6) = (mu/detF+dw1(1)) *(Bbar(4:6))
&           + dw1(2)*(A(1,4:6))

! *** Jaumann tangent stiffness in spatial frame
!
! factors
C1 = 2._RK/3._RK*mu/detF
C2 = 3._RK/4._RK*C1
!
! isotropic deviatoric components
!
M(1,1) = C1 * (Bbar(1) + I1bar3)
M(2,2) = C1 * (Bbar(2) + I1bar3)
M(3,3) = C1 * (Bbar(3) + I1bar3)

!
M(2,1) = -C1 * (Bbar(1) + Bbar(2) - I1bar3)
M(3,1) = -C1 * (Bbar(1) + Bbar(3) - I1bar3)
M(3,2) = -C1 * (Bbar(2) + Bbar(3) - I1bar3)

!
M(4,1) = C1 * Bbar(4) / 2._RK
M(6,1) = C1 * Bbar(6) / 2._RK
M(4,2) = C1 * Bbar(4) / 2._RK
M(5,2) = C1 * Bbar(5) / 2._RK
M(5,3) = C1 * Bbar(5) / 2._RK
M(6,3) = C1 * Bbar(6) / 2._RK

!
M(5,1) = -C1 * Bbar(5)
M(6,2) = -C1 * Bbar(6)
M(4,3) = -C1 * Bbar(4)

!
M(4,4) = C2 * (Bbar(1) + Bbar(2))

```

```

M(5,5) = C2 * (Bbar(2) + Bbar(3))
M(6,6) = C2 * (Bbar(1) + Bbar(3))

!-----
M(5,4) = C2 * Bbar(6)
M(6,4) = C2 * Bbar(5)
M(6,5) = C2 * Bbar(4)

! anisotropic deviatoric components
!-----

M(1,1)=M(1,1) + dw2(1)*(Bbar(1)-I1bar3)**2
& + dw2(2)*(A(1,1)-I4bar(1)/3._RK)**2
& +2._RK*dw2(3)*(Bbar(1)-I1bar3)*(A(1,1)-I4bar(1)/3._RK)
& +4._RK/3._RK*(dw1(1)*(2._RK*I1bar3-Bbar(1))
& +dw1(2)*(2._RK*I4bar(1)/3._RK-A(1,1)))
M(2,2)=M(2,2) + dw2(1)*(Bbar(2)-I1bar3)**2
& + dw2(2)*(A(1,2)-I4bar(1)/3._RK)**2
& +2._RK*dw2(3)*(Bbar(2)-I1bar3)*(A(1,2)-I4bar(1)/3._RK)
& +4._RK/3._RK*(dw1(1)*(2._RK*I1bar3-Bbar(2))
& +dw1(2)*(2._RK*I4bar(1)/3._RK-A(1,2)))
M(3,3)=M(3,3) + dw2(1)*(Bbar(3)-I1bar3)**2
& + dw2(2)*(A(1,3)-I4bar(1)/3._RK)**2
& +2._RK*dw2(3)*(Bbar(3)-I1bar3)*(A(1,3)-I4bar(1)/3._RK)
& +4._RK/3._RK*(dw1(1)*(2._RK*I1bar3-Bbar(3))
& +dw1(2)*(2._RK*I4bar(1)/3._RK-A(1,3)))

