Material Models Used in NairnMPM and NairnFEA

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Contents

Chapter 1

Linear Elastic Hypoelastic Materials

1.1 Introduction

The `Isotropic`, `TransIsotropic`, and `Orthotropic` classes all inherit from the `Elastic` class and implement linear elastic materials. The constitutive law is in the `Elastic` class and implemented for an orthotropic material. The isotropic and transversely isotropic materials are special cases of the orthotropic material. In MPM, isotropic materials have a separate constitutive law to enhance efficiency by ignoring terms that only apply to anisotropic materials. For such a material, the 3D stiffness equation in the material axis system is

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy} - \varepsilon_{yy}^{(res)} \\ \varepsilon_{zz} - \varepsilon_{zz}^{(res)} \\ \gamma_{xz} \\ \gamma_{yz} \\ \gamma_{xy} \end{pmatrix} \tag{1.1}$$

The elements of the **C** matrix can be found from all engineering properties. Where $\varepsilon_{ii}^{(res)}$ are residual strains in the normal directions. Here they may be caused by either thermal expansion or moisture expansion:

$$\begin{pmatrix} \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy}^{(res)} \\ \varepsilon_{zz}^{(res)} \end{pmatrix} = \begin{pmatrix} \alpha_{xx}\Delta T + \beta_{xx}\Delta c \\ \alpha_{yy}\Delta T + \beta_{yy}\Delta c \\ \alpha_{zz}\Delta T + \beta_{zz}\Delta c \end{pmatrix} \tag{1.2}$$

where α_{ii} and β_{ii} are thermal and moisture expansion coefficients, and ΔT and Δc are temperature and moisture change from reference conditions. FEA has only thermal expansion while MPM may have both thermal and moisture expansion.

1.2 Generalized Plane Stress Equations

For potential inclusion of through-the-thickness stress, we assume the σ_{zz} is a function of x and y only while $\tau_{xz} = \tau_{yz} = 0$. The code is written to allow σ_{zz} to vary with position, but need to check if any restrictions are variation that make sense for plane stress analysis (*e.g.*, $\nabla^2\sigma_{zz} = 0$). In any case the output σ_{zz} is the average out-if-plane stress through thickness of the model.

Extracting the in-plane strains from the 3D compliance equation and inverting, the 2D, plane stress stiffness equations for in-plane stresses become:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} Q_{xx} & Q_{xy} & 0 \\ Q_{xy} & Q_{yy} & 0 \\ 0 & 0 & Q_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - S_{13}\sigma_{zz} - \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy} - S_{23}\sigma_{zz} - \varepsilon_{yy}^{(res)} \\ \gamma_{xy} \end{pmatrix} \tag{1.3}$$

The elements of the **Q** and **S** matrices are found from

$$Q_{xx} = C_{11} - \frac{C_{13}^2}{C_{33}} = \frac{E_{xx}}{1 - \nu_{xy}\nu_{yx}} \tag{1.4}$$

$$Q_{yy} = C_{22} - \frac{C_{23}^2}{C_{33}} = \frac{E_{yy}}{1 - \nu_{xy}\nu_{yx}} \tag{1.5}$$

$$Q_{xy} = C_{12} - \frac{C_{13}C_{23}}{C_{33}} = \frac{E_{xx}\nu_{yx}}{1 - \nu_{xy}\nu_{yx}} = \frac{E_{yy}\nu_{xy}}{1 - \nu_{xy}\nu_{yx}} \tag{1.6}$$

$$Q_{xyxy} = G_{xy}, \qquad S_{13} = -\frac{\nu_{xz}}{E_{xx}}, \qquad S_{23} = -\frac{\nu_{yz}}{E_{yy}} \tag{1.7}$$

For incremental elasticity calculations in the code, the stress increment is:

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} Q_{xx} & Q_{xy} & 0 \\ Q_{xy} & Q_{yy} & 0 \\ 0 & 0 & Q_{xyxy} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx} - S_{13}d\sigma_{zz} - d\varepsilon_{xx}^{(res)} \\ d\varepsilon_{yy} - S_{23}d\sigma_{zz} - d\varepsilon_{yy}^{(res)} \\ d\gamma_{xy} \end{pmatrix} \tag{1.8}$$

These equation are assuming no rotation off orthotropic axes. See below for off-axis equations.

These terms needed for these calculation for small-strain, anisotropic materials are calculated in `SetAnalysisProps()` as `C11` $= Q_{xx}$, `C12` $= Q_{xy}$, `C22` $= Q_{yy}$, and `C66` $= Q_{xyxy}$. The thermal and moisture expansion coefficients are equal to the material thermal and moisture expansion coefficients and set as `CTE1` $= \alpha_{xx}$, `CTE2` $= \alpha_{yy}$, `CME1` $= \beta_{xx}$, and `CME2` $= \beta_{yy}$, also in `SetAnalysisProps()`. To account for $\sigma_{zz} \neq 0$, `S13` and `S23` are also set in `SetAnalysisProps()`.

In generalized plane stress analysis, σ_{zz} is fixed (at some input function of x and y), but $\varepsilon_{zz} \neq 0$ will depend on other in-plane stresses. The out-of-plane strain increment is found from the 3D stiffness matrix by solving the σ_{zz} equation for ε_{zz}:

$$d\sigma_{zz} = C_{13}(d\varepsilon_{xx} - d\varepsilon_{xx}^{(res)}) + C_{23}(d\varepsilon_{yy} - d\varepsilon_{yy}^{(res)}) + C_{33}(d\varepsilon_{zz} - d\varepsilon_{zz}^{(res)}) \tag{1.9}$$

$$d\varepsilon_{zz} = \frac{1}{C_{33}}d\sigma_{zz} - \frac{C_{13}}{C_{33}}(d\varepsilon_{xx} - d\varepsilon_{xx}^{(res)}) - \frac{C_{23}}{C_{33}}(d\varepsilon_{yy} - d\varepsilon_{yy}^{(res)}) + d\varepsilon_{zz}^{(res)} \tag{1.10}$$

The new terms are set in `SetAnalysisProps()` as `C13` $= -C_{13}/C_{33}$, `C23` $= -C_{23}/C_{33}$, `CTE3` $= \alpha_{zz}$, and `CME3` $= \beta_{zz}$.

1.3 Generalized Plane Strain Equations

For potential inclusion of through-the-thickness strain, we assume the ε_{zz} is a function of x and y only while $\gamma_{xz} = \gamma_{yz} = 0$. The code is written to allow ε_{zz} to vary with position, but need to check if there or any restrictions on variation that make sense for plane strain analysis). In any case the output σ_{zz}

and ε_{zz} is the average out-if-plane strain through thickness of the model. From compliance equation, we solve for σ_{zz}:

$$\begin{aligned} \varepsilon_{zz} &= S_{13}\sigma_{xx} + S_{23}\sigma_{yy} + S_{33}\sigma_{zz} + \varepsilon_{zz}^{(res)} && (1.11) \\ \sigma_{zz} &= -\frac{S_{13}}{S_{33}}\sigma_{xx} - \frac{S_{23}}{S_{33}}\sigma_{yy} + \frac{1}{S_{33}}\left(\varepsilon_{zz} - \varepsilon_{zz}^{(res)}\right) && (1.12) \end{aligned}$$

Substituting into compliance equation leaves equation for in-plane strains

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} S_{11} - \frac{S_{13}^2}{S_{33}} & S_{12} - \frac{S_{13}S_{23}}{S_{33}} & 0 \\ S_{12} - \frac{S_{13}S_{23}}{S_{33}} & S_{22} - \frac{S_{23}^2}{S_{33}} & 0 \\ 0 & 0 & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} + \begin{pmatrix} \varepsilon_{xx}^{(res)} + \frac{S_{13}}{S_{33}}\left(\varepsilon_{zz} - \varepsilon_{zz}^{(res)}\right) \\ \varepsilon_{yy}^{(res)} + \frac{S_{23}}{S_{33}}\left(\varepsilon_{zz} - \varepsilon_{zz}^{(res)}\right) \\ 0 \end{pmatrix} \quad (1.13)$$

Solve for stress and casting in incremental form Reduce 3D stiffness equation to in-plane stresses, the 2D equations are:

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)} + \nu_{zx} d\varepsilon_{zz} \\ d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)} + \nu_{zy} d\varepsilon_{zz} \\ d\gamma_{xy} \end{pmatrix} \quad (1.14)$$

where residual strains now depend on reduced residual strains

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \varepsilon_{xx}^{(res)} + \nu_{zx}\varepsilon_{zz}^{(res)} \\ \varepsilon_{yy}^{(res)} + \nu_{zy}\varepsilon_{zz}^{(res)} \end{pmatrix} \quad (1.15)$$

which is equivalent to using reduced expansion properties

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \alpha_{xx}^{(r)}\Delta T + \beta_{xx}^{(r)}\Delta c \\ \alpha_{yy}^{(r)}\Delta T + \beta_{xx}^{(r)}\Delta c \end{pmatrix} \quad (1.16)$$

The reduced expansion coefficients are

$$\alpha_{xx}^{(r)} = \alpha_{xx} + \nu_{zx}\alpha_{zz}, \;\; \alpha_{yy}^{(r)} = \alpha_{yy} + \nu_{zy}\alpha_{zz}, \;\; \beta_{xx}^{(r)} = \beta_{xx} + \nu_{zx}\beta_{zz}, \;\; \beta_{yy}^{(r)} = \beta_{yy} + \nu_{zy}\beta_{zz} \quad (1.17)$$

These elements are calculated in `SetAnalysisProps()` as `C11` $= C_{11}$, `C12` $= C_{12}$, `C22` $= C_{22}$, and `C66` $= C_{66}$. The reduced expansion coefficients are set as `CTE1` $= \alpha_{xx}^{(r)}$, `CTE2` $= \alpha_{yy}^{(r)}$, `CME1` $= \beta_{xx}^{(r)}$, and `CME2` $= \beta_{yy}^{(r)}$, also in `SetAnalysisProps()`.

The out-of-plane stress is found from the 3D stiffness matrix by setting $\varepsilon_{zz} = 0$:

$$\begin{aligned} d\sigma_{zz} &= C_{13}\left(d\varepsilon_{xx} - (\alpha_{xx}^{(r)} - \nu_{zx}\alpha_{zz})\Delta T - (\beta_{xx}^{(r)} - \nu_{zx}\beta_{zz})\Delta c\right) \\ &\quad + C_{23}\left(d\varepsilon_{yy} - (\alpha_{yy}^{(r)} - \nu_{zy}\alpha_{zz})\Delta T - (\beta_{yy}^{(r)} - \nu_{zy}\beta_{zz})\Delta c\right) + C_{33}\left(d\varepsilon_{zz} - \varepsilon_{zz}^{(res)}\right) \quad (1.18) \end{aligned}$$

The new terms are set in `SetAnalysisProps()` as `C13` $= C_{13}$, `C23` $= C_{23}$, and `C33` $= C_{33}$. Notice that this equation needs actual residual expansion coefficients and thus the reduced expansion coefficients must be *unreduced* by subtracting terms. For these calculations (more details in next section), the following expansion properties are set as `CTE3` $= \alpha_{zz}$, `CME3` $= \beta_{zz}$, `prop1` $= \nu_{zx}$, and `prop2` $= \nu_{zy}$.

