Implementation of the Compressible Mooney-Rivlin Material in the `imitor` Finite Element Code

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Material Model

A compressible Mooney-Rivlin material is defined by the following relationship:

$$W = C_1(\overline{I_1} - 3) + C_2(\overline{I_2} - 3) + D_1(J - 1)^2 \tag{1}$$

where W is the strain energy density, C_1 and C_2 are constants related to distortional response, and D_1 is a constant related to volumetric response. The quantities $\overline{I_1} = J^{-2/3}I_1$, $\overline{I_2} = J^{-4/3}I_2$, where I_1 and I_2 are the first and second invariants of $\mathbf{B} = \mathbf{F}\mathbf{F}^{\mathbf{T}}$, and $J = \det(\mathbf{F})$. Specifically, $I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$ and $I_2 = \lambda_1^2\lambda_2^2 + \lambda_2^2\lambda_3^2 + \lambda_1^2\lambda_3^2 = \frac{1}{2}[(\mathrm{tr}\mathbf{B})^2 - \mathrm{tr}(\mathbf{B}^2)]$, where λ_i are the eigenvalues of the deformation gradient $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$.

The relationship between Cauchy stress $\mathbf{T}$ and strain energy density W is as follows:

$$\mathbf{T} = \frac{1}{J}\frac{\partial W}{\partial \mathbf{F}}\mathbf{F}^T \tag{2}$$

Using this relationship, one may obtain a direct expression for the Cauchy stress $\mathbf{T}$ in terms of the deformation gradient:

$$\mathbf{T} = \frac{2}{J}\left[\frac{1}{J^{2/3}}(C_1 + \overline{I_1}C_2)\mathbf{B} - \frac{1}{J^{4/3}}C_2\mathbf{B}^2\right] + \left[2D_1(J-1) - \frac{2}{3J}(C_1\overline{I_1} + 2C_2\overline{I_2})\right]\mathbf{I} \tag{3}$$

which can be written in index notation as:

$$T_{ij} = \frac{2}{J}\left[\frac{1}{J^{2/3}}(C_1 + \overline{I_1}C_2)B_{ij} - \frac{1}{J^{4/3}}C_2B_{ik}B_{kj}\right] + \left[2D_1(J-1) - \frac{2}{3J}(C_1\overline{I_1} + 2C_2\overline{I_2})\right]\delta_{ij} \tag{4}$$

Using the relationships $\overline{I_1} = J^{-2/3}I_1$ and $\overline{I_2} = J^{-4/3}I_2$ and reorganizing, the relationship that will be used moving forward is as follows:

$$T_{ij} = 2C_1J^{-5/3}\left[B_{ij} - \frac{1}{3}I_1\delta_{ij}\right] + 2C_2J^{-7/3}\left[I_1B_{ij} - B_{im}B_{mj} - \frac{2}{3}I_2\delta_{ij}\right] + 2D_1(J-1)\delta_{ij} \tag{5}$$

In the limit of small strains, this relationship reduces to a linear elastic material when the bulk modulus $K = 2D_1$ and the shear modulus $\mu = 2(C_1 + C_2)$.

Calculating Unrotated Stresses

In the absence of rotation, $\mathbf{L} = \mathbf{D} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{U}}\mathbf{U}^{-1}$. Thus, the following ODE must be solved to find the appropriate $\hat{\mathbf{U}}$ that produces the same stretch that $\hat{\mathbf{F}}$ does.

$$\dot{\mathbf{U}} = \mathbf{D}\mathbf{U} \tag{6}$$
$$\mathbf{U}(t_n) = \mathbf{I} \tag{7}$$
$$\mathbf{U}(t_{n+1}) = \hat{\mathbf{U}} \tag{8}$$

The solution to this ODE is

$$\hat{\mathbf{U}} = \exp(\mathbf{D}\Delta t) \tag{9}$$

We now redefine $\mathbf{D}$ as the stretch rate *multiplied by the time step*. Thus, in terms of the original definition of $\mathbf{D}$ as the stretch rate, $\mathbf{D} \leftarrow \mathbf{D}\Delta t$. The previous relationship now becomes

$$\hat{\mathbf{U}} = \exp(\mathbf{D}) \tag{10}$$

The Taylor expansion of this relationship is then:

$$\hat{\mathbf{U}} = \mathbf{I} + \mathbf{D} + \frac{1}{2}\mathbf{D}^2 + \frac{1}{6}\mathbf{D}^3 \tag{11}$$
$$\tag{12}$$