!-----
M(2,1)=M(2,1) + dw2(1)*(Bbar(1)-I1bar3)*(Bbar(2)-I1bar3)
& + dw2(2)*(A(1,1)-I4bar(1)/3._RK)*(A(1,2)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(1)-I1bar3)*(A(1,2)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(2)-I1bar3)*(A(1,1)-I4bar(1)/3._RK)
& +2._RK/3._RK*dw1(1)*(I1bar3-Bbar(1)-Bbar(2))
& +2._RK/3._RK*dw1(2)*(I4bar(1)/3._RK-A(1,1)-A(1,2))
M(3,1)=M(3,1) + dw2(1)*(Bbar(1)-I1bar3)*(Bbar(3)-I1bar3)
& + dw2(2)*(A(1,1)-I4bar(1)/3._RK)*(A(1,3)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(1)-I1bar3)*(A(1,3)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(3)-I1bar3)*(A(1,1)-I4bar(1)/3._RK)
& +2._RK/3._RK*dw1(1)*(I1bar3-Bbar(1)-Bbar(3))
& +2._RK/3._RK*dw1(2)*(I4bar(1)/3._RK-A(1,1)-A(1,3))
M(3,2)=M(3,2) + dw2(1)*(Bbar(2)-I1bar3)*(Bbar(3)-I1bar3)
& + dw2(2)*(A(1,2)-I4bar(1)/3._RK)*(A(1,3)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(2)-I1bar3)*(A(1,3)-I4bar(1)/3._RK)
& + dw2(3)*(Bbar(3)-I1bar3)*(A(1,2)-I4bar(1)/3._RK)
& +2._RK/3._RK*dw1(1)*(I1bar3-Bbar(2)-Bbar(3))
& +2._RK/3._RK*dw1(2)*(I4bar(1)/3._RK-A(1,2)-A(1,3))

!-----
M(4,1)=M(4,1) + dw2(1)*(Bbar(1)-I1bar3)*Bbar(4)
& + dw2(2)*(A(1,1)-I4bar(1)/3._RK)*A(1,4)
& + dw2(3)*(Bbar(1)-I1bar3)*A(1,4)
& + dw2(3)*(A(1,1)-I4bar(1)/3._RK)*Bbar(4)
& -2._RK/3._RK*(dw1(1)*Bbar(4)+dw1(2)*A(1,4))
M(6,1)=M(6,1) + dw2(1)*(Bbar(1)-I1bar3)*Bbar(6)
& + dw2(2)*(A(1,1)-I4bar(1)/3._RK)*A(1,6)
& + dw2(3)*(Bbar(1)-I1bar3)*A(1,6)
& + dw2(3)*(A(1,1)-I4bar(1)/3._RK)*Bbar(6)
& -2._RK/3._RK*(dw1(1)*Bbar(6)+dw1(2)*A(1,6))
M(4,2)=M(4,2) + dw2(1)*(Bbar(2)-I1bar3)*Bbar(4)
& + dw2(2)*(A(1,2)-I4bar(1)/3._RK)*A(1,4)
& + dw2(3)*(Bbar(2)-I1bar3)*A(1,4)
& + dw2(3)*(A(1,2)-I4bar(1)/3._RK)*Bbar(4)
& -2._RK/3._RK*(dw1(1)*Bbar(4)+dw1(2)*A(1,4))
M(5,2)=M(5,2) + dw2(1)*(Bbar(2)-I1bar3)*Bbar(5)
& + dw2(2)*(A(1,2)-I4bar(1)/3._RK)*A(1,5)
& + dw2(3)*(Bbar(2)-I1bar3)*A(1,5)
& + dw2(3)*(A(1,2)-I4bar(1)/3._RK)*Bbar(5)
& -2._RK/3._RK*(dw1(1)*Bbar(5)+dw1(2)*A(1,5))
M(5,3)=M(5,3) + dw2(1)*(Bbar(3)-I1bar3)*Bbar(5)
& + dw2(2)*(A(1,3)-I4bar(1)/3._RK)*A(1,5)
& + dw2(3)*(Bbar(3)-I1bar3)*A(1,5)
& + dw2(3)*(A(1,3)-I4bar(1)/3._RK)*Bbar(5)
& -2._RK/3._RK*(dw1(1)*Bbar(5)+dw1(2)*A(1,5))
M(6,3)=M(6,3) + dw2(1)*(Bbar(3)-I1bar3)*Bbar(6)
& + dw2(2)*(A(1,3)-I4bar(1)/3._RK)*A(1,6)
& + dw2(3)*(Bbar(3)-I1bar3)*A(1,6)
& + dw2(3)*(A(1,3)-I4bar(1)/3._RK)*Bbar(6)
& -2._RK/3._RK*(dw1(1)*Bbar(6)+dw1(2)*A(1,6))

```

