# EN234: Computational methods in Structural and Solid Mechanics 

## Homework 7: Large deformation elasticity

Due Fri Nov 3, 2017

School of Engineering
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In this homework you will implement a finite element method to solve problems involving large-deformations of elastic materials (hyperelasticity).

The calculations in this homework will show that there are a large number of equivalent ways to solve large deformation problems, depending on what stress and strain measures you choose to use. You will come across all of them in the mechanics literature.

As a specific choice, we will consider the generalized 'Fung' hyperelastic material.
 This model specifies the second Piola-
Kirchhoff stress (or 'material stress', which is related to Cauchy stress by $\boldsymbol{\Sigma}=\mathbf{F}^{-1} J \boldsymbol{\sigma} \mathbf{F}^{-T}$ ) as a function of the jacobian $J=\operatorname{det}(\mathbf{F})$ and the deviatoric right Cauchy-Green deformation tensor $\mathbf{C}=\mathbf{F}^{T} \mathbf{F}$ as

$$
\begin{aligned}
& \Sigma_{i j}=\mu \exp (Q) P_{i j}+K J(J-1) C_{i j}^{-1} \\
& Q=\frac{1}{4}\left(\bar{C}_{i j}-\delta_{i j}\right) G_{i j k l}\left(\bar{C}_{k l}-\delta_{k l}\right) \quad P_{i j}=\frac{\partial Q}{\partial C_{i j}}=\frac{1}{2 J^{2 / 3}}\left\{G_{i j k l}\left(\bar{C}_{k l}-\delta_{k l}\right)-\frac{1}{3} C_{m n} G_{m n k l}\left(\bar{C}_{k l}-\delta_{k l}\right) C_{i j}^{-1}\right\}
\end{aligned}
$$

where $\bar{C}_{i j}=C_{i j} / J^{2 / 3} ; \mu, G_{i j k l}$ are two constants that control the anisotropic elastic moduli and the rate of stiffening of the material with stretch, and $K \gg \mu \exp (Q)$ is the bulk modulus.
The material has a strain energy density $W=\frac{\mu}{2}(\exp (Q)-1)+\frac{K}{2}(J-1)^{2}$. To interpret the constants $\mu, G_{i j k l}$, note that for small strains the stress is

$$
\Sigma_{i j} \approx \sigma_{i j}=\mu G_{i j k l} \varepsilon_{k l}-\frac{1}{3} G_{n n k l} \varepsilon_{k l}+K \delta_{i j} \varepsilon_{k k}
$$

In this homework, we will assume for simplicity that the components of $\mathbf{G}$ in the global basis (with the usual convention for storing the modulus tensor as a 6x6 matrix) have the form

$$
\left[\begin{array}{cccccc}
G_{11} & 0 & 0 & 0 & 0 & 0 \\
0 & G_{22} & 0 & 0 & 0 & 0 \\
0 & 0 & G_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & G_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & G_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & G_{44}
\end{array}\right]
$$

1. In this problem we will implement a finite element method for this material directly, by coding an ABAQUS format UEL. This problem is meant to illustrate the general Newton-Raphson method for finite strain hyperelasticity problems, so we will not try to correct for volumetric locking in the element. To use this approach for most real hyperelastic materials (which are usually close to incompressible) it would be essential to correct for volumetric locking.

Since the stress-strain law is expressed in terms of the second Piola-Kircchoff stress, it is simplest to proceed by re-writing the finite element equilibrium equations in terms of this stress measure. It is straightforward to show that the equilibrium equations reduce to a set of nonlinear equations for the displacements of the form

$$
R_{i}^{a}-F_{i}^{a}=0 \quad F_{i}^{a}=\int_{\partial_{2} V_{0}} t_{i}^{*} N^{a} d A_{0} \quad R_{i}^{a}=\int_{V_{0}} \frac{\partial N^{a}}{\partial x_{j}} \Sigma_{j k} F_{i k} d V_{0}
$$

The nonlinear equations must be solved using Newton-Raphson iteration: as always this involves repeatedly computing a correction to the approximation to the displacement field by solving a set of linear equations

$$
K_{a i b k} d w_{k}^{b}=-R_{i}^{a}+F_{i}^{a}
$$

1.1 Follow the procedure in class to show that the tangent matrix can be expressed as

$$
K_{a i b k}^{e l}=\int_{V_{0}} \frac{\partial N^{a}}{\partial x_{j}} F_{i p} 2 \frac{\partial \boldsymbol{\Sigma}_{p j}}{\partial C_{l n}} F_{k n} \frac{\partial N^{b}}{\partial x_{l}} d V_{0}+\int_{V_{0}} \frac{\partial N^{a}}{\partial x_{j}} \Sigma_{j n} \frac{\partial N^{b}}{\partial x_{n}} \delta_{i k} d V_{0}
$$