1.4 Rotated Stiffness Equations in 2D MPM

For orthotropic materials with material angle not zero, the stiffness equations must be rotated counter-clockwise by the material point angle to transpose to the analysis coordinate systems. The initial material point angle is stored for anisotropic materials. To account for large rotations, the total angle from material axes to current axes must be found by polar decomposition of $\mathbf{F}$ (which can find $\sin\theta$ and $\cos\theta$ easily in 2D). Thus prior to calling `MPMConstitutiveLaw()`, the equations are rotated (if needed) to obtain:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & \texttt{C[1][3]} \\ \texttt{C[1][2]} & \texttt{C[2][2]} & \texttt{C[2][3]} \\ \texttt{C[1][3]} & \texttt{C[2][3]} & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \texttt{C[5][1]}(\sigma_{zz}/\varepsilon_{zz}) - \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy} - \texttt{C[5][2]}(\sigma_{zz}/\varepsilon_{zz}) - \varepsilon_{yy}^{(res)} \\ \gamma_{xx} - \texttt{C[5][3]}(\sigma_{zz}/\varepsilon_{zz}) - \varepsilon_{xy}^{(res)} \end{pmatrix} \tag{1.19}$$

where for plane stress $\texttt{C[5][1]} = \overline{S}_{13}$, $\texttt{C[5][2]} = \overline{S}_{23}$, and $\texttt{C[5][3]} = \overline{S}_{36}$ are rotated elements of the compliance matrix and use σ_{zz} but for plane strain $\texttt{C[5][1]} = \overline{S}_{13}/S_{33}$, $\texttt{C[5][2]} = \overline{S}_{23}/S_{33}$, and $\texttt{C[5][3]} = \overline{S}_{36}S_{33}$ are rotated and normalized elements of the compliance matrix and use ε_{zz}. The rotated residual strains (which become reduced residual strains when in plane strain) are

$$\begin{pmatrix} \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy}^{(res)} \\ \varepsilon_{xy}^{(res)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \texttt{alpha[3]}\Delta T + \texttt{beta[3]}\Delta c \end{pmatrix} \tag{1.20}$$

The rotated elements are found by standard in-plane rotation in the counter-clockwise direction in `FillElasticProperties2D()`. Rotation is only needed for anistotropic materials and thus this method is in the `TransIsotropic` class, which is parent to all anisotropic materials. For isotropic materials, the `C[][]`, `alpha[]`, and `beta[]` elements are calculated once for zero rotation angle in `FillUnrotated-ElasticProperties()`. For MPM, the elements of `C[][]` are also made specific by dividing by material density. The constitutive law should only use specific properties to have the proper specific stress.

Calculation of out-of-plane values requires rotation of the 3D stiffness matrix counter-clockwise around the z axis. The results for plane stress are

$$\begin{aligned} \varepsilon_{zz} \;=\; & \frac{1}{\texttt{C[4][4]}}\sigma_{zz} + \texttt{C[4][1]}(\varepsilon_{xx} - \varepsilon_{xx}^{(res)}) + \texttt{C[4][2]}(\varepsilon_{yy} - \varepsilon_{yy}^{(res)}) \\ & + \texttt{C[4][3]}(\gamma_{xy} - \varepsilon_{xy}^{(res)}) + \varepsilon_{zz}^{(res)} \end{aligned} \tag{1.21}$$

where

$$\texttt{C[4][4]} = C_{33} = \texttt{C33} \tag{1.22}$$

$$\texttt{C[4][1]} = -\left(\frac{C_{13}}{C_{33}}\cos^2\theta + \frac{C_{23}}{C_{33}}\sin^2\theta\right) = \texttt{C13}\cos^2\theta + \texttt{C23}\sin^2\theta \tag{1.23}$$

$$\texttt{C[4][2]} = -\left(\frac{C_{13}}{C_{33}}\sin^2\theta + \frac{C_{23}}{C_{33}}\cos^2\theta\right) = \texttt{C13}\sin^2\theta + \texttt{C23}\cos^2\theta \tag{1.24}$$

$$\texttt{C[4][3]} = \left(\frac{C_{13}}{C_{33}} - \frac{C_{23}}{C_{33}}\right)\sin\theta\cos\theta = -(\texttt{C13} - \texttt{C23})\sin\theta\cos\theta \tag{1.25}$$

and $\texttt{CTE3} = \texttt{alpha[4]} = \alpha_{zz}$ and $\texttt{CME3} = \texttt{beta[4]} = \beta_{zz}$ hold out-of-plane thermal expansion coefficients needed to find $\varepsilon_{zz}^{(res)}$, which was defined earlier.

The problem in plane strain is that the calculation of σ_{zz} requires rotated expansion coefficients while the `alpha[1]` to `alpha[3]` and `beta[1]` to `beta[3]` have rotated *reduced* expansion coefficients.

The solution is to define some new terms such that

$$\begin{aligned}\sigma_{zz} &= \texttt{C[4][1]}(\varepsilon_{xx}-(\varepsilon_{xx}^{(res,r)}-\texttt{alpha[5]}\varepsilon_{zz}^{(res)}))+\texttt{C[4][2]}(\varepsilon_{yy}-(\varepsilon_{yy}^{(res,r)}-\texttt{alpha[6]}\varepsilon_{zz}^{(res)}))\\ &\quad+\texttt{C[4][3]}(\gamma_{xx}-(\varepsilon_{xy}^{(res,r)}-\texttt{alpha[7]}\varepsilon_{zz}^{(res)}))-\texttt{C[4][4]}\varepsilon_{zz}^{(res)} \end{aligned} \tag{1.26}$$

where

$$\rho\,\texttt{C[4][1]} = C_{13}\cos^2\theta + C_{23}\sin^2\theta = \texttt{C13}\cos^2\theta + \texttt{C23}\sin^2\theta \tag{1.27}$$

$$\rho\,\texttt{C[4][2]} = C_{13}\sin^2\theta + C_{23}\cos^2\theta = \texttt{C13}\sin^2\theta + \texttt{C23}\cos^2\theta \tag{1.28}$$

$$\rho\,\texttt{C[4][3]} = -(C_{13}-C_{23})\sin\theta\cos\theta = -(\texttt{C13}-\texttt{C23})\sin\theta\cos\theta \tag{1.29}$$

$$\rho\,\texttt{C[4][4]} = C_{33} \tag{1.30}$$

$$\texttt{alpha[5]} = \nu_{zx}\cos^2\theta + \nu_{zy}\sin^2\theta = \texttt{prop1}\cos^2\theta + \texttt{prop2}\sin^2\theta \tag{1.31}$$

$$\texttt{alpha[6]} = \nu_{zx}\sin^2\theta + \nu_{zy}\cos^2\theta = \texttt{prop1}\sin^2\theta + \texttt{prop2}\cos^2\theta \tag{1.32}$$

$$\texttt{alpha[7]} = -2\left(\nu_{zx}-\nu_{zy}\right)\sin\theta\cos\theta = -2(\texttt{prop1}-\texttt{prop2})\sin\theta\cos\theta \tag{1.33}$$

Again, $\texttt{CTE3} = \texttt{alpha[4]} = \alpha_{zz}$ and $\texttt{CME3} = \texttt{beta[4]} = \beta_{zz}$ hold out-of-plane expansion coefficients needed to find $\varepsilon_{zz}^{(res)}$, which was defined earlier. In these terms, $\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)}$ (and similarly for $(yy, 6)$ and $(xy, 7)$ pairs) evaluate to the rotated, but *unreduced* expansion strains.

1.5 Rotated Stiffness Equations in 3D MPM

To be added.

1.6 Rotated Stiffness Equations in FEA

To be added.

1.7 Two-State Isotropic Material

The `BistableIsotropic` class inherits from `Isotropic`. It allows two different isotropic states and transitions between the states based on various criteria. The two options are to have a jump to a new linear stress-strain curve (`DILATION_RULE`) or to simply change the slope (`DISTORTION_RULE` or `VONMISES_RULE`). When jumping to a new curve (`DILATION_RULE`), the deformed state can additionally define a new origin by adding an offset volumetric strain. The only new calculations needed are to change properties when a transition occurs and if there is a new stress-strain curve to calculate a jump in stresses to the new curve. The 3D stiffness equations with an offset volumetric strain for an isotropic material are

$$\begin{pmatrix}\sigma_{xx}\\ \sigma_{yy}\\ \sigma_{zz}\\ \tau_{xz}\\ \tau_{yz}\\ \tau_{xy}\end{pmatrix} = \begin{pmatrix}C_{11} & C_{12} & C_{12} & 0 & 0 & 0\\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0\\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & C_{66} & 0 & 0\\ 0 & 0 & 0 & 0 & C_{66} & 0\\ 0 & 0 & 0 & 0 & 0 & C_{66}\end{pmatrix}\begin{pmatrix}\varepsilon_{xx}-\frac{\Delta}{3}-\varepsilon^{(res)}\\ \varepsilon_{yy}-\frac{\Delta}{3}-\varepsilon^{(res)}\\ \varepsilon_{zz}-\frac{\Delta}{3}-\varepsilon^{(res)}\\ \gamma_{xz}\\ \gamma_{yz}\\ \gamma_{xy}\end{pmatrix} \tag{1.34}$$

where $\varepsilon^{(res)} = \alpha\Delta T + \beta\Delta c$. Whenever a change in state occurs in the `DILATION_RULE`, these equations must be used to recalculate all components of stress.

1.7.1 Plane Stress Equations

The plane stress stiffness equations for in-plane stresses are

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} Q_{xx} & Q_{xy} & 0 \\ Q_{xy} & Q_{xx} & 0 \\ 0 & 0 & Q_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \gamma_{xx} \end{pmatrix} \tag{1.35}$$

with out-of-plane strain given by

$$\varepsilon_{zz} = -\frac{C_{12}}{C_{11}}(\varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)}) - \frac{C_{12}}{C_{11}}(\varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)}) + \frac{\Delta}{3} + \varepsilon^{(res)} \tag{1.36}$$

For the super-class `Isotropic` material, the needed terms are stored as `C[1][1]` $= $ `C[2][2]` $= Q_{xx}/\rho$, `C[1][2]` $= Q_{xy}/\rho$, `C[3][3]` $= Q_{xyxy}/\rho$, `C[4][1]` $=$ `C[4][2]` $= -C_{12}/C_{11}$, `alpha[1]` $=$ `alpha[2]` $=$ `alpha[4]` $=$ `CTE3` $= \alpha$, `beta[1]` $=$ `beta[2]` $=$ `beta[4]` $=$ `CME3` $= \beta$, `C[1][3]` $=$ `C[2][3]` $=$ `alpha[3]` $=$`beta[3]` $= 0$, and `normOffset` $= \Delta/3$.

1.7.2 Plane Strain Equations

The plane strain stiffness equations for in-plane stresses are

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \frac{\Delta}{3}(1+\nu) - \varepsilon^{(res,r)} \\ \varepsilon_{yy} - \frac{\Delta}{3}(1+\nu) - \varepsilon^{(res,r)} \\ \gamma_{xx} \end{pmatrix} \tag{1.37}$$

where $\varepsilon^{(res,r)} = \alpha^{(r)}\Delta T + \beta^{(r)}\Delta c$. In other words, a reduced offset and residual strains are needed. The out-of-plane stress is found from 3D equation and without reduced terms:

$$\sigma_{zz} = C_{12}\left(\varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)}\right) + C_{12}\left(\varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)}\Delta T\right) - C_{11}\left(\frac{\Delta}{3} + \varepsilon^{(res)}\right) \tag{1.38}$$

For the super-class `Isotropic` material, the needed terms are stored as `C[1][1]` $=$ `C[2][2]` $=$ `C[4][4]` $= C_{11}/\rho$, `C[1][2]` $= C_{12}/\rho$, `C[3][3]` $= C_{66}/\rho$, `C[4][1]` $=$ `C[4][2]` $= C_{12}/\rho$, `alpha[1]` $=$ `alpha[2]` $= \alpha(1+\nu)$, `beta[1]` $=$ `beta[2]` $= \beta(1+\nu)$, `alpha[4]` $=$ `CTE3` $= \alpha$, `beta[4]` $=$ `CME3` $= \beta$, `alpha[5]` $=$ `alpha[6]` $= \nu$, `C[1][3]` $=$ `C[2][3]` $=$ `C[4][3]` $=$ `alpha[3]` $=$ `alpha[7]` $= 0$, `normOffset` $= \Delta/3$, and `nu` $= \nu$.