```

M(5,1)=M(5,1) + dw2(1)*(Bbar(1)-I1bar3)*Bbar(5)
&      + dw2(2)*(A(1,1)-I4bar(1)/3._RK)*A(1,5)
&      + dw2(3)*(Bbar(1)-I1bar3)*A(1,5)
&      + dw2(3)*(A(1,1)-I4bar(1)/3._RK)*Bbar(5)
&      -2._RK/3._RK*(dw1(1)*Bbar(5)+dw1(2)*A(1,5))
M(6,2)=M(6,2) + dw2(1)*(Bbar(2)-I1bar3)*Bbar(6)
&      + dw2(2)*(A(1,2)-I4bar(1)/3._RK)*A(1,6)
&      + dw2(3)*(Bbar(2)-I1bar3)*A(1,6)
&      + dw2(3)*(A(1,2)-I4bar(1)/3._RK)*Bbar(6)
&      -2._RK/3._RK*(dw1(1)*Bbar(6)+dw1(2)*A(1,6))
M(4,3)=M(4,3) + dw2(1)*(Bbar(3)-I1bar3)*Bbar(4)
&      + dw2(2)*(A(1,3)-I4bar(1)/3._RK)*A(1,4)
&      + dw2(3)*(Bbar(3)-I1bar3)*A(1,4)
&      + dw2(3)*(A(1,3)-I4bar(1)/3._RK)*Bbar(4)
&      -2._RK/3._RK*(dw1(1)*Bbar(4)+dw1(2)*A(1,4))

```

```

!-----
M(4,4)=M(4,4) + dw2(1)*(Bbar(4))**2
&      + dw2(2)*(A(1,4))**2
&      + 2._RK*dw2(3)*Bbar(4)*A(1,4)
&      +1._RK/3._RK*(dw1(1)*I1bar+dw1(2)*I4bar(1))
M(5,5)=M(5,5) + dw2(1)*(Bbar(5))**2
&      + dw2(2)*(A(1,5))**2
&      + 2._RK*dw2(3)*Bbar(5)*A(1,5)
&      +1._RK/3._RK*(dw1(1)*I1bar+dw1(2)*I4bar(1))
M(6,6)=M(6,6) + dw2(1)*(Bbar(6))**2
&      + dw2(2)*(A(1,6))**2
&      + 2._RK*dw2(3)*Bbar(6)*A(1,6)
&      +1._RK/3._RK*(dw1(1)*I1bar+dw1(2)*I4bar(1))

```

```

!-----
M(5,4)=M(5,4) + dw2(1)*Bbar(4)*Bbar(5)
&      + dw2(2)*A(1,4)*A(1,5)
&      + dw2(3)*(Bbar(4)*A(1,5)+Bbar(5)*A(1,4))
M(6,4)=M(6,4) + dw2(1)*Bbar(4)*Bbar(6)
&      + dw2(2)*A(1,4)*A(1,6)
&      + dw2(3)*(Bbar(4)*A(1,6)+Bbar(6)*A(1,4))
M(6,5)=M(6,5) + dw2(1)*Bbar(5)*Bbar(6)
&      + dw2(2)*A(1,5)*A(1,6)
&      + dw2(3)*(Bbar(5)*A(1,6)+Bbar(6)*A(1,5))
*****
```

```
endif
```

```
! symmetries
```

```

M(1,2) = M(2,1)
M(1,3) = M(3,1)
M(2,3) = M(3,2)
M(1,4) = M(4,1)
M(2,4) = M(4,2)
M(3,4) = M(4,3)
M(1,5) = M(5,1)
M(2,5) = M(5,2)
M(3,5) = M(5,3)
M(4,5) = M(5,4)
M(1,6) = M(6,1)
M(2,6) = M(6,2)
M(3,6) = M(6,3)
M(4,6) = M(6,4)
M(5,6) = M(6,5)

```