We now define $\tilde{\mathbf{F}}$ as the deformation gradient at time t_{n+1} prior to applying the rotation increment $\hat{\mathbf{R}}$. Specifically,

$$\tilde{\mathbf{F}} = \hat{\mathbf{U}}\bar{\mathbf{F}} \tag{13}$$
$$\mathbf{F} = \hat{\mathbf{R}}\tilde{\mathbf{F}} \tag{14}$$

where $\bar{\mathbf{F}} = \partial\bar{\mathbf{u}}/\partial\mathbf{X}$ is the deformation gradient at time t_n.

Thus, when calculating stresses for the new time step, rather than feed $\mathbf{F}$ to calculate $\mathbf{T}$, $\tilde{\mathbf{F}}$ is fed into the constitutive model to produce $\hat{\mathbf{T}}$, and then $\mathbf{T} = \hat{\mathbf{R}}\hat{\mathbf{T}}\hat{\mathbf{R}}^T$.

Tangent Modulus

If we are stepping from time t_n to t_{n+1}, we seek the derivatives $\partial\hat{\mathbf{T}}/\partial\mathbf{D}$, where $\hat{\mathbf{T}}$ is the the Cauchy stress at time t_{n+1} prior to applying the rotation increment $\hat{\mathbf{R}}$, and $\mathbf{D}$ retains the new definition from the previous section, as stretch rate *multiplied by the time step.*

Successive use of chain rule will be used:

$$\frac{\partial\hat{\mathbf{T}}}{\partial\mathbf{D}} = \frac{\partial\hat{\mathbf{T}}}{\partial\tilde{\mathbf{F}}}\frac{\partial\tilde{\mathbf{F}}}{\partial\mathbf{D}} \tag{15}$$

$$\frac{\partial\hat{T}_{ij}}{\partial D_{kl}} = \frac{\partial\hat{T}_{ij}}{\partial\tilde{F}_{mn}}\frac{\partial\tilde{F}_{mn}}{\partial D_{kl}} \tag{16}$$

again where $\tilde{\mathbf{F}}$ is defined in the previous section.

Chain rule is used on the derivative $\partial\tilde{\mathbf{F}}/\partial\mathbf{D}$ as follows:

$$\frac{\partial\tilde{\mathbf{F}}}{\partial\mathbf{D}} = \frac{\partial\tilde{\mathbf{F}}}{\partial\hat{\mathbf{U}}}\frac{\partial\hat{\mathbf{U}}}{\partial\mathbf{D}} \tag{17}$$

$$\frac{\partial\tilde{F}_{ij}}{\partial D_{kl}} = \frac{\partial\tilde{F}_{ij}}{\partial\hat{U}_{mn}}\frac{\partial\hat{U}_{mn}}{\partial D_{kl}} \tag{18}$$

The following tensor derivatives will be used repeatedly in what follows:

$$\text{if } \mathbf{A} \neq \mathbf{A}^T, \quad \frac{\partial A_{ij}}{\partial A_{kl}} = \delta_{ik}\delta_{jl} \tag{19}$$

$$\text{if } \mathbf{A} = \mathbf{A}^T, \quad \frac{\partial A_{ij}}{\partial A_{kl}} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{20}$$

Note, *these definitions are not the same for a symmetric tensor.* If a tensor is symmetric, the appropriate definition for symmetric tensors *must* be used.