1.7.3 Special Cases for $E = 0$

If either K or G in any state is zero then the tensile modulus E is also zero. Although this state is easy to derive in theory, in practice, it rarely gives useful results in dynamic MPM (except maybe as an inclusion in a composite material). A second problem is that it requires special cases to make it work with the super `Isotropic` class because that class has equations requiring $E \neq 0$. For these reasons, NairnMPM does not support zero modulus states in this material. It is easy to approximate such a state simply by setting K and/or G to a very small number.

Chapter 2

Plasticity Materials

2.1 Introduction

This sections gives general plasticity results, which are later specialized for implementation in various material types. Some parts were adapted from text book "Computational methods for plasticity: theory and applications" (Eduardo de Souza Neto, Djordje Peric, and David Owens, John Wiley & Sons, 2008).

Plastic materials are assumed to have a Helmholz free energy (per unit volume) that depends on $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_p$, $\boldsymbol{\alpha}$, and T:

$$A(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\alpha}, T) = A_e(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p, T) + A_p(\boldsymbol{\alpha}, T) = A_e(\boldsymbol{\varepsilon}^e, T) + A_p(\boldsymbol{\alpha}, T) \tag{2.1}$$

Here $\boldsymbol{\varepsilon}$ is total strain, $\boldsymbol{\varepsilon}^p$ is plastic strain, and $\boldsymbol{\alpha}$ are internal variables, and T is temperature (A is ψ in Neto and that is free energy per unit mass). The elastic strain is $\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p$. The stress, $\boldsymbol{\sigma}$, and plastic forces, $\boldsymbol{\psi}$ (which are $\boldsymbol{A}$ in Neto), are found from

$$\boldsymbol{\sigma} = \left(\frac{\partial A_e}{\partial \boldsymbol{\varepsilon}^e}\right)_{\boldsymbol{\alpha},T} \quad \text{and} \quad \boldsymbol{\psi} = \left(\frac{\partial A_p}{\partial \boldsymbol{\alpha}}\right)_{\boldsymbol{\varepsilon}^e,T} \tag{2.2}$$

The plastic dissipation function is

$$D^p = \sigma \cdot \frac{d\varepsilon^p}{dt} + \boldsymbol{\psi} * \frac{d\boldsymbol{\alpha}}{dt} \tag{2.3}$$

For linear elastic, small strain materials:

$$A_e(\boldsymbol{\varepsilon}^e, T) = \frac{1}{2}\varepsilon^e \cdot \mathbf{C}\varepsilon^e \tag{2.4}$$

(Neto uses D^e for $\mathbf{C}$). For isotropic materials, the energy becomes

$$A_e(\boldsymbol{\varepsilon}^e, T) = G\varepsilon^d \cdot \varepsilon^d + \frac{1}{2}K(\varepsilon^v)^2 \tag{2.5}$$

where G and K are shear and bulk moduli, ε^d is deviatoric, elastic strain, and ε^v is the dilational, elastic strain. For these energies, the stress is

$$\boldsymbol{\sigma} = \mathbf{C}\varepsilon^e \tag{2.6}$$

For isotropic materials, the stress becomes

$$\boldsymbol{\sigma} = 2G\varepsilon^d + K\varepsilon^v \mathsf{I} \tag{2.7}$$

Next, let $\Phi(\boldsymbol{\sigma}, \boldsymbol{\psi})$ be a plastic potential function that depends on components of stress and plastic forces. The potential function is defined such that $\Phi = 0$ is the yield surface, $\Phi < 0$ is the elastic region,

and $\Phi > 0$ is not allowed. Plasticity is characterized by defining evolution laws for plastic strain (ε_p) and hardening variables ($\boldsymbol{\alpha}$). To start with general expressions, the evolution laws are:

$$d\boldsymbol{\varepsilon}^p = \lambda \boldsymbol{N}(\boldsymbol{\sigma}, \boldsymbol{\psi}) \quad \text{and} \quad d\alpha = \lambda \boldsymbol{H}(\boldsymbol{\sigma}, \boldsymbol{\psi}) \tag{2.8}$$

where $\boldsymbol{N}(\boldsymbol{\sigma}, \boldsymbol{\psi})$ is the flow vector and $\boldsymbol{H}(\boldsymbol{\sigma}, \boldsymbol{\psi})$ is the generalized hardening modulus (also $d\boldsymbol{\varepsilon}^p$ is $\dot{\boldsymbol{\varepsilon}}^p$, $d\boldsymbol{\alpha}$ is $\dot{\boldsymbol{\alpha}}$, and λ is $\dot{\gamma}$ in Neto). Finally, the yield surface is described by loading/unloading conditions:

$$\Phi \leq 0, \qquad \lambda \geq 0, \qquad \text{and} \qquad \Phi\lambda = 0 \tag{2.9}$$

It is usual to assume $\boldsymbol{N}$ and $\boldsymbol{H}$ are defined by a plastic potential $\Psi(\boldsymbol{\sigma}, \boldsymbol{\psi})$ using:

$$\boldsymbol{N}(\boldsymbol{\sigma}, \boldsymbol{\psi}) = \frac{\partial \Psi}{\partial \boldsymbol{\sigma}} \quad \text{and} \quad \boldsymbol{H}(\boldsymbol{\sigma}, \boldsymbol{\psi}) = -\frac{\partial \Psi}{\partial \boldsymbol{\psi}} \tag{2.10}$$

If $\Psi = \Phi$, the plastic flow is associative plasticity, otherwise it is non-associative plasticity.

2.2 Incremental Plasticity Constitutive Problem

Once it is determined (by trial stress state), that plastic deformation is occurring, the task is to solve for updated state using:

$$\begin{aligned}
\Phi(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\psi}_{n+1}) &= 0 && (2.11)\\
d\boldsymbol{\varepsilon}^p &= \lambda \boldsymbol{N}(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\psi}_{n+1}) && (2.12)\\
d\boldsymbol{\varepsilon}^e &= d\boldsymbol{\varepsilon}^{tot} - d\boldsymbol{\varepsilon}^p && (2.13)\\
\boldsymbol{\alpha}_{n+1} &= \boldsymbol{\alpha}_n + \lambda \boldsymbol{H}(\boldsymbol{\sigma}_{n+1}, \boldsymbol{\psi}_{n+1}) && (2.14)\\
\boldsymbol{\sigma}_{n+1} &= \left(\frac{\partial A_e}{\partial \boldsymbol{\varepsilon}^e_{n+1}} \right)_{\boldsymbol{\alpha}_{n+1}, T} = \boldsymbol{\sigma}_n + \mathbf{C} d\boldsymbol{\varepsilon}^e && (2.15)\\
\boldsymbol{\psi}_{n+1} &= \left(\frac{\partial A_p}{\partial \boldsymbol{\alpha}_{n+1}} \right)_{\boldsymbol{\varepsilon}^e_{n+1}, T} && (2.16)
\end{aligned}$$

Ideally this problem is solved implicitly.

As a return mapping method, the algorithm is expression:

1. Give a total strain increment of $d\boldsymbol{\varepsilon}^{tot}$, get trial update of

$$\boldsymbol{\varepsilon}^{e,trial}_{n+1} = \varepsilon^e_n + d\boldsymbol{\varepsilon}^{tot} \quad \text{and} \quad \boldsymbol{\alpha}^{trial}_{n+1} = \boldsymbol{\alpha}_n \tag{2.17}$$

   and find corresponding trial $\boldsymbol{\sigma}$ and $\boldsymbol{\psi}$.

2. If $\Phi(\boldsymbol{\sigma}^{trial}, \boldsymbol{\psi}^{trial}) \leq 0$ than the step is elastic. Accept the trial state and update is done.

3. Otherwise, solve:

$$\begin{pmatrix} \boldsymbol{\varepsilon}^e_{n+1} - \boldsymbol{\varepsilon}^{e,trial}_{n+1} + \lambda \boldsymbol{N}_{n+1} \\ \boldsymbol{\alpha}_{n+1} - \boldsymbol{\alpha}^{trial}_{n+1} - \lambda \boldsymbol{H}_{n+1} \\ \Phi(\sigma_{n+1}, \boldsymbol{\psi}_{n+1}) \end{pmatrix} = \begin{pmatrix} \lambda \boldsymbol{N}_{n+1} - d\boldsymbol{\varepsilon}^p \\ d\boldsymbol{\alpha} - \lambda \boldsymbol{H}_{n+1} \\ \Phi(\sigma_{n+1}, \boldsymbol{\psi}_{n+1}) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.18}$$

   for $\boldsymbol{\varepsilon}^e_{n+1}$, $\boldsymbol{\alpha}_{n+1}$, and λ with

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_n + \mathbf{C} d\boldsymbol{\varepsilon}^e_{n+1} \quad \text{and} \quad \boldsymbol{\psi}_{n+1} = \left(\frac{\partial A_p}{\partial \boldsymbol{\alpha}_{n+1}} \right)_{\boldsymbol{\varepsilon}^e_{n+1}, T} \tag{2.19}$$

2.3 IsoPlasticity Material

This material implements associative, J_2 plasticity for isotropic materials with isotropic hardening. This material uses a single internal variable, α, and assumes the plastic potential is a function only of $J_2 = (1/2)\|\mathbf{s}\|^2$ expressed as

$$\Phi = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}K(\alpha) = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}(\sigma_y + \psi) \tag{2.20}$$

where $\mathbf{s}$ is the deviatoric stress tensor and $K(\alpha)$ defines the tensile yield stress as a function of the hardening variable and possibly other variables (*e.g.*, plastic strain rate or temperature, or probably not pressure). The plastic force, ψ, as function of α is

$$\psi = K(\alpha) - \sigma_y \quad \text{and} \quad A_p = \int_0^\alpha (K(\alpha) - \sigma_y) d\alpha \tag{2.21}$$

All materials that fit this mold are handled in `NairnMPM` by the `IsoPlasticity` class. The implementation of hardening law ($K(\alpha)$) is handled by a separate subclass of the `HardeningLawBase` class. Combining `IsoPlasticity` class with various hardening laws gives a series of materials. The only materials that need to subclass `IsoPlasticity` is if they need a different equation of state to handle elastic parts differently.

For pure shear loading, $\|\mathbf{s}\| = \sqrt{2}\tau$ and yielding occurs when $\tau = \tau_y = K(\alpha)/\sqrt{3}$. For uniaxial loading of σ, the deviatoric stress is:

$$\mathbf{s} = \begin{pmatrix} \frac{2}{3}\sigma & 0 & 0 \\ 0 & -\frac{1}{3}\sigma & 0 \\ 0 & 0 & -\frac{1}{3}\sigma \end{pmatrix}, \quad \|\mathbf{s}\|^2 = \frac{2}{3}\sigma^2, \quad \text{and} \quad J_2 = \frac{1}{3}\sigma^2 \tag{2.22}$$

For this loading, yielding occurs when $\sigma = \sigma_y = K(\alpha)$.

In terms of the deviatoric stress

$$2J_2 = \|\mathbf{s}\|^2 = s_{xx}^2 + s_{yy}^2 + s_{zz}^2 + 2s_{xy}^2 + 2s_{xz}^2 + 2s_{yz}^2 \tag{2.23}$$

During plastic deformation, the first equation in return mapping simplifies to:

$$d\boldsymbol{\varepsilon}^p = \lambda \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} = \lambda \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} = \lambda \mathbf{n} \tag{2.24}$$

where $\mathbf{s}_{trial}$ is the deviatoric stress calculated by assuming no plastic deformation. Importantly, this normal is constant, which greatly simplifies radial return mapping for this type of material. The second return mapping equation simplifies, or associative plasticity, to:

$$d\alpha = \lambda \boldsymbol{H} = -\lambda \frac{\partial \Phi}{\partial \psi} = \lambda \sqrt{\frac{2}{3}} \tag{2.25}$$

Since $\|d\boldsymbol{\varepsilon}^p\| = \|\lambda(\partial\Phi/\partial\boldsymbol{\sigma})\| = \lambda$, this result corresponds to

$$d\alpha = \sqrt{\frac{2}{3}}\|d\boldsymbol{\varepsilon}^p\| \tag{2.26}$$

where $\sqrt{\frac{2}{3}}\|d\boldsymbol{\varepsilon}^p\|$ is known as the equivalent plastic strain increment. In other words, α is the cumulative equivalent plastic strain. During uniaxial plastic deformation, the equivalent plastic strain will equal the axial plastic strain (*i.e.* when $d\varepsilon_{xx} = d\varepsilon$ and $d\varepsilon_{yy} = d\varepsilon_{zz} = -d\varepsilon/2$, $\sqrt{\frac{2}{3}}\|d\boldsymbol{\varepsilon}^p\| = d\varepsilon$).