1.2 Show that the elastic tangent modulus is something like (I don't guarantee that the result below is correct, but it is close enough to pass the stiffness check in EN234FEA and for the Newton iterations to converge):

$$
\begin{aligned}
& 2 \frac{\partial \boldsymbol{\Sigma}_{i j}}{\partial C_{k l}}=2 \mu \exp (Q)\left[P_{i j} P_{k l}+\Lambda_{i j k l}\right]+K J\left((2 J-1) C_{i j}^{-1} C_{k l}^{-1}+2[J-1] \boldsymbol{\Omega}_{i j k l}\right) \\
& \boldsymbol{\Omega}_{i j k l}=\frac{\partial C_{i j}^{-1}}{\partial C_{k l}}=-\frac{1}{2}\left[C_{i k}^{-1} C_{j l}^{-1}+C_{i l}^{-1} C_{j k}^{-1}\right] \\
& \boldsymbol{\Lambda}_{i j k l}=\frac{\partial P_{i j}}{\partial C_{k l}} \\
& =\frac{1}{2 J^{4 / 3}} G_{i j k l}-\frac{1}{3} P_{i j} C_{k l}^{-1}-\frac{1}{2 J^{2 / 3}} \frac{1}{3} C_{i j}^{-1} G_{k l p q}\left(\bar{C}_{p q}-\delta_{p q}\right) \\
& +\frac{1}{2 J^{4 / 3}}\left\{-\frac{1}{3}\left[G_{i j p q} C_{p q} C_{k l}^{-1}+G_{k l p q} C_{p q} C_{i j}^{-1}\right]-\frac{J^{2 / 3}}{3} C_{m n} G_{m n p q}\left(\bar{C}_{p q}-\delta_{p q}\right) \boldsymbol{\Omega}_{i j k l}+\frac{1}{9} C_{m n} G_{m n p q} C_{p q} C_{i j}^{-1} C_{k l}^{-1}\right\}
\end{aligned}
$$

The following identities are useful

$$
\frac{\partial J}{\partial C_{i j}}=\frac{1}{2} J C_{i j}^{-1} \quad \frac{\partial \bar{C}_{i j}}{\partial C_{k l}}=\frac{1}{J^{2 / 3}}\left(\frac{\delta_{i k} \delta_{j l}+\delta_{i l} \delta_{j k}}{2}-\frac{1}{3} C_{i j} C_{k l}^{-1}\right)
$$

1.3 Now, implement this procedure as an ABAQUS UEL (you can use EN234FEA to do this, there is no need to run your code in ABAQUS.)

As always, your UEL will need to calculate the element internal force vector and stiffness matrix. The general structure of your code will be very similar to those you have written in previous assignments (and you could start by copying the small strain linear elastic UEL into a new file). The stiffness and internal force vectors can be expressed in matrix form as

$$
\begin{gathered}
\mathbf{R}=\int_{V_{0}} \mathbf{B}^{* T} \mathbf{q} d V_{0} \\
\mathbf{K}=\int_{V_{0}} \mathbf{B}^{* T} \mathbf{H}^{T} \mathbf{D} \mathbf{H} \mathbf{B}^{*} d V_{0}+\int_{V_{0}} \mathbf{Y} d V_{0}
\end{gathered}
$$

Here, $\mathbf{B}^{*}$ is a modified $\mathbf{B}$ matrix that maps the displacements onto the deformation gradient (for a 3D element with $n$ nodes this is a $9 \times 3 n$ matrix) as

$$
\mathbf{B}^{*}=\left[\begin{array}{cccccc}
\frac{\partial N^{1}}{\partial x_{1}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{1}} & 0 & 0 \\
0 & \frac{\partial N^{1}}{\partial x_{2}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{2}} & 0 \\
0 & 0 & \frac{\partial N^{1}}{\partial x_{3}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{3}} \\
\frac{\partial N^{1}}{\partial x_{2}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{2}} & 0 & 0 \\
0 & \frac{\partial N^{1}}{\partial x_{1}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{1}} & 0 \\
\frac{\partial N^{1}}{\partial x_{3}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{3}} & & \\
0 & 0 & \frac{\partial N^{1}}{\partial x_{1}} & 0 & 0 & \frac{\partial N^{2}}{\partial x_{1}} \\
0 & \frac{\partial N^{1}}{\partial x_{3}} & 0 & & & \\
0 & 0 & \frac{\partial N^{1}}{\partial x_{2}} & & &
\end{array}\right]
$$

The vector $\mathbf{q}$ stores the (unsymmetric) nominal stress $\Sigma_{i k} F_{j k}$ as a 9 dimensional vector

$$
\mathbf{q}=\left[\Sigma_{1 k} F_{1 k}, \Sigma_{2 k} F_{2 k}, \Sigma_{3 k} F_{3 k}, \Sigma_{2 k} F_{1 k}, \Sigma_{1 k} F_{2 k}, \Sigma_{3 k} F_{1 k}, \Sigma_{1 k} F_{3 k}, \Sigma_{3 k} F_{2 k}, \Sigma_{2 k} F_{3 k}\right]
$$

You can compute $\mathbf{q}$ by:
(i) Find the deformation gradient $\mathbf{F}$, which can be assembled as a $3 \times 3$ matrix by first computing the shape function derivatives $\frac{\partial N^{a}}{\partial x_{j}}$ in the usual way, then multiply by the displacement vector

$$
F_{i j}=\delta_{i j}+\frac{\partial N^{a}}{\partial x_{j}} u_{i}^{a} \text { (you can use a Fortran matmul to do this) }
$$

(ii) Calculate the material stress $\boldsymbol{\Sigma}$, and store it as a $3 \times 3$ matrix
(iii) Find $\boldsymbol{\Sigma} \mathbf{F}^{T}$ (use matmul)
(iv) Assemble $\mathbf{q}$ (be careful to get the order right, or your code will bomb...)

The matrix $\mathbf{H}$ in the stiffness is a $6 \times 9$ matrix with components

$$
\mathbf{H}=\left[\begin{array}{ccccccccc}
F_{11} & 0 & 0 & 0 & F_{21} & 0 & F_{31} & 0 & 0 \\
0 & F_{22} & 0 & F_{12} & 0 & 0 & 0 & 0 & F_{32} \\
0 & 0 & F_{33} & 0 & 0 & F_{13} & 0 & F_{23} & 0 \\
F_{12} & F_{21} & 0 & F_{11} & F_{22} & 0 & F_{32} & 0 & F_{31} \\
F_{13} & 0 & F_{31} & 0 & F_{23} & F_{11} & F_{33} & F_{21} & 0 \\
0 & F_{23} & F_{32} & F_{13} & 0 & F_{12} & 0 & F_{22} & F_{33}
\end{array}\right]
$$

It is best to calculate the stress and the material tangent matrix $\mathbf{D}$ in a separate subroutine (which takes $\mathbf{F}$ and the material properties as input, and returns $\mathbf{\Sigma}$ and $\mathbf{D}$ ). It is helpful to define vectors

$$
\mathbf{C}=\left[C_{11}, \mathrm{C}_{22}, C_{33}, C_{12}, C_{13}, C_{23}\right], \quad \overline{\mathbf{C}}=\mathbf{C} / J^{2 / 3}, \quad \mathbf{C}^{-1}=\left[C_{11}^{-1}, C_{22}^{-1}, \cdots\right], \quad \mathbf{P}=\left[P_{11}, P_{22}, P_{33}, \cdots\right]
$$

where $\mathbf{C}=\mathbf{F}^{T} \mathbf{F}$. We also need two stretch vectors with the shear terms doubled

$$
\mathbf{C}^{*}=\left[C_{11}, \mathrm{C}_{22}, C_{33}, 2 C_{12}, 2 C_{13}, 2 C_{23}\right], \quad \overline{\mathbf{C}}^{*}=\mathbf{C}^{*} / J^{2 / 3}
$$

Then (assuming you agree with the result in problem 1.2 - if not, you will need to change what is below)

$$
\begin{aligned}
\boldsymbol{\Sigma} & =\mu \exp (Q) \mathbf{P}+K J(J-1) \mathbf{C}^{-1} \\
\mathbf{D} & =\mu \exp (Q)\left(\frac{1}{J^{4 / 3}}\left[\mathbf{G}-\frac{1}{3}\left(\mathbf{G} \mathbf{C}^{*} \otimes \mathbf{C}^{-1}+\mathbf{C}^{-1} \otimes \mathbf{G} \mathbf{C}^{*}\right)-\frac{J^{2 / 3}}{3}\left(\mathbf{C}^{*} \cdot \mathbf{G}\left(\overline{\mathbf{C}}^{*}-\mathbf{I}\right)\right) \mathbf{\Omega}+\frac{1}{9}\left(\mathbf{C}^{*} \cdot \mathbf{G} \mathbf{C}^{*}\right) \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}\right]\right) \\
& +\mu \exp (Q)\left(2 \mathbf{P} \otimes\left(\mathbf{P}-\frac{1}{3} \mathbf{C}^{-1}\right)-\frac{1}{3 J^{2 / 3}} \mathbf{C}^{-1} \otimes \mathbf{G}\left(\overline{\mathbf{C}}^{*}-\mathbf{I}\right)\right)+K J\left((2 J-1) \mathbf{C}^{-1} \otimes \mathbf{C}^{-1}+2[J-1] \mathbf{\Omega}\right)
\end{aligned}
$$

where
$\boldsymbol{\Omega}=-\left[\begin{array}{cccccc}C_{11}^{-1} C_{11}^{-1} & C_{12}^{-1} C_{12}^{-1} & C_{13}^{-1} C_{13}^{-1} & C_{11}^{-1} C_{12}^{-1} & \left.\mathbf{G}\left(\overline{\mathbf{C}}^{*}-\mathbf{I}\right)-\frac{1}{3}\left[\mathbf{C}^{*} \cdot \mathbf{G}\left(\overline{\mathbf{C}}^{*}-\mathbf{I}\right)\right] \mathbf{C}^{-1}\right\} \\ & C_{22}^{-1} C_{22}^{-1} & C_{23}^{-1} C_{23}^{-1} & C_{21}^{-1} C_{22}^{-1} & C_{11}^{-1} C_{13}^{-1} & \\ & & C_{33}^{-1} C_{33}^{-1} & C_{31}^{-1} C_{32}^{-1} & C_{21}^{-1} C_{23}^{-1} & C_{12}^{-1} C_{13}^{-1} \\ & & & \left(C_{11}^{-1} C_{22}^{-1}+C_{12}^{-1} C_{12}^{-1}\right) / 2 & \left(C_{11}^{-1} C_{23}^{-1}+C_{13}^{-1} C_{12}^{-1}\right) / 2 & \left(C_{12}^{-1} C_{23}^{-1}+C_{13}^{-1} C_{22}^{-1}\right) / 2 \\ & & & & \left(C_{11}^{-1} C_{33}^{-1}+C_{13}^{-1} C_{13}^{-1}\right) / 2 & \left(C_{12}^{-1} C_{33}^{-1}+C_{13}^{-1} C_{23}^{-1}\right) / 2 \\ & & & & \left(C_{22}^{-1} C_{33}^{-1}+C_{23}^{-1} C_{23}^{-1}\right) / 2\end{array}\right]$

Note that in Fortran the outer product of two 6 dimensional vectors $\mathbf{a} \otimes \mathbf{b}$ can be calculated quickly using D = spread(a,dim=2, ncopies=6)*spread(b,dim=1,ncopies=6)

Finally the geometric stiffness can be constructed by first computing the matrix

$$
k_{a b}=\frac{\partial N^{a}}{\partial x_{j}} \Sigma_{j n} \frac{\partial N^{b}}{\partial x_{n}}
$$

which can be assembled using standard matrix multiplications. The full $3 n x 3 n$ matrix follows by expanding this

$$
\mathbf{Y}=\left[\begin{array}{cccccc}
k_{11} & 0 & 0 & k_{12} & & \\
0 & k_{11} & 0 & & k_{12} & \\
0 & 0 & k_{11} & & & k_{12} \\
k_{21} & & & k_{22} & & \\
& k_{21} & & & & \\
& & k_{21} & & & \ddots
\end{array}\right]
$$

When you write your UEL, store the components of Cauchy stress

$$
\sigma=\mathbf{F} \boldsymbol{\Sigma} \mathbf{F}^{T} / J
$$

at each integration point as state variables (using the usual vector notation), so EN234FEA can print the stress components to the tecplot format output file.

1.4 Test your UEL by using the input file Abaqus_uel_hyperelastic.in provided with EN234FEA. The file sets up a problem in which a bar is subjected to a sequence of a stretch, followed by a rotation. Check the file to determine the order of the material properties in the PROPS vector in the UMAT subroutine.

Use the CHECK STIFFNESS to make sure that the stiffness matrix for your element is consistent with the internal force vector. You can use Tecplot to visualize the deformed mesh

As a solution to this problem (i) Upload your derivations of 1.1 and 1.2 and include a short summary of tests you have run to verify your code; and (ii) push your code to Github.