The Taylor expansion definition of $\hat{\mathbf{U}}$ from the previous section is repeated here in index notation:

$$\hat{U}_{ij} = \delta_{ij} + D_{ij} + \frac{1}{2}D_{im}D_{mj} + \frac{1}{6}D_{im}D_{mn}D_{nj} \tag{21}$$

The derivative $\partial\hat{\mathbf{U}}/\partial\mathbf{D}$ is then:

$$\begin{aligned}\frac{\partial\hat{U}_{ij}}{\partial D_{kl}} =& \frac{1}{2}\Bigg[\delta_{ik}\delta_{jl} + \frac{1}{2}\delta_{ik}\delta_{ml}D_{mj} + \frac{1}{2}D_{im}\delta_{mk}\delta_{jl} + \\ & \frac{1}{6}\delta_{ik}\delta_{ml}D_{mn}D_{nj} + \frac{1}{6}D_{im}\delta_{mk}\delta_{nl}D_{nj} + \frac{1}{6}D_{im}D_{mn}\delta_{nk}\delta_{jl}\Bigg] + \\ & \frac{1}{2}\Bigg[\delta_{il}\delta_{jk} + \frac{1}{2}\delta_{il}\delta_{mk}D_{mj} + \frac{1}{2}D_{im}\delta_{ml}\delta_{jk} + \\ & \frac{1}{6}\delta_{il}\delta_{mk}D_{mn}D_{nj} + \frac{1}{6}D_{im}\delta_{ml}\delta_{nk}D_{nj} + \frac{1}{6}D_{im}D_{mn}\delta_{nl}\delta_{jk}\Bigg]\end{aligned} \tag{22}$$

Further simplifying,

$$\frac{\partial \hat{U}_{ij}}{\partial D_{kl}} = \frac{1}{2}\left[\delta_{ik}\delta_{jl} + \frac{1}{2}\delta_{ik}D_{lj} + \frac{1}{2}D_{ik}\delta_{jl} + \frac{1}{6}\delta_{ik}D_{ln}D_{nj} + \frac{1}{6}D_{ik}D_{lj} + \frac{1}{6}D_{im}D_{mk}\delta_{jl}\right] + \tag{23}$$

$$\frac{1}{2}\left[\delta_{il}\delta_{jk} + \frac{1}{2}\delta_{il}D_{kj} + \frac{1}{2}D_{il}\delta_{jk} + \frac{1}{6}\delta_{il}D_{kn}D_{nj} + \frac{1}{6}D_{il}D_{kj} + \frac{1}{6}D_{im}D_{ml}\delta_{jk}\right] \tag{24}$$

Now, repeating the definition for $\tilde{\mathbf{F}}$ in index notation,

$$\tilde{F}_{ij} = \hat{U}_{im}\overline{F}_{mj} \tag{25}$$

The derivative $\partial\tilde{\mathbf{F}}/\partial\hat{\mathbf{U}}$ is

$$\frac{\partial \tilde{F}_{ij}}{\partial \hat{U}_{kl}} = \frac{1}{2}\left(\delta_{ik}\delta_{ml}\overline{F}_{mj} + \delta_{il}\delta_{mk}\overline{F}_{mj}\right) \tag{26}$$

and finally,

$$\frac{\partial \tilde{F}_{ij}}{\partial \hat{U}_{kl}} = \frac{1}{2}\left(\delta_{ik}\overline{F}_{lj} + \delta_{il}\overline{F}_{kj}\right) \tag{27}$$

With $\partial\tilde{\mathbf{F}}/\partial\hat{\mathbf{U}}$ and $\partial\hat{\mathbf{U}}/\partial\mathbf{D}$ specified, $\partial\tilde{\mathbf{F}}/\partial\mathbf{D}$ is fully defined. What remains to fully define the tangent modulus $\partial\hat{\mathbf{T}}/\partial\mathbf{D}$ is to calculate $\partial\hat{\mathbf{T}}/\partial\tilde{\mathbf{F}}$.

In what follows, we assume J and $\mathbf{B}$ are independent variables, and that the tensor invariants of $\mathbf{B}$ are functions of $\mathbf{B}$, i.e., $I_1 = I_1(\mathbf{B})$ and $I_2 = I_2(\mathbf{B})$. Then, one may write

$$\frac{\partial \hat{\mathbf{T}}}{\partial \tilde{\mathbf{F}}} = \frac{\partial \hat{\mathbf{T}}}{\partial J}\frac{\partial J}{\partial \tilde{\mathbf{F}}} + \frac{\partial \hat{\mathbf{T}}}{\partial \mathbf{B}}\frac{\partial \mathbf{B}}{\partial \tilde{\mathbf{F}}} \tag{28}$$

$$\frac{\partial \hat{T}_{ij}}{\partial \tilde{F}_{kl}} = \frac{\partial \hat{T}_{ij}}{\partial J}\frac{\partial J}{\partial \tilde{F}_{kl}} + \frac{\partial \hat{T}_{ij}}{\partial B_{mn}}\frac{\partial B_{mn}}{\partial \tilde{F}_{kl}} \tag{29}$$