Once λ is known, the final deviatoric stress is written as

$$\mathbf{s} = \mathbf{s}_{trial} - \lambda 2G\mathbf{n} = \left(1 - \frac{\lambda 2G}{\|\mathbf{s}_{trial}\|}\right)\mathbf{s}_{trial} \tag{2.27}$$

which by using $\mathbf{s}_{trial} \cdot \mathbf{s}_{trial} = \|\mathbf{s}_{trial}\|^2$, $\mathbf{s}_{trial} \cdot \mathbf{n} = \|\mathbf{s}_{trial}\|$, and $\mathbf{n} \cdot \mathbf{n} = 1$, leads to

$$\|\mathbf{s}\| = \|\mathbf{s}_{trial}\| - \lambda 2G \qquad \text{and} \qquad \frac{\mathbf{s}}{\|\mathbf{s}\|} = \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} \tag{2.28}$$

which confirms that normal is independent of λ.

The final return mapping equation is used to find λ. The above results simplify it to depend only on $\|\mathbf{s}_{trial}\|$, G, and the hardening law:

$$\Phi_{n+1} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}K(\alpha_{n+1}) = \|\mathbf{s}_{trial}\| - \lambda 2G - \sqrt{\frac{2}{3}}K(\alpha_{n+1}) = 0 \tag{2.29}$$

Sometimes this equation can be solved analytically (see below). Otherwise is can be solved using Newton's method. Start with $\Phi^{(0)} = \Phi^{trial}$ and then iterate using:

$$\frac{d\Phi^{(k)}}{d\lambda} = -2G - \sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = -2G - \frac{2}{3}\frac{dK(\alpha^{(k)})}{d\alpha} \tag{2.30}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)}\sqrt{\frac{2}{3}} \tag{2.31}$$

where $K'(\alpha^{(k)}) = dK(\alpha^{(k)})/d\alpha$ is the derivative with respect to α. This solution is implemented by hardening law classes. The `HardeningLawBase` class solves this equation numerically by having a subclass providing for calculation of $K(\alpha^{(k)})$ (in `GetYield()`) and $\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda}$ (in `GetKPrime()`). The base class uses Newton's method with bracketing; the bracketing is needed because some yield functions are unstable by the unbracketed Newton's method. The solution is done in `SolveForLambdaBracketed()` as follows:

1. The result for $\lambda = 0$ is known to have $\Phi > 0$.
2. Set the plastic strain rate $d\alpha/dt$ to 1 sec^{-1} where dt is time step and then trial $\lambda = d\alpha/\sqrt{2/3}$.
3. Evaluate Φ; if it is negative, λ is between current value and previous order of magnitude; if it is positive, increase the strain rate by a factor or 10 and go back to beginning of this step.

If any subclass hardening law can bracket the solution faster (or find the solution with an unbracketed method), it can override `SolveForLambdaBracketed()` and provide a new method (which may be as simple as calling the unbracketed method in `SolveForLambda()` or devising a better bracketing method in `BracketSolution()`). For example, for a linear hardening law, λ can be found in a closed-form expression — when $K(\alpha) = \sigma_Y + E_p\alpha$, the task is to solve

$$\Phi = \|\mathbf{s}_{trial}\| - \lambda 2G - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\left(\alpha^0 + \lambda\sqrt{\frac{2}{3}}\right)\right) = 0 \tag{2.32}$$

The analytical solution is

$$\lambda = \frac{\|\mathbf{s}_{trial}\| - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\alpha^0\right)}{2G + \frac{2E_p}{3}} \tag{2.33}$$

2.3.1 Plane Strain and Axisymmetric Analysis

Plane strain and axisymmetric analysis can follow the above analysis. For isotropic material models, it is convenient to formulate in terms of bulk and shear moduli (K and G) and track pressure and deviatoric stress. The stress update is

$$\frac{\Delta V}{V} = d\varepsilon_{xx} + d\varepsilon_{yy} + d\varepsilon_{zz} - 3d\varepsilon^{(res)} \tag{2.34}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.35}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i=j=x,y,z \tag{2.36}$$

$$d\tau_{xy} = ds_{xy} = Gd\gamma_{xy} \tag{2.37}$$

where

$$d\varepsilon_{xx}^{(tot)} = d\varepsilon_{xx} - d\varepsilon^{(res)}, \quad d\varepsilon_{yy}^{(tot)} = d\varepsilon_{yy} - d\varepsilon^{(res)}, \quad \text{and} \quad d\varepsilon_{zz}^{(tot)} = d\varepsilon_{zz} - d\varepsilon^{(res)} \tag{2.38}$$

are the strain increments relative to the increment in residual strain (note that in plane strain, $d\varepsilon_{zz} = 0$, but it may be nonzero when axisymmetric). For isotropic materials, only normal residual strains exist and they are all equal to

$$d\varepsilon^{(res)} = \alpha\Delta T + \beta\Delta c \tag{2.39}$$

If the updated stress has $\Phi < 0$, the analysis uses the new stress state.

If $\Phi > 0$, the equations in the previous section are used to find λ. Once λ is known, the initial update is modified using

$$ds_{ij} = ds_{ij}^{trial} - 2Gd\varepsilon_{ij}^{p} \tag{2.40}$$

while the pressure update is unchanged. By including σ_{zz} in the calculations, the out-of-plane stress is correctly updated. In general, the plastic strain will include plastic strain in the z direction, even in plane strain. To keep zero total strain when in plane strain analysis, the out-of-plane elastic strain update will be

$$d\varepsilon_{ij}^{e} = -d\varepsilon_{ij}^{p} \tag{2.41}$$

For the `IsoPlasticity` class, $K =$ `Kred`, $G =$ `Gred`, $\alpha =$ `CTE3`, and $\beta =$ `CME3`. The default implementation assumes these are constant and they are calculated once in `VerifyAndLoadProperties()`. A subclass can implement non-linear materials two ways. To let K, G, α, and β, depend on particle state, calculate their state-dependent values in `LoadMechanicalProps()` and/or `GetTransportProps()`. An alternative approach for more complicated materials is to replace the pressure calculation by overriding `UpdatePressure()` . This method is called after finding $\Delta V/V$, but before any other calculations. It must update the particle pressure and particle strain energy due to dilation. It should also calculate G (in `Gred`) if it depends on particle state. It need not calculate K (in `Kred`) because it is not needed after new pressure is found.

2.3.2 Plane Stress Analysis

Unfortunately, plane stress analysis requires some additional steps and always requires numerical solution for λ. First, by requiring $\sigma_{zz} = 0$, the 3D equations can be solved to show

$$d\varepsilon_{zz}^{(tot)} = -\frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.42}$$

Using this relation, the stress update for the in-plane terms only are

$$\frac{\Delta V}{V} = d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)} + d\varepsilon_{zz}^{(tot)} = \left(\frac{1-2\nu}{1-\nu}\right)\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.43}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.44}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i = j = x, y \tag{2.45}$$

$$ds_{zz}^{trial} = ds_{zz} = dP \tag{2.46}$$

$$d\tau_{xy}^{trial} = ds_{xy}^{trial} = Gd\gamma_{xy} \tag{2.47}$$

$$\tag{2.48}$$

The `IsoPlasticity` class is based on K and G (in `Kred` and `Gred`). For calculation efficiency, two above terms and one term defined below are stored in variables:

$$\texttt{psRed} = \left(\frac{1-2\nu}{1-\nu}\right) = \frac{1}{\frac{K}{2G}+\frac{2}{3}} \tag{2.49}$$

$$\texttt{psLr2G} = \frac{\nu}{1-\nu} = \frac{\frac{K}{2G}-\frac{1}{3}}{\frac{K}{2G}+\frac{2}{3}} \tag{2.50}$$

$$\texttt{psKred} = \frac{E}{3(1-\nu)} = K * \texttt{psRed} = \frac{K}{\frac{K}{2G}+\frac{2}{3}} \tag{2.51}$$

Note that plane stress analysis assumes incrementally linear-elastic response (although the linear terms can depend on particle state) and also needs to know `psRed` *before* finding the pressure change. Materials that override `LoadMechanicaProps()` must calculate `psRed`, `psLr2G`, and `psKred` along with `Kred` and `Gred`. Materials that override `UpdatePressure()` instead will need to deal with these terms differently. For such materials, the incremental volumetric strain passed to `UpdatePressure()` depends on `psRed` (see Eq. (2.43)). The best approach is to set `psRed` $= 1$ and then scale `delV` by the current $(1-2\nu)/(1-\nu)$ in `UpdatePressure()`. That method can leave `psRed` $= 1$ (because it is no longer needed) and calculate `psLr2G` (for normal stress update) and `psKred` (for finding λ) needed in subsequent calculations. It should also calculate `Gred`, but `Kred` is not needed.

When $\Phi > 0$, the process (following Simo and Hughes), effectively (or equivalently) revises Φ using squares to be

$$\Phi = \|\mathbf{s}\|^2 - \frac{2}{3}K^2(\alpha) = \sigma\mathbf{P}\sigma - \frac{2}{3}K^2(\alpha) \tag{2.52}$$

where $\mathbf{P}$ is a transformation matrix on the plane stress vector $\sigma = (\sigma_{xx}, \sigma_{yy}, \tau_{xy})$ given by

$$\mathbf{P} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & 0 \\ -\frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{2.53}$$

such that $\sigma\mathbf{P}\sigma = \|\mathbf{s}\|^2$. The plastic strain update from this Φ, and using engineering shear strain, is

$$(d\varepsilon_{xx}^p, d\varepsilon_{yy}^p, d\gamma_{xy}^p) = \lambda\frac{\partial\Phi}{\partial\boldsymbol{\sigma}} = \lambda\mathbf{P}\sigma \tag{2.54}$$

Now, in this flow theory, the total volume change due to plastic strains is zero; thus this plastic strain increment implies $d\varepsilon_{zz}^p = -(d\varepsilon_{xx}^p + d\varepsilon_{yy}^p)$. The full 3D plastic strain increment tensor using tensorial

strains is

$$d\boldsymbol{\varepsilon}^p = \lambda \begin{pmatrix} \frac{1}{3}(2\sigma_{xx}-\sigma_{yy}) & \tau_{xy} & 0 \\ \tau_{xy} & \frac{1}{3}(2\sigma_{yy}-\sigma_{xx}) & 0 \\ 0 & 0 & -\frac{1}{3}(\sigma_{xx}+\sigma_{yy}) \end{pmatrix} \tag{2.55}$$

This traceless tensor has inner product

$$\begin{aligned} \|d\boldsymbol{\varepsilon}^p\|^2 &= \lambda^2\left(\frac{2}{3}(\sigma_{xx}^2+\sigma_{yy}^2-\sigma_{xx}\sigma_{yy})+2\tau_{xy}^2\right) = \lambda^2\sigma\mathbf{P}\sigma & (2.56)\\ &= \lambda^2\left(s_{xx}^2+s_{yy}^2+s_{zz}^2+2s_{xy}^2\right) & (2.57)\end{aligned}$$

Requiring $d\alpha$ to equal the equivalent plastic strain increment (as it does in plane strain and 3D), leads to

$$d\alpha = \sqrt{\frac{2}{3}}\lambda\sqrt{\sigma\mathbf{P}\sigma} \tag{2.58}$$

When $\Phi > 0$, the task is to find the $(n+1)^{st}$ stress and strain state in terms of the n^{th} state. In terms of the to-be-determined λ, the stress update is

$$\begin{aligned} \sigma_{n+1}^{trial} &= \sigma_n + \mathbf{C}(d\varepsilon_{xx}^{(tot)}, d\varepsilon_{yy}^{(tot)}, d\gamma_{xy}^{(tot)}) & (2.59)\\ \sigma_{n+1} &= \sigma_{n+1}^{trial} - \mathbf{C}d\boldsymbol{\varepsilon}^p = \sigma_{n+1}^{trial} - \mathbf{C}\lambda\mathbf{P}\sigma_{n+1} & (2.60)\end{aligned}$$

where $\mathbf{C}$ is the plane stress stiffness matrix:

$$\mathbf{C} = \begin{pmatrix} \frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\ \frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & G \end{pmatrix} \quad \text{with} \quad \mathbf{C}^{-1} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & 0 \\ 0 & 0 & \frac{1}{G} \end{pmatrix} \tag{2.61}$$

Solving the second equation the required stress is:

$$\sigma_{n+1} = \left[\mathbf{C}^{-1}+\lambda\mathbf{P}\right]^{-1}\mathbf{C}^{-1}\sigma_{n+1}^{trial} \tag{2.62}$$

This general result applied to isotropic materials leads to

$$\begin{aligned} \sigma_{xx}^{(n+1)}+\sigma_{yy}^{(n+1)} &= \frac{1}{1+\frac{E}{3(1-\nu)}\lambda}\left(\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right) & (2.63)\\ -\sigma_{xx}^{(n+1)}+\sigma_{yy}^{(n+1)} &= \frac{1}{1+2G\lambda}\left(-\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right) & (2.64)\\ \tau_{xy}^{(n+1)} &= \frac{\tau_{xy}^{trial}}{1+2G\lambda} & (2.65)\end{aligned}$$

and

$$\|\mathbf{s}\|^2 = \sigma_{n+1}\mathbf{P}\sigma_{n+1} = \frac{\frac{1}{6}\left(\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right)^2}{\left(1+\frac{E}{3(1-\nu)}\lambda\right)^2} + \frac{\frac{1}{2}\left(-\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right)^2+2\tau_{xy}^{trial\,2}}{(1+2G\lambda)^2} \tag{2.66}$$

The task is to find λ by Newton's method with the key equations being:

$$\Phi^{(k)} = \frac{1}{2}\|\mathbf{s}^{(k)}\|^2 - \frac{1}{3}K^2(\alpha^{(k)}) = 0 \tag{2.67}$$

$$\frac{d\Phi^{(k)}}{d\lambda} = -\left[\frac{E}{3(1-\nu)}\frac{\frac{1}{6}\left(\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right)^2}{\left(1+\frac{E}{3(1-\nu)}\lambda^{(k)}\right)^3} + 2G\frac{\frac{1}{2}\left(-\sigma_{xx}^{trial}+\sigma_{yy}^{trial}\right)^2 + 2\tau_{xy}^{trial\,2}}{\left(1+2G\lambda^{(k)}\right)^3}\right] - \frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} \tag{2.68}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)}\sqrt{\frac{2}{3}}\|\mathbf{s}^{(k+1)}\| \tag{2.69}$$

A `HardeningLawBase` subclass attached to an `IsoPlasticity` material can implement this numerical solution simply by providing for calculation of $K(\alpha^{(k)})$ (in `GetYield()`) and $\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda}$ (in `GetK2Prime()`). To keep the analysis in terms of K and G, the modulus term above can be found from

$$\texttt{psKred} = \frac{E}{3(1-\nu)} = \frac{K}{\frac{K}{2G}+\frac{2}{3}} \tag{2.70}$$

When a material class is working in deviatoric stress ($\mathbf{s} = \boldsymbol{\sigma} + P$), the key terms needed above are

$$\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{xx}^{trial} + s_{yy}^{trial} - 2P_{final} \tag{2.71}$$

$$-\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{yy}^{trial} - s_{xx}^{trial} \tag{2.72}$$

$$s_{xx}^{(n+1)} = \sigma_{xx}^{(n+1)} + P_{final} \tag{2.73}$$

$$s_{yy}^{(n+1)} = \sigma_{yy}^{(n+1)} + P_{final} \tag{2.74}$$

$$s_{zz}^{(n+1)} = P_{final} \tag{2.75}$$

$$s_{xy}^{(n+1)} = \tau_{xy}^{(n+1)} \tag{2.76}$$

The special hardening laws that allow a closed-form expression in plane strain will still require numerical solution in plane stress. The example given above used $K(\alpha) = \sigma_Y + E_p\alpha$. The equation for λ will be quartic expression. The one key derivative needed, however, simplifies to:

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}\left(\sigma_Y + E_p\alpha^{(k)}\right)E_p\|\mathbf{s}^{(k)}\| \tag{2.77}$$

2.3.3 3D Analysis

This analysis follows the plane strain and axisymmetric section except includes direct updates for γ_{xz}, γ_{yz}, τ_{xz}, and τ_{yz}.

2.3.4 Examples of J_2 Hardening Laws

From the previous sections, analysis with materials that can use J_2 flow theory only require code implementation of the yield stress ($K(\alpha)$) and its derivatives. For plane strain or 3D, the code only needs $\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda}$. To handle plane stress as well, the code needs $\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda}$. When the yield stress depends on strain rate, that rate is $\dot{\varepsilon}_p = d\alpha/dt$ where dt is the time step. When evaluating in plane strain or 3D code $\alpha'(\lambda) = \sqrt{2/3}$ and $\dot{\varepsilon}_p'(\lambda) = \sqrt{2/3}/dt$. In plane stress code $\alpha'(\lambda) = \sqrt{2/3}\|\mathbf{s}\|$ and $\dot{\varepsilon}_p'(\lambda) = \sqrt{2/3}\|\mathbf{s}\|/dt$.

All hardening laws are implemented as subclasses of the `HardeningLawBase` class. The `Isoplasticity` class, or any of its subclasses, can use any hardening law by picking it when defining material parameters. Thus, the total number of available materials in this group is number of hardening laws × number of `Isoplasticity` classes. The following sections list the current hardening laws and the equations that are implemented.

Linear Work Hardening

$$K(\alpha) = \sigma_y(1+\beta\alpha) = \sigma_y + E_p\alpha \tag{2.78}$$

$$A_p = \frac{1}{2}E_p\alpha^2 \tag{2.79}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}E_p \tag{2.80}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}(\sigma_y + E_p\alpha)E_p\|\mathbf{s}\| \tag{2.81}$$

Non-Linear Work Hardening

$$K(\alpha) = \sigma_y(1+\beta\alpha)^n \tag{2.82}$$

$$A_p = \sigma_y\left(\frac{(1+\alpha\beta)^{1+n} - (1+(1+n)\alpha\beta)}{(1+n)\beta}\right) \tag{2.83}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}\sigma_y\beta n(1+\beta\alpha)^{n-1} \tag{2.84}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}\sigma_y^2\beta n(1+\beta\alpha)^{2n-1}\|\mathbf{s}\| \tag{2.85}$$

Alternate Non-Linear Work Hardening

$$K(\alpha) = \sigma_y(1+\beta\alpha^n) \tag{2.86}$$

$$A_p = \frac{\alpha^{1+n}\beta\sigma_y}{1+n} \tag{2.87}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}\sigma_y\beta n\alpha^{n-1} \tag{2.88}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}\sigma_y^2\beta n\alpha^{n-1}(1+\beta\alpha^n)\|\mathbf{s}\| \tag{2.89}$$

Johnson-Cook

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.90}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}\left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\left(1-(T^*)^m\right) \tag{2.91}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right)^2 \left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\|\mathbf{s}\| \tag{2.92}$$

This law has numerical issues as $\dot{\varepsilon}_p \to 0$ because the $\ln\dot{\varepsilon}_p$ can cause the yield stress to be nonphysically negative. One solution is to truncate at $\dot{\varepsilon}_{p,min}$ within $\dot{\varepsilon}_0 e^{-1/C} < \dot{\varepsilon}_{p,min} < \dot{\varepsilon}_0$; the lower limit is when the rate term becomes zero and the upper is when it is one. Below $\dot{\varepsilon}_{p,min}$, the rate term can be taken as a constant using that minimum strain rate. The resulting yield functions are

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.93}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.94}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}Bn\alpha^{n-1}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)^2\left(1-(T^*)^m\right)^2\|\mathbf{s}\| \tag{2.95}$$

2.4 Drucker-Prager Plasticity

The Drucker-Prager yield function can be expressed as:

$$\Phi(\boldsymbol{\sigma},\boldsymbol{\psi}) = \sqrt{J_2} - \eta p - \xi c(\alpha) = \sqrt{\frac{1}{2}\|\mathbf{s}\|^2} - \eta p - \xi(c_0+\psi) \tag{2.96}$$

where $c(\alpha) = c_0+\psi$ is a yield stress with hardening, c_0 is initial cohesive stress, and η and ξ are material properties (commonly set by analogy to Mohr-Coulomb law). Note that p is pressure (which is positive in compression) while Neto book calls it pressure, but defines it as $1/3$ trace of stress tensor (which is positive for tension). For pure shear stress, $J_2 = \tau^2$ and $p = 0$, yielding occurs when $\tau = \tau_y = \xi c(\alpha)$. For uniaxial tensile stress, $J_2 = \sigma^2/3$ and $p = -\sigma/3$, yielding occurs when:

$$\sigma = \sigma_y = \frac{3\xi}{\sqrt{3}+\eta}c(\alpha) = \frac{3}{\sqrt{3}+\eta}\tau_y \tag{2.97}$$

For hydrostatic pressure, $J_2 = 0$ and yielding occurs when $p = p_y = -\xi K(\alpha)/\eta$. Finally, if Mohr-Coulomb law evolves to a Tresca condition, common choices for η and ξ evolve to $\eta \to 0$ and $\xi \to 2/\sqrt{3}$. The yield condition becomes $\Phi = \|\mathbf{s}\|/\sqrt{2} - K(\alpha)/\sqrt{3}$ and $\sigma_y = \sqrt{3}\tau_y = 2c(\alpha)$, which matches the von Mises criterion.

The plastic flow commonly uses a non-associative law where

$$\Psi = \sqrt{\frac{1}{2}\|\mathbf{s}\|^2} - \bar{\eta}p \tag{2.98}$$

$$d\boldsymbol{\varepsilon}^p = \lambda \boldsymbol{N}(\boldsymbol{\sigma},\boldsymbol{\psi}) = \lambda \frac{d\Psi}{d\boldsymbol{\sigma}} = \lambda\left(\frac{\mathbf{s}}{2\sqrt{\frac{1}{2}\|\mathbf{s}\|^2}} + \frac{\overline{\eta}}{3}\mathsf{I}\right) \tag{2.99}$$

Note that positive sign on the second term is because it is derivative with respect to stress and not pressure. The hardening by associative, isotropic hardening is

$$d\alpha = \lambda \boldsymbol{H} = -\lambda \frac{\partial \Phi}{\partial \psi} = \lambda \xi \tag{2.100}$$

Starting with $\boldsymbol{\sigma}_{n+1}^{trial}$ and after finding λ, the updated stress is

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{trial} - \lambda\left(\frac{G\mathbf{s}_{n+1}}{\sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}\|^2}} + \frac{K\overline{\eta}}{3}\mathsf{I}\right) \tag{2.101}$$

where G and K and shear and bulk moduli. Noting that

$$\mathbf{s}_{n+1} = \boldsymbol{\sigma}_{n+1} - \frac{1}{3}\mathrm{tr}(\boldsymbol{\sigma}_{n+1})\mathsf{I} \tag{2.102}$$

$$= \mathbf{s}_{n+1}^{trial} - \lambda \frac{G\mathbf{s}_{n+1}}{\sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}\|^2}} \tag{2.103}$$

$$\mathbf{s}_{n+1}^{trial} = \left(1 + \lambda \frac{G}{\sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}\|^2}}\right)\mathbf{s}_{n+1} \tag{2.104}$$

$$\frac{\mathbf{s}_{n+1}^{trial}}{\|\mathbf{s}_{n+1}^{trial}\|} = \frac{\mathbf{s}_{n+1}}{\|\mathbf{s}_{n+1}\|} \tag{2.105}$$

The stress update can be rewritten as

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_{n+1}^{trial} - \lambda\left(\frac{G\mathbf{s}_{n+1}^{trial}}{\sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}^{trial}\|^2}} + \frac{K\overline{\eta}}{3}\mathsf{I}\right) \tag{2.106}$$

Splitting into updates for deviatoric stress and pressure gives:

$$\mathbf{s}_{n+1} = \left(1 - \frac{\lambda G}{\sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}^{trial}\|^2}}\right)\mathbf{s}_{n+1}^{trial} \tag{2.107}$$

$$p_{n+1} = p_{n+1}^{trial} + \lambda\overline{\eta}K \tag{2.108}$$

Substituting into yield function gives

$$\Phi(\boldsymbol{\sigma},\boldsymbol{\psi}) = \sqrt{\frac{1}{2}\left(\|\mathbf{s}_{n+1}^{trial}\| - \frac{\lambda G}{\sqrt{\frac{1}{2}}}\right)^2} - \eta\left(p_{n+1}^{trial} + \lambda\overline{\eta}K\right) - \xi c(\alpha_n + \lambda\xi) = 0 \tag{2.109}$$

$$= \sqrt{\frac{1}{2}\|\mathbf{s}_{n+1}^{trial}\|^2} - \lambda G - \eta\left(p_{n+1}^{trial} + \lambda\overline{\eta}K\right) - \xi c(\alpha_n + \lambda\xi) = 0 \tag{2.110}$$

Sometimes this equation can be solved analytically (see below). Otherwise is can be solved using Newton's method. Start with $\Phi^{(0)} = \Phi^{trial}$ and then iterate using:

$$\frac{d\Phi^{(k)}}{d\lambda} = -G - \eta\overline{\eta}K - \xi\frac{dc(\alpha^{(k)})}{d\lambda} = -G - \eta\overline{\eta}K - \xi^2\frac{dc(\alpha^{(k)})}{d\alpha} \tag{2.111}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)}\xi \tag{2.112}$$

where $c'(\alpha^{(k)}) = dc(\alpha^{(k)})/d\alpha$ is the derivative with respect to α. For example, for a linear hardening law, λ can be found in a closed-form expression — when $c(\alpha) = c_0 + E_p\alpha$, the task is to solve

$$\Phi = \sqrt{J_2^{trial}} - \lambda G - \eta\left(p_{n+1}^{trial} + \lambda K\overline{\eta}\right) - \xi(c_0 + E_p\alpha^0 + E_p\lambda\xi) = 0 \tag{2.113}$$

The analytical solution is

$$\lambda = \frac{\sqrt{J_2^{trial}} - \eta p_{n+1}^{trial} - \xi(c_0 + E_p\alpha^0)}{G + \eta\overline{\eta}K + \xi^2 E_p} \tag{2.114}$$

2.5 Anisotropic Plasticity

Anisotropic Plasticity is best done in the material axes, because otherwise many properties and the yield criterion will need rotation in current configuration. In other words, this material will always use the large rotation mode (see Chapter 3).

One yield criterion for anisotropic plasticity is the quadratic Hill yield criterion. It can implement anisotropic plasticity and hardening terms can be added to include hardening as well. For 3D analysis, the Hill yield function with arbitrary hardening function (defined later) reduces to:

$$f = \sqrt{F\left(\sigma_{yy} - \sigma_{zz}\right)^2 + G(\sigma_{xx} - \sigma_{zz})^2 + H\left(\sigma_{yy} - \sigma_{xx}\right)^2 + 2L{\tau_{yz}}^2 + 2M{\tau_{xz}}^2 + 2N{\tau_{xy}}^2} - g(\boldsymbol{\alpha}) \tag{2.115}$$

$$= \Big[(G+H){\sigma_{xx}}^2 + (F+H){\sigma_{yy}}^2 + (F+G)\sigma_{zz}^2 - 2F\sigma_{yy}\sigma_{zz} - 2G\sigma_{xx}\sigma_{zz} - 2H\sigma_{xx}\sigma_{yy} + 2L{\tau_{yz}}^2 + 2M{\tau_{xz}}^2 + 2N{\tau_{xy}}^2\Big]^{1/2} - g(\boldsymbol{\alpha}) \tag{2.116}$$

$$= \sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}} - g(\boldsymbol{\alpha}) = \sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}} - \frac{\sigma_{ref}^Y + \sqrt{\frac{2}{3}}\boldsymbol{\psi}(\boldsymbol{\alpha})}{\sigma_{ref}^Y} \tag{2.117}$$

where $\boldsymbol{\sigma}$ is stress in the material axis system, $g(\boldsymbol{\alpha})$ is a hardening function, $\boldsymbol{\psi}$ is plastic force for hardening, σ_{ref}^Y is a reference tensile yield strength, and

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.118}$$

As explained below, the $\sqrt{2/3}$ is used to have model reduce to isotropic yield and same hardening parameter if the material is isotropic. For 2D, plane strain, $\boldsymbol{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \tau_{xy})$ and

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 \\ -H & F+H & -F & 0 \\ -G & -F & F+G & 0 \\ 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.119}$$

Formal plasticity theory has $\mathbf{A}$ as fourth-rank tensor and $\boldsymbol{\sigma}$ as second rank tensor. To recover the same f, we need

$$A_{xxxx} = G+H,\ A_{xxyy} = A_{yyxx} = -H,\ A_{xxzz} = A_{zzxx} = -G,\ A_{yyyy} = F+H, \tag{2.120}$$

$$A_{yyzz} = A_{zzyy} = -F,\ A_{zzzz} = F+G,\ A_{yzyz} = \frac{L}{2},\ A_{xzxz} = \frac{M}{2},\ A_{xyxy} = \frac{N}{2} \tag{2.121}$$

such that

$$\mathbf{A}\boldsymbol{\sigma} = \begin{pmatrix} (G+H)\sigma_{xx} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + (F+H)\sigma_{yy} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + (F+G)\sigma_{zz} \end{pmatrix} \tag{2.122}$$

and $\boldsymbol{\sigma} \cdot \mathbf{A}\boldsymbol{\sigma}$ recovers the yield criterion.

The elements of the $\mathbf{A}$ matrix are physically defined by directionally dependent yield stresses prior to any hardening:

$$(G+H) = \frac{1}{(\sigma^Y_{xx})^2} \qquad (F+H) = \frac{1}{(\sigma^Y_{yy})^2} \qquad (F+G) = \frac{1}{(\sigma^Y_{zz})^2} \tag{2.123}$$

$$F = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{yy})^2} + \frac{1}{(\sigma^Y_{zz})^2} - \frac{1}{(\sigma^Y_{xx})^2}\right) \qquad G = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{zz})^2} + \frac{1}{(\sigma^Y_{xx})^2} - \frac{1}{(\sigma^Y_{yy})^2}\right) \tag{2.124}$$

$$H = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{xx})^2} + \frac{1}{(\sigma^Y_{yy})^2} - \frac{1}{(\sigma^Y_{zz})^2}\right) \quad L = \frac{1}{2(\tau^Y_{yz})^2} \quad M = \frac{1}{2(\tau^Y_{xz})^2} \quad N = \frac{1}{2(\tau^Y_{xy})^2} \tag{2.125}$$

To make physical sense, the $\mathbf{A}$ matrix must be positive semidefinite (so square root will always be of a non-negative number). The determinant of $\mathbf{A}$ is zero, but it can be diagonalized using its eigenvalues and three linearly independent eigenvectors. The calculations were done separately, but show that for $\mathbf{A}$ to be positive semidefinite, requires both:

$$F^2 + G^2 + H^2 - FH - GH - FG \geq 0 \tag{2.126}$$

$$F + G + H \geq \sqrt{F^2 + G^2 + H^2 - FH - GH - FG} \tag{2.127}$$

Substituting yield stresses, the conditions can be recast as

$$\left(\frac{1}{\sigma^Y_{xx}} - \frac{1}{\sigma^Y_{yy}}\right)^2 \leq \frac{1}{(\sigma^Y_{zz})^2} \leq \left(\frac{1}{\sigma^Y_{xx}} + \frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.128}$$

$$\left(\frac{1}{\sigma^Y_{xx}} - \frac{1}{\sigma^Y_{zz}}\right)^2 \leq \frac{1}{(\sigma^Y_{yy})^2} \leq \left(\frac{1}{\sigma^Y_{xx}} + \frac{1}{\sigma^Y_{zz}}\right)^2 \tag{2.129}$$

$$\left(\frac{1}{\sigma^Y_{zz}} - \frac{1}{\sigma^Y_{yy}}\right)^2 \leq \frac{1}{(\sigma^Y_{xx})^2} \leq \left(\frac{1}{\sigma^Y_{zz}} + \frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.130}$$

Two special cases are mentioned. If one yield stress is infinite (*e.g.*, $\sigma^Y_{xx} = \infty$), the other two must be equal (*e.g.*, $\sigma^Y_{yy} = \sigma^Y_{zz}$). If two yield stresses are related by $\sigma^Y_{yy}/\sigma^Y_{xx} = R$ then the other is bracketed by:

$$\frac{\sigma^Y_{yy}}{(1+R)} \leq \sigma^Y_{zz} \leq \frac{\sigma^Y_{yy}}{|1-R|} \tag{2.131}$$

For examples: if $R = 1$ then $\sigma^Y_{yy}/2 \le \sigma^Y_{zz} \le \infty$; if $R = 0$ or $R = \infty$ then $\sigma^Y_{yy} = \sigma^Y_{zz}$.

The implemented hardening with a single hardening variable is effective isotropic. Perhaps more anisotropic methods would be better. With a single variable, a reasonable choice for reference tensile yield strength is

$$\frac{1}{\sigma^Y_{ref}} = \sqrt{F+G+H} = \sqrt{\frac{1}{2}\left(\frac{1}{(\sigma^Y_{xx})^2} + \frac{1}{(\sigma^Y_{yy})^2} + \frac{1}{(\sigma^Y_{yy})^2}\right)} \tag{2.132}$$

For an isotropic material (*i.e.*, the Von Mises criterion), the key terms are

$$(G+H) = (F+H) = (F+G) = 2F = 2G = 2H = \frac{1}{\sigma_Y^2}, \tag{2.133}$$

$$L = M = N = \frac{1}{2\tau_Y^2} = \frac{3}{2\sigma_Y^2}, \quad \text{and} \quad \sigma^Y_{ref} = \sqrt{\frac{2}{3}}\sigma_Y \tag{2.134}$$

leading to:

$$\begin{aligned} f &= \sqrt{\frac{\left(\sigma_{yy}-\sigma_{zz}\right)^2}{2\sigma_Y^2} + \frac{(\sigma_{xx}-\sigma_{zz})^2}{2\sigma_Y^2} + \frac{\left(\sigma_{yy}-\sigma_{xx}\right)^2}{2\sigma_Y^2} + \frac{3{\tau_{yz}}^2}{\sigma_Y^2} + \frac{3{\tau_{xz}}^2}{\sigma_Y^2} + \frac{3{\tau_{xy}}^2}{\sigma_Y^2}} - g(\boldsymbol{\alpha}) \\ &= \frac{1}{\sigma_Y}\sqrt{3J_2} - g(\boldsymbol{\alpha}) = \frac{1}{\sigma_Y}\sqrt{\frac{3}{2}}\left(\sqrt{2J_2} - \sqrt{\frac{2}{3}}(\sigma_Y + \psi)\right) \end{aligned} \tag{2.135}$$

This is equivalent to isotropic J_2 plasticity with f scaled by and the $\sqrt{2/3}$ factors reproduces physical interpretation α as cumulative plastic strain..

The derivatives with respect to material axes are found by differentiating with respect to material stress. The result is

$$\frac{d\boldsymbol{f}}{d\boldsymbol{\sigma}} = \frac{\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.136}$$

In the material axis system, the tensorial plastic strain increment is found from tensor product $\mathbf{A}\boldsymbol{\sigma}$ from above:

$$d\boldsymbol{\varepsilon}^p = \lambda d\boldsymbol{f} = \frac{\lambda\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.137}$$

This strain results in a traceless tensor (*i.e.*, only deviatoric plastic strains):

$$d\boldsymbol{\varepsilon}^p = \frac{\lambda}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}}\begin{pmatrix} \frac{\sigma_{xx}}{(\sigma^Y_{xx})^2} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + \frac{\sigma_{yy}}{(\sigma^Y_{yy})^2} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + \frac{\sigma_{zz}}{(\sigma^Y_{zz})^2} \end{pmatrix} \tag{2.138}$$

The engineering plastic strain increment is

$$d\boldsymbol{\varepsilon}^p = \frac{\lambda}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}}\begin{pmatrix} \frac{\sigma_{xx}}{(\sigma^Y_{xx})^2} - H\sigma_{yy} - G\sigma_{zz} \\ -H\sigma_{xx} + \frac{\sigma_{yy}}{(\sigma^Y_{yy})^2} - F\sigma_{zz} \\ -G\sigma_{xx} - F\sigma_{yy} + \frac{\sigma_{zz}}{(\sigma^Y_{zz})^2} \\ \frac{\tau_{yz}}{(\tau^Y_{yz})^2} \\ \frac{\tau_{xz}}{(\tau^Y_{yx})^2} \\ \frac{\tau_{xy}}{(\tau^Y_{xy})^2} \end{pmatrix} \tag{2.139}$$

The usual assumption for associative flow is to take

$$d\boldsymbol{\alpha} = -\lambda \frac{\partial f}{\partial \psi} = \frac{\lambda}{\sigma^Y_{ref}} \sqrt{\frac{2}{3}} \tag{2.140}$$

Solving for $\boldsymbol{\psi}$ gives

$$\boldsymbol{\psi} = \sigma^Y_{ref} \sqrt{\frac{3}{2}} (g(\boldsymbol{\alpha}) - 1) \quad \text{and} \quad \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}} = \sigma^Y_{ref} \sqrt{\frac{3}{2}} g'(\alpha) \tag{2.141}$$

The plasticity term needed in Newton's method of solution is

$$\frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}^{(k)}} \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} = \frac{g'(\alpha)}{\sigma^Y_{ref}} \sqrt{\frac{2}{3}} \tag{2.142}$$

The current code implements several hardening laws. Originally, the only law available was:

$$g(\alpha) = 1 + K\alpha^n, \quad g'(\alpha) = nK\alpha^{n-1}, \quad K_n = K_1 \alpha^{1-n} \tag{2.143}$$

which is linear when $n = 1$. If K_1 is the hardening term when $n = 1$ and then a new value of n is selected, then then given K_n is the value of K for the new n to match the amount of hardening that occurs up to any specified α between the $n = 1$ and n laws. Compared to linear hardening law defined by

$$\sigma_y = \sigma_{y0}(1 + K'\alpha) \quad \text{with} \quad \psi = \sigma_y(\alpha) - \sigma_{y0} = \sigma_{y0} K'\alpha \tag{2.144}$$

The use of $g(\alpha)$ to get same K' should select:

$$K = K' \frac{\sigma_{y0}}{\sigma^Y_{ref}} \sqrt{\frac{2}{3}} \quad (= K') \quad \text{and} \quad K = \frac{E_p}{\sigma^Y_{ref}} \sqrt{\frac{2}{3}} \quad \left(= \frac{E_p}{\sigma_{y0}} \right) \tag{2.145}$$

where second form is for linear hardening with plastic modulus E_p (and parenthetical forms are if material is isotropic too).

The nonlinear law above as $g'(\alpha) \to \infty$ when $n < 1$. This high slope causes problems in numerical method used to calculate plastic strain. A hack is used such that it seems to work for $n > 0.7$, but not for smaller n. A reason to use $n < 1$ is to model material where slope decreases with strain. Two harding laws that can alternatively model that behavior without numerical instabilities are:

$$g(\alpha) = (1 + K\alpha)^n, \; g'(\alpha) = nK(1 + K\alpha)^{n-1}, \; g'(0) = nK \tag{2.146}$$

and

$$g(\alpha) = 1 + \frac{K}{k}\big(1 - \exp(-k\alpha)\big), \; g'(\alpha) = K \exp(-k\alpha), \; g'(0) = K \tag{2.147}$$

2.6 Anisotropic 2D Plane Strain and Axisymmetric Analysis - Material Axes

In is most convenient to implement to constitutive law in the material axes and here the material is assumed to be orthotropic. In general plane strain or axisymmetric analysis, the matrix equation for update is:

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}^{tot} + \boldsymbol{c}_{excess} \tag{2.148}$$

The key terms are

$$\mathbf{C} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 & 0 \\ \texttt{C[4][1]} & \texttt{C[4][2]} & 0 & \texttt{C[4][4]} \\ 0 & 0 & \texttt{C[3][3]} & 0 \end{pmatrix} \tag{2.149}$$

$$d\boldsymbol{\varepsilon}^{tot} = \left(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)},\, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)},\, d\varepsilon_{zz} - \varepsilon_{zz}^{(res)},\, d\gamma_{xy}\right) \tag{2.150}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.151}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res)} \\ \gamma_{xy}^{(res)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \alpha_{zz}\Delta T + \beta_{zz}\Delta c \\ 0 \end{pmatrix} \tag{2.152}$$

The term $d\varepsilon_{zz}$ is zero for plane strain, but incremental hoop strain of axisymmetry, while the term $\boldsymbol{c}_{excess}$ is zero for axisymmetry but is needed for plane strain analysis to compensate for use of reduced thermal and moisture expansion coefficients in the x-y terms. The only non-zero component is:

$$\boldsymbol{c}_{excess}[3] = \left(\texttt{C[4][1]alpha[5]} + \texttt{C[4][2]alpha[6]}\right)\varepsilon_{zz}^{(res)} \tag{2.153}$$

Note that in the code, `alpha[5]` and `alpha[6]` hold out-of-plane Poisson ratios (or rotated ratios) and not thermal expansion coefficients. This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx}, \quad d\varepsilon_{yy}^{(p)} = \lambda df_{yy}, \quad d\gamma_{xy}^{(p)} = \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(p)} = \lambda df_{zz} \tag{2.154}$$

where df_{xy} is evaluated to give engineering plastic shear strain. The elastic strain increments are:

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(e)} = -\lambda df_{zz} \tag{2.155}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 \\ 0 & 0 & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\gamma_{xx}^{(e)} \end{pmatrix} \tag{2.156}$$

For plane strain analysis, $d\sigma_{zz}$ is similar to an elastic material using elastic strains:

$$\begin{aligned} d\sigma_{zz} = {} & \texttt{C[4][1]}\left(d\varepsilon_{xx}^{(e)} - (\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)})\right) + \texttt{C[4][2]}\left(d\varepsilon_{yy}^{(e)} - (\varepsilon_{yy}^{(res,r)} - \texttt{alpha[6]}\varepsilon_{zz}^{(res)})\right) \\ & - \texttt{C[4][4]}(d\varepsilon_{zz}^{(e)} - \varepsilon^{(res)}) \end{aligned} \tag{2.157}$$

The $d\varepsilon_{zz}^{(e)}$ term may be non zero even though it is plane strain. The total z direction strain is zero because $d\varepsilon_{zz}^{(e)} = -d\varepsilon_{zz}^{(p)}$.

2.7 Anisotropic 2D Plane Stress Analysis

Plane stress analysis is currently not supported for anisotropic plastic materials.

2.8 Anisotropic 3D Analysis - Material Axes

In 3D strain analysis in orthotropic material axes, the matrix equation for update is

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}^{tot} \tag{2.158}$$

The key terms are

$$\mathbf{C} = \texttt{C[i][j]} \quad \text{for i} = 0,5 \text{ and j} = 0,5 \tag{2.159}$$

$$d\boldsymbol{\varepsilon}^{tot} = \left(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{zz}^{(res)}, d\gamma_{yz}, d\gamma_{xz}, d\gamma_{xy} \right) \tag{2.160}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{yz}, df_{xz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{yz}}, \frac{\partial f}{\tau_{xz}}, \frac{\partial f}{\tau_{xy}} \right) \tag{2.161}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[0]}\Delta T + \texttt{beta[0]}\Delta c \\ \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \end{pmatrix} \tag{2.162}$$

This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx},\ d\varepsilon_{yy}^{(p)} = \lambda df_{yy},\ d\varepsilon_{zz}^{(p)} = \lambda df_{zz}, \tag{2.163}$$

$$d\gamma_{yz}^{(p)} = \lambda df_{yz},\ d\gamma_{xz}^{(p)} = \lambda df_{xz},\ d\gamma_{xy}^{(p)} = \lambda df_{xy}, \tag{2.164}$$

where df_{yz}, df_{xz}, and df_{xy} are evaluated to give engineering plastic shear strain. The elastic strain increments are:

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\varepsilon_{zz}^{(e)} = d\varepsilon_{yy} - \lambda df_{zz} \tag{2.165}$$

$$d\gamma_{yz}^{(e)} = d\gamma_{yz} - \lambda df_{yz}, \quad d\gamma_{xz}^{(e)} = d\gamma_{xz} - \lambda df_{xz}, \quad \text{and} \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy} \tag{2.166}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \\ d\tau_{xz} \\ d\tau_{xy} \end{pmatrix} = \left(\texttt{C[i][j]} \quad \text{for i} = 0,5 \text{ and j} = 0,5 \right) \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\varepsilon_{zz}^{(e)} - \varepsilon_{zz}^{(res,r)} \\ d\gamma_{yz}^{(e)} \\ d\gamma_{xz}^{(e)} \\ d\gamma_{xy}^{(e)} \end{pmatrix} \tag{2.167}$$

2.9 More General Plasticity Methods

We define several variables (6 components of stress and λ) and need to solve the simultaneous equations:

$$0 = \Delta\boldsymbol{\sigma} - \mathsf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_p) = \Delta\boldsymbol{\sigma} - \mathsf{C}d\boldsymbol{\varepsilon} + \lambda \mathsf{C} \nabla f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) \tag{2.168}$$

$$0 = f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) = f\left(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + \sqrt{\frac{3}{2}} \lambda \|\nabla f\| \right) \tag{2.169}$$

We convert to $F(\boldsymbol{x})=0$ where x_1 to x_6 are components of stress increment and x_7 is λ. The Newton's method solution is:

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)}-\boldsymbol{x}^{(n)}\right)=-F(\boldsymbol{x}^{(n)}) \tag{2.170}$$

Here $J(\boldsymbol{x}^{(n)})$ is the Jacobian of $F(\boldsymbol{x}^{(n)})$. The equation can be written as

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)}-\boldsymbol{x}^{(n)}\right)=\begin{bmatrix} \mathsf{I}+\lambda\mathsf{C}\frac{d\nabla f}{d\Delta\boldsymbol{\sigma}} & \mathsf{C}\nabla f \\ \nabla f & \frac{df}{d\alpha}\frac{d\alpha}{d\lambda}\end{bmatrix}^{(n)}\begin{bmatrix}\delta\boldsymbol{\sigma}^{(n)}\\ \delta\lambda^{(n)}\end{bmatrix}=-\begin{bmatrix}\boldsymbol{p}^{(n)}\\ q^{(n)}\end{bmatrix} \tag{2.171}$$

where

$$\begin{aligned}\boldsymbol{p}^{(n)} &= \Delta\boldsymbol{\sigma}^{(n)}-\mathsf{C}d\boldsymbol{\varepsilon}+\lambda^{(n)}\mathsf{C}\nabla f(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)}) &(2.172)\\ q^{(n)} &= f\left(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)}\right) &(2.173)\\ d\alpha^{(n)} &= \sqrt{\frac{3}{2}}\lambda\left\|\nabla f(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)})\right\| &(2.174)\end{aligned}$$

The next iteration for stress and λ are

$$\begin{aligned}\Delta\boldsymbol{\sigma}^{(n+1)} &= \Delta\boldsymbol{\sigma}^{(n)}+\delta\boldsymbol{\sigma}^{(n)} &(2.175)\\ \delta\lambda^{(n+1)} &= \lambda^{(n)}+\delta\lambda^{(n)} &(2.176)\end{aligned}$$

For the special case of J_2 plasticity, the gradient ∇f is independent of the increment, which implies $d\nabla f/d\Delta\boldsymbol{\sigma}=0$. The incremental resulgts can be solved as:

$$\delta\boldsymbol{\sigma}^{(n)}=-\boldsymbol{p}^{(n)}-\delta\lambda^{(n)}\mathsf{C}\nabla f \qquad \text{and} \qquad \delta\lambda^{(n)}=-\frac{q^{(n)}-\nabla f\cdot\boldsymbol{p}^{(n)}}{\nabla f\cdot\mathsf{C}\nabla f-\frac{df}{d\alpha}\frac{d\alpha}{d\lambda}} \tag{2.177}$$

For next increment:

$$\begin{aligned}\boldsymbol{p}^{(n+1)} &= \Delta\boldsymbol{\sigma}^{(n+1)}-\mathsf{C}d\boldsymbol{\varepsilon}+\lambda^{(n+1)}\mathsf{C}\nabla f &(2.178)\\ &= \Delta\boldsymbol{\sigma}^{(n)}-\boldsymbol{p}^{(n)}-\delta\lambda^{(n)}\mathsf{C}\nabla f-\mathsf{C}d\boldsymbol{\varepsilon}+(\lambda^{(n)}+\delta\lambda^{(n)})\mathsf{C}\nabla f &(2.179)\\ &= 0 &(2.180)\end{aligned}$$

We thus seed the numerical solution with $\Delta\boldsymbol{\sigma}^{(n)}=\mathsf{C}d\boldsymbol{\varepsilon}$ and $\lambda^{(0)}=0$ leading to $\boldsymbol{p}^{(0)}=0$ and all other $\boldsymbol{p}^{(n)}=0$. The final stress increment becomes:

$$\Delta\boldsymbol{\sigma}^{(n)}=-\sum_{i=0}^{n}\delta\lambda^{(i)}\mathsf{C}\nabla f=-\lambda^{(n)}\mathsf{C}\nabla f \tag{2.181}$$

The analysis reduces to a single equation, which may need numerical solution, of

$$0=f\left(\boldsymbol{\sigma}+\mathsf{C}d\boldsymbol{\varepsilon}-\lambda^{(n)}\mathsf{C}\nabla f,\alpha+d\alpha^{(n)}\right)=f_{trial}-\lambda^{(n)}\left(\nabla f\cdot\mathsf{C}\nabla-\frac{df}{d\alpha}\frac{d\alpha}{d\lambda}\right) \tag{2.182}$$

Starting with $\lambda^{(0)}$ and $q^{(0)}=f_{trial}$ leads to Newton's method with step increment:

$$\delta\lambda^{(n)}=-\frac{q^{(n)}}{\nabla f\cdot\mathsf{C}\nabla f-\frac{df}{d\alpha}\frac{d\alpha}{d\lambda}} \tag{2.183}$$

which is identical to J_2 plasticity methods defined above. The derivation assumes a single hardening variable, α but can easily be generalized to more than one.

2.9.1 Old Notes, May Be Cutting Algorithm

We begin with trial state as the initial state in explicit integrations:

$$\begin{aligned}
\boldsymbol{\sigma}^{(0)} = \boldsymbol{\sigma}_{trial} &= \boldsymbol{\sigma}_n + \mathbf{C} d\boldsymbol{\varepsilon}^{tot} && (2.184)\\
d\boldsymbol{\varepsilon}_p^{(0)} &= 0 && (2.185)\\
\boldsymbol{\lambda}^{(0)} &= 0 && (2.186)\\
\boldsymbol{\alpha}^{(0)} = \boldsymbol{\alpha}_{trial} &= \boldsymbol{\alpha}_n && (2.187)\\
\boldsymbol{\psi}^{(0)} = \boldsymbol{\psi}_{trial} &= \boldsymbol{\psi}_n && (2.188)\\
f^{(0)} = f_{trial} &= f(\boldsymbol{\varepsilon}_{e,trial}, \boldsymbol{\psi}_{trial}) > 0 && (2.189)
\end{aligned}$$

Imagine step k in sequence of Newton's steps to the solution. The next step can be expanded in a Taylor series to give:

$$f^{(k+1)} = f(\boldsymbol{\sigma}^{(k)} + d\boldsymbol{\sigma}, \boldsymbol{\psi}^{(k)} + d\boldsymbol{\psi}) = f^{(k)} + \frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} d\boldsymbol{\sigma} + \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} d\boldsymbol{\psi} \tag{2.190}$$

where stress differential is

$$\begin{aligned}
d\boldsymbol{\sigma} &= \boldsymbol{\sigma}^{(k+1)} - \boldsymbol{\sigma}^{(k)} && (2.191)\\
&= \boldsymbol{\sigma}_n + \mathbf{C} d\boldsymbol{\varepsilon}^{tot} - \lambda^{(k+1)} \mathbf{C} N(\boldsymbol{\sigma}^{(k+1)}, \boldsymbol{\psi}^{(k+1)}) - \boldsymbol{\sigma}_n - \mathbf{C} d\boldsymbol{\varepsilon}^{tot} + \lambda^{(k)} \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.192)\\
&\approx -d\lambda\, \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.193)
\end{aligned}$$

The last step is forward, explicit approximation and $d\lambda = \lambda^{(k+1)} - \lambda^{(k)}$. The plastic differential is

$$\begin{aligned}
d\boldsymbol{\psi} &= \boldsymbol{\psi}^{(k+1)} - \boldsymbol{\psi}^{(k)} \approx \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}} (\boldsymbol{\alpha}^{(k+1)} - \boldsymbol{\alpha}^{(k)}) && (2.194)\\
&= \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}} \left(\boldsymbol{\alpha}_n + \lambda^{(k+1)} H(\boldsymbol{\sigma}^{(k+1)}, \boldsymbol{\psi}^{(k+1)}) - \boldsymbol{\alpha}_n - \lambda^{(k)} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \right) && (2.195)\\
&\approx d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.196)
\end{aligned}$$

The last step is forward, explicit approximation. The updated potential function is:

$$f^{(k+1)} = f^{(k)} - d\lambda \left(\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) - \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \right) \tag{2.197}$$

Solving for $f^{(k+1)} = 0$ for $d\lambda$ gives

$$d\lambda = \frac{f^{(k)}}{\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \cdot \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) - \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\alpha}^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)})} \tag{2.198}$$

For associative plasticity, the result is:

$$d\lambda = \frac{f^{(k)}}{\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \cdot \mathbf{C} \frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} + \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}^{(k)}} \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}}} \tag{2.199}$$

From the solved increment, update the variables using:

$$\lambda^{(k+1)} = \lambda^{(k)} + d\lambda \tag{2.200}$$
$$d\boldsymbol{\varepsilon}_p^{(k+1)} = d\boldsymbol{\varepsilon}_p^{(k)} + d\lambda N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \tag{2.201}$$
$$\boldsymbol{\alpha}^{(k+1)} = \boldsymbol{\alpha}^{(k)} + d\lambda H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \tag{2.202}$$
$$\boldsymbol{\sigma}^{(k+1)} = \boldsymbol{\sigma}^{(k)} - d\lambda \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \tag{2.203}$$
$$\boldsymbol{\psi}^{(k+1)} = \boldsymbol{\psi}^{(k)} + d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \tag{2.204}$$

Finally, find $f(\boldsymbol{\sigma}^{(k+1)}, \boldsymbol{\psi}^{(k+1)})$. If it is sufficiently close to zero, the problem is done. If not, continue to the next step.

This above analysis is assuming common decoupling between elasticity and hardening. Some plasticity models could violate this assumption. This assumption is used implicitly in finding $d\boldsymbol{\sigma}$ and $d\boldsymbol{\psi}$.

Chapter 3

Small Strain Materials with Large Rotation

3.1 Introduction

Beginning in `NairnMPM`, version 11 and `OSParticulas`, version 2, all small strain materials were converted to new methods that track strain better and have two options to better account for large rotations. In brief, all materials track total deformation gradient. In the new "large rotation" mode, on each time step the deformation gradient is decomposed to get rotation matrix and small strain increment in material axes, in initial axes, or in material axes (depending on material type). After performing the constitutive law, the updated results are rotated to the current analysis coordinates. In addition, output of strains (as global quantities or VTK archive) calculate the strain in the current coordinates. This conversion works for both elastic and plastic strains and now makes tracking of strains much better. The visualization tools also extract all strains correctly from the tracked deformation gradient.

The default mode is a "small rotation" mode which is similar to before, but was updated to track deformation gradient better and to track strains correctly. The main difference between large and small rotation is that the small rotation method uses an approximation to the incremental rotation rather the finding it by polar decomposition. The small rotation mode is therefore more efficient and may be very close to the large rotation mode for many problems (especially if problem has little rotation). When rotation is crucial (such as when modeling anisotropic materials and materials that become anisotropic due to damage), the new method is probably better (and would have similar efficiency because handling anisotropy uses polar decomposition as well).

3.2 Small Strain Increment

In small strain elasticity, the strain tensor in the initial configuration is give by Biot strain:

$$\varepsilon_n^{(0)} = \mathbf{U}_n^{(0)} - \mathbf{I} \tag{3.1}$$

where $\mathbf{U}_n^{(0)}$ is stretch tensor in the initial configuration (the superscript) and time step n (the subscript). The strain increment between two states (in the initial configuration) becomes

$$d\varepsilon_n^{(0)} = \mathbf{U}_n^{(0)} - \mathbf{U}_{n-1}^{(0)} \tag{3.2}$$

If *both* total strain and total rotation are small, the deformation gradient can be written as

$$\mathbf{F} = \mathbf{I} + \varepsilon + \boldsymbol{\omega} \tag{3.3}$$

where $\boldsymbol{\omega} = (1/2)(\nabla \boldsymbol{u} - \nabla \boldsymbol{u}^T)$ is the infinitesimal rotation tensor. For small terms, this deformation can be decomposed to:

$$\mathbf{F} = (\mathbf{I} + \boldsymbol{\omega})(\mathbf{I} + \varepsilon) = \mathbf{RU} \qquad \text{or} \qquad \mathbf{R} = \mathbf{I} + \boldsymbol{\omega} \quad \text{and} \quad \mathbf{U} = \mathbf{I} + \varepsilon \tag{3.4}$$

Now imagine a small increment between two small deformation states $n-1$ and n of $\mathbf{dF}$ such that $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$. With all small deformations and rotations, this state can be written as:

$$\mathbf{F} = \mathbf{I} + \varepsilon_{n-1} + d\varepsilon + \boldsymbol{\omega}_{n-1} + d\boldsymbol{\omega} \approx (\mathbf{I} + d\varepsilon + d\boldsymbol{\omega})(\mathbf{I} + \varepsilon_{n-1} + \boldsymbol{\omega}_{n-1}) = \mathbf{dF}\mathbf{F}_{n-1} \tag{3.5}$$

In other words, both strain increment and rotation tensor can be found from $\mathbf{dF}$ using:

$$\nabla d\boldsymbol{u} = \mathbf{dF} - \mathbf{I}, \qquad d\varepsilon = \frac{1}{2}\left(\nabla d