```
! isotropic volumic components
```

```
M(1:3,1:3) = M(1:3,1:3) + bm*(2._RK*detF - 1._RK)
```

```
! change from spatial to corotated frame
```

```
! rotation from polar decomposition
```

```
call polarRU(F1,R,U)
```

```
! dim 6 rotation matrix
```

```
call trans_mattrx_6(Q,transpose(R))
```

```
! corotated stress
```

```
stressfull(:) = matmul(Q,sigma)
```

```
! corotated tangent
```

```
dsdePlfull(:,:) = matmul(Q,matmul(M,transpose(Q)))
```

```
if (ncomp .eq. 4) then
```

```

stress(:) = stressfull(1:4)
dsdePl = dsdePlfull(1:4,1:4)
else
  stress = stressfull
  dsdePl = dsdePlfull
end if
! transverse shear stiffness
tsstif(:) = dsdePlfull(6,6)
!-----!
! state variables
!-----!
*** orientation vector E_theta
ustatev(1) = EVT(1)
ustatev(2) = EVT(2)
!-----!
normspaevt = sqrt( (F1(1,1)*EVT(1)+F1(1,2)*EVT(2))**2
&           + (F1(2,1)*EVT(1)+F1(2,2)*EVT(2))**2 )
spaevt(1) = (F1(1,1)*EVT(1)+F1(1,2)*EVT(2))/normspaevt
spaevt(2) = (F1(2,1)*EVT(1)+F1(2,2)*EVT(2))/normspaevt
! *** radial stress sigma_rr
ustatev(3) = sigma(1)*(spaevt(2))**2
&           + sigma(2)*(spaevt(1))**2
&           - 2._RK * sigma(4)*spaevt(1)*spaevt(2)
! *** circumferential stress sigma_tt
ustatev(4) = sigma(1)*(spaevt(1))**2
&           + sigma(2)*(spaevt(2))**2
&           + 2._RK * sigma(4)*spaevt(1)*spaevt(2)
!-----!
end subroutine usermat3d
!*****
! *** subroutines ***
! author:          JM GeRKen, ANSYS, Inc.
! creation date:   17/12/2008
!*****
```

```

subroutine polarRU(F,R,U)
!-----!
*** Polar decomposition, F=RU
References :
JC Simo & TJR Hughes, Computational Inelasticity, 1998, Springer
!-----!
```

```

IMPLICIT NONE
integer,parameter :: RK=KIND(1.D0) ! real kind
! arguments
real(RK),intent(IN) :: F(3,3) ! matrix to decompose
real(RK),intent(OUT) :: R(3,3) !rotation
real(RK),intent(OUT) :: U(3,3) !stretch
! local
real(RK), parameter :: pi    = 3.14159265358979324_RK
real(RK),parameter ::I(3,3)=reshape((/1._RK,0._RK,0._RK,
&                                0._RK,1._RK,0._RK,
&                                0._RK,0._RK,1._RK/),(3,3))
real(RK) :: C(3,3),CC(3,3) ! right Cauchy-Green, squared
real(RK) :: Ui(3,3) ! U inverse
real(RK) :: IC, IIC, IIIC ! invariants of C
real(RK) :: IU, IIU, IIIU ! invariants of U
real(RK) :: l1,l2,l3 ! eigenvalues
real(RK) :: p,q,m,n,t,D ! constants
!-----!
```

```

! right Cauchy-Green
C(:,:,)=matmul(transpose(F),F)
CC(:,:,)=matmul(C,C)
! invariants
IC = C(1,1) + C(2,2) + C(3,3)
IIC = 0.5_RK*(IC**2 - (CC(1,1) + CC(2,2) + CC(3,3)))
IIIC = C(1,1) * (C(2,2)*C(3,3) - C(2,3)*C(3,2))
&   + C(1,2) * (C(2,3)*C(3,1) - C(2,1)*C(3,3))
&   + C(1,3) * (C(2,1)*C(3,2) - C(2,2)*C(3,1))
! eigenvalues of sqrt(C)
p = IIC - (IC**2)/3._RK
q = -(2._RK/27._RK)*IC**3+IC*IIC/3._RK-IIIC
if(abs(p)<epsilon(1._RK))then
  l1 = sqrt( abs(-abs(q)**(1._RK/3._RK) + IC/3._RK) )
```