If one looks at the definition for T in Equation 5, it is clear that calculating derivatives in this way is equivalent to simply taking the derivative directly and making use of the product rule.

For convenience, in what follows it will be assumed that $\mathbf{F}$ and associated quantities in fact refer to $\tilde{\mathbf{F}}$ and its respective quantities. That is, we are redefining $\mathbf{F} \leftarrow \tilde{\mathbf{F}}$ from here on. The tensors $\hat{\mathbf{T}}$ and $\mathbf{T}$ will also be interchangeable. The following definitions will be needed:

$$J = \det(\mathbf{F}) \tag{30}$$

$$B_{ij} = F_{im}F_{jm} \tag{31}$$

The corresponding derivatives are then:

$$\frac{\partial J}{\partial F_{kl}} = JF^{-1}_{lk} \tag{32}$$

$$\frac{\partial B_{ij}}{\partial F_{kl}} = \delta_{ik}\delta_{ml}F_{jm} + F_{im}\delta_{jk}\delta_{ml} \tag{33}$$

$$= \delta_{ik}F_{jl} + F_{il}\delta_{jk} \tag{34}$$

The relationship for the updated Cauchy stress is repeated here:

$$\begin{aligned} T_{ij} = 2C_1 J^{-5/3} &\left[B_{ij} - \frac{1}{3}I_1\delta_{ij}\right] + \\ &2C_2 J^{-7/3}\left[I_1 B_{ij} - B_{im}B_{mj} - \frac{2}{3}I_2\delta_{ij}\right] + \\ &2D_1(J-1)\delta_{ij} \end{aligned} \tag{35}$$

Then,

$$\begin{aligned} \frac{\partial \hat{T}_{ij}}{\partial J} =& \frac{-10}{3}C_1 J^{-8/3}\left[B_{ij} - \frac{1}{3}I_1\delta_{ij}\right] + \\ &\frac{-14}{3}C_2 J^{-10/3}\left[I_1 B_{ij} - B_{im}B_{mj} - \frac{2}{3}I_2\delta_{ij}\right] + \\ &2D_1\delta_{ij} \end{aligned} \tag{36}$$

To calculate the derivative $\partial\hat{\mathbf{T}}/\partial\mathbf{B}$, the following relationships will be needed:

$$\frac{\partial I_1}{\partial B_{kl}} = \delta_{lk} \tag{37}$$

$$\frac{\partial I_2}{\partial B_{kl}} = I_1\delta_{kl} - B_{lk} \tag{38}$$

Finally,

$$\begin{aligned} \frac{\partial \hat{T}_{ij}}{\partial B_{kl}} = 2C_1 J^{-5/3} &\left[\frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) - \frac{1}{3}\delta_{ij}\delta_{kl}\right] + \\ 2C_2 J^{-7/3} &\left[\delta_{kl}B_{ij} + \frac{1}{2}I_1\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) - \frac{1}{2}\left(\delta_{ik}\delta_{ml} + \delta_{ik}\delta_{ml}\right)B_{mj} + \right. \\ &\left. -\frac{1}{2}B_{im}\left(\delta_{mk}\delta_{jl} + \delta_{ml}\delta_{jk}\right) - \frac{2}{3}I_1\delta_{ij}\delta_{kl} + \frac{2}{3}\delta_{ij}B_{lk}\right] \end{aligned} \tag{39}$$

And simplifying,

$$\begin{aligned} \frac{\partial \hat{T}_{ij}}{\partial B_{kl}} = 2C_1 J^{-5/3} &\left[\frac{1}{2}\delta_{ik}\delta_{jl} + \frac{1}{2}\delta_{il}\delta_{jk} - \frac{1}{3}\delta_{ij}\delta_{kl}\right] + \\ 2C_2 J^{-7/3} &\left[\delta_{kl}B_{ij} + \frac{1}{2}I_1\delta_{ik}\delta_{jl} + \frac{1}{2}I_1\delta_{il}\delta_{jk} - \frac{1}{2}\delta_{ik}B_{lj} - \frac{1}{2}\delta_{il}B_{kj} + \right. \\ &\left. -\frac{1}{2}B_{ik}\delta_{jl} - \frac{1}{2}B_{il}\delta_{jk} - \frac{2}{3}I_1\delta_{ij}\delta_{kl} + \frac{2}{3}\delta_{ij}B_{lk}\right] \end{aligned} \tag{40}$$

Thus, all terms have been defined in the calculation of the tangent modulus in Equation 16.

Implementation

Population of tensors

Populating these rank-four tensor derivatives can be performed efficiently by taking advantage of Kronecker-delta properties. For demonstration purposes, the code snippet for forming $\partial \hat{U}_{ij}/\partial D_{kl}$ is shown and explained. Its definition is repeated below:

$$\begin{aligned}\frac{\partial \hat{U}_{ij}}{\partial D_{kl}} =& \frac{1}{2}\left[\delta_{ik}\delta_{jl} + \frac{1}{2}\delta_{ik}D_{lj} + \frac{1}{2}D_{ik}\delta_{jl} + \frac{1}{6}\delta_{ik}D_{ln}D_{nj} + \frac{1}{6}D_{ik}D_{lj} + \frac{1}{6}D_{im}D_{mk}\delta_{jl}\right] + \\ & \frac{1}{2}\left[\delta_{il}\delta_{jk} + \frac{1}{2}\delta_{il}D_{kj} + \frac{1}{2}D_{il}\delta_{jk} + \frac{1}{6}\delta_{il}D_{kn}D_{nj} + \frac{1}{6}D_{il}D_{kj} + \frac{1}{6}D_{im}D_{ml}\delta_{jk}\right]\end{aligned} \tag{41}$$

The code to fill this tensor is as follows:

```
DU_DD = ZERO
DO I = 1, 3
   DO J = 1, 3
      DU_DD(I,J,I,J) = DU_DD(I,J,I,J) + HALF
      DU_DD(I,J,J,I) = DU_DD(I,J,J,I) + HALF
         DO K = 1, 3
            DU_DD(I,J,I,K) = DU_DD(I,J,I,K) + HALF *
                             (HALF * STRN_INC(IJ(K,J)) +
                             SIXTH * DSQ(IJ(K,J)))
             DU_DD(I,J,K,I) = DU_DD(I,J,K,I) + HALF *
                             (HALF * STRN_INC(IJ(K,J)) +
                             SIXTH * DSQ(IJ(K,J)))
             DU_DD(I,J,K,J) = DU_DD(I,J,K,J) + HALF *
                             (HALF * STRN_INC(IJ(I,K)) +
                             SIXTH * DSQ(IJ(I,K)))
             DU_DD(I,J,J,K) = DU_DD(I,J,J,K) + HALF *
                             (HALF * STRN_INC(IJ(I,K)) +
                             SIXTH * DSQ(IJ(I,K)))
             DO L = 1, 3
                DU_DD(I,J,K,L) = DU_DD(I,J,K,L) + HALF *
                                 (SIXTH * STRN_INC(IJ(I,K)) *
                                 STRN_INC(IJ(L,J)) +
                                 (SIXTH * STRN_INC(IJ(I,L)) *
                                 STRN_INC(IJ(K,J))
             END DO
          END DO
      END DO
  END DO
```

Note, the variables ZERO, ONE, HALF, and SIXTH are REALs that have the corresponding number stored in them. STRN_INC is the stretch rate multiplied by the time step, and DSQ is that quantity squared. The rank-two matrix IJ that is used in indexing STRN_INC AND DSQ is a 3×3 matrix that makes use of the symmetry of STRN_INC and DSQ. Rather than store these variables as 3×3, they are stored as 6×1, and are indexed using this IJ matrix. The index pairs are stored in the following order: 11, 22, 33, 23, 13, 21. For reference, IJ(1:3,1) = (/ 1, 6, 5 /), IJ(1:3,2) = (/ 6, 2, 4 /), IJ(1:3,3) = (/ 5, 4, 3 /). Thus, when the index pair (I,J) = (2,3), for example, IJ(2,3) = 4. This is not particularly relevant to the purpose of this discussion.

DU_DD is a 3×3×3×3 matrix, that is first initialized as all zeros in line 1. Let us consider the first term of Equation 41: $\frac{1}{2}\delta_{ik}\delta_{jl}$. When index $k = i$ and $l = j$, the term is $\frac{1}{2}$, and for any other combination, it is 0. More generally, when the third index equals the first index, and the fourth index equals the second index, the term is $\frac{1}{2}$, and otherwise it is 0. Thus, in line 4, when the first and third indices are the same, and the second and fourth indices are the same, we add $\frac{1}{2}$ to that particular location of the tensor.

The assignment in line 5 follows the same rules, where now we deal with $\frac{1}{2}\delta_{il}\delta_{jk}$.

Consider now the following terms in Equation 41 (the second and fourth terms): $\frac{1}{2}\left(\frac{1}{2}\delta_{ik}D_{lj} + \frac{1}{6}\delta_{ik}D_{ln}D_{nj}\right)$. When $k = i$, these terms amount to: $\frac{1}{2}\left(\frac{1}{2}D_{lj} + \frac{1}{6}D_{ln}D_{nj}\right)$, and when they are not equal, the terms amount to 0. Thus, when the first and third indices are the same, these terms must be added into the appropriate locations of the tensor derivative. When we access them, we are interested in the (4th index of DU_DD, 2nd index of DU_DD) elements of STRN_INC and of DSQ. In lines 7-9, the first and third index of DU_DD are the same, the second index is J and the fourth index is K. Thus, the (K,J) indices of STRN_INC and DSQ are accessed (with the help of the IJ matrix).

The other assignments in lines 10-18 behave in a similar manner for terms multiplied by δ_{il}, δ_{jl}, and δ_{jk} for the corresponding terms in Equation 41.

Finally, the term $\frac{1}{2}\left(\frac{1}{6}D_{ik}D_{lj} + \frac{1}{6}D_{il}D_{kj}\right)$ is added into DU_DD in a straightforward manner, looping L = 1, 3 in lines 20-24.

A similar strategy is used for populating the other tensor derivatives that were mentioned in the previous section.

Note the symmetry in U and in D are *not* taken advantage of here. DU_DD indeed could be stored as a 6×6, although the following procedure would not apply any more, and it is not necessarily trivial to loop minimally over the indices and still add terms in the same way.

Round-off issues

Referring again to the definition of Cauchy stress in terms of deformation gradient:

$$T_{ij} = 2C_1 J^{-5/3}\left[B_{ij} - \frac{1}{3}I_1\delta_{ij}\right] + 2C_2 J^{-7/3}\left[I_1 B_{ij} - B_{im}B_{mj} - \frac{2}{3}I_2\delta_{ij}\right] + 2D_1(J-1)\delta_{ij} \tag{42}$$

For $\mathbf{F} = \mathbf{I}$, each of the terms in the brackets (or parentheses) goes to $\mathbf{0}$ (or 0). Subtraction of two numbers that differ in magnitude by a very small number can lead to an undesirable round-off error. Thus, some of the expressions must be implemented in a slightly different manner than simply direct computation.

Given $\bar{\mathbf{F}} - \mathbf{I}$, let us define the following, which are mathematically equivalent to previous relations stated in this document:

$$(\hat{\mathbf{U}} - \mathbf{I}) = \mathbf{D} + \frac{1}{2}\mathbf{D}^2 + \frac{1}{6}\mathbf{D}^3 \tag{43}$$

$$(\tilde{\mathbf{F}} - \mathbf{I}) = (\hat{\mathbf{U}} - \mathbf{I})(\bar{\mathbf{F}} - \mathbf{I}) + (\hat{\mathbf{U}} - \mathbf{I}) + (\bar{\mathbf{F}} - \mathbf{I}) \tag{44}$$

Rename $\tilde{\mathbf{F}}$ as $\mathbf{F}$ for simplicity as before, and

$$(\mathbf{B} - \mathbf{I}) = (\mathbf{F} - \mathbf{I})(\mathbf{F} - \mathbf{I})^T + (\mathbf{F} - \mathbf{I}) + (\mathbf{F} - \mathbf{I})^T \tag{45}$$

$$(\mathbf{B}^2 - \mathbf{I}) = (\mathbf{B} - \mathbf{I})^2 + 2(\mathbf{B} - \mathbf{I}) \tag{46}$$

$$(\mathbf{F}^2 - \mathbf{I}) = (\mathbf{F} - \mathbf{I})^2 + 2(\mathbf{F} - \mathbf{I}) \tag{47}$$

$$I_1 = \mathrm{tr}(\mathbf{B} - \mathbf{I}) + 3 \tag{48}$$

$$I_2 = \frac{1}{2}[(\mathrm{tr}(\mathbf{B} - \mathbf{I}))^2 + 6\mathrm{tr}(\mathbf{B} - \mathbf{I}) - \mathrm{tr}(\mathbf{B}^2 - \mathbf{I}) + 6] \tag{49}$$

Using these relationships, we may recast the expressions in parenthesis at the beginning of this subsection.

$$\mathbf{B} - \frac{1}{3}(\mathrm{tr}\mathbf{B})\mathbf{I} = (\mathbf{B} - \mathbf{I}) - \frac{1}{3}\mathrm{tr}(\mathbf{B} - \mathbf{I})\mathbf{I} \tag{50}$$

$$\begin{aligned} I_1\mathbf{B} - \mathbf{B}^2 - \frac{2}{3}I_2\mathbf{I} &= (\mathbf{B} - \mathbf{I})[\mathrm{tr}(\mathbf{B} - \mathbf{I}) + 1] - (\mathbf{B} - \mathbf{I})^2 \\ &\quad - \mathbf{I}\left[\mathrm{tr}(\mathbf{B} - \mathbf{I}) + \frac{1}{3}(\mathrm{tr}(\mathbf{B} - \mathbf{I}))^2 - \frac{1}{3}\mathrm{tr}(\mathbf{B}^2 - \mathbf{I})\right] \end{aligned} \tag{51}$$

$$J - 1 = \det(\mathbf{F} - \mathbf{I}) + \frac{1}{2}(\mathrm{tr}(\mathbf{F} - \mathbf{I}))^2 - \frac{1}{2}\mathrm{tr}(\mathbf{F}^2 - \mathbf{I}) + 2\mathrm{tr}(\mathbf{F} - \mathbf{I}) \tag{52}$$

These expressions are used to compute $\hat{T}_{ij}$ as well as $\partial\hat{T}_{ij}/\partial J$ in the previous sections. No other computations are affected by this round-off error.

Round off continued

For problems with large rotation increments, the term $\mathbf{F} - \mathbf{I}$ is not necessarily small. A more appropriate term to use as a state variable is $\mathbf{F} - \mathbf{R}$. In order to update this term, however, one must be able to store and update $\mathbf{U} - \mathbf{I}$ and $\mathbf{R}$ on every time step. This is not in general a straightforward task, as a polar decomposition would be required for every time step. This may be something to reconsider in the future, but for double precision arithmetic, the roundoff error is not particularly significant.

Updating state variables

In the spirit of modeling this material by use of incremental kinematics, the deformation gradient should be stored as a state variable. In order to do so, $\mathbf{F}$ must be forward rotated at the end of every time step. Because the state variable is being stored as $\mathbf{F} - \mathbf{I}$, the state variable update is performed as follows $(\mathbf{F}_1 - \mathbf{I}) = \hat{\mathbf{R}}\,[(\mathbf{F_0} - \mathbf{I}) + \mathbf{I}] - \mathbf{I}$. This of course thwarts any efforts toward preventing the round-off errors mentioned above, but again for double precision it is a non-issue. For simplicity's sake in the code, keeping the state variable as $\mathbf{F} - \mathbf{I}$ is still more convenient, though, so that it can be initialized as zero.