```

l2 = l1
l3 = l2
else
  m = 2._RK*sqrt(abs(p)/3._RK)
  n = 3._RK*q/(m*p)
  if(abs(n)>1._RK) n = sign(1._RK, n)
  t = atan2(sqrt(1._RK-n**2),n)/3._RK
  l1 = sqrt( abs(m*cos(t) + IC/3._RK) )
  l2 = sqrt( abs(m*cos(t+2._RK/3._RK*pi) + IC/3._RK) )
  l3 = sqrt( abs(m*cos(t+4._RK/3._RK*pi) + IC/3._RK) )
endif
! stretch and inverse
!invariants
IU = l1 + l2 + l3
IIU = l1*l2 + l1*l3 + l2*l3
IIIU = l1*l2*l3
D = IU*IIU-IIIU

U(:,:) = (-CC(:,:)+ (IU**2-IIU)*C(:,:)+ IU*IIIU*I(:,:))/D
Ui(:,:) = (C(:,:)- IU*U(:,:)+ IIU*I(:,:))/IIIU

! rotation
R(:,:) = matmul(F,Ui)
end subroutine polarRU
!-----
SUBROUTINE trans_matrix_6(Q,R)
!-----
! construct the 6x6 Voigt rotation matrix
!-----
IMPLICIT NONE
integer,parameter :: RK=KIND(1.D0) ! real kind
! arguments
real(RK), intent(OUT) :: Q(6,6)
real(RK), intent(IN) :: R(3,3)
!-----
Q(1,1) = R(1,1)**2
Q(2,1) = R(2,1)**2
Q(3,1) = R(3,1)**2
Q(4,1) = R(1,1)*R(2,1)
Q(5,1) = R(2,1)*R(3,1)
Q(6,1) = R(3,1)*R(1,1)

Q(1,2) = R(1,2)**2
Q(2,2) = R(2,2)**2
Q(3,2) = R(3,2)**2
Q(4,2) = R(1,2)*R(2,2)
Q(5,2) = R(2,2)*R(3,2)
Q(6,2) = R(3,2)*R(1,2)

Q(1,3) = R(1,3)**2
Q(2,3) = R(2,3)**2
Q(3,3) = R(3,3)**2
Q(4,3) = R(1,3)*R(2,3)
Q(5,3) = R(2,3)*R(3,3)
Q(6,3) = R(3,3)*R(1,3)

Q(1,4) = R(1,1)*R(1,2)*2._RK
Q(2,4) = R(2,1)*R(2,2)*2._RK
Q(3,4) = R(3,1)*R(3,2)*2._RK
Q(4,4) = R(1,1)*R(2,2)+R(1,2)*R(2,1)
Q(5,4) = R(2,1)*R(3,2)+R(2,2)*R(3,1)
Q(6,4) = R(3,1)*R(1,2)+R(3,2)*R(1,1)

Q(1,5) = R(1,2)*R(1,3)*2._RK
Q(2,5) = R(2,2)*R(2,3)*2._RK
Q(3,5) = R(3,2)*R(3,3)*2._RK
Q(4,5) = R(1,2)*R(2,3)+R(1,3)*R(2,2)
Q(5,5) = R(2,2)*R(3,3)+R(2,3)*R(3,2)
Q(6,5) = R(3,2)*R(1,3)+R(3,3)*R(1,2)

Q(1,6) = R(1,1)*R(1,3)*2._RK
Q(2,6) = R(2,1)*R(2,3)*2._RK
Q(3,6) = R(3,1)*R(3,3)*2._RK
Q(4,6) = R(1,1)*R(2,3)+R(1,3)*R(2,1)
Q(5,6) = R(2,1)*R(3,3)+R(2,3)*R(3,1)

```

```
Q(6,6) = R(3,1)*R(1,3)+R(3,3)*R(1,1)
END SUBROUTINE trans_matrix_6
```

!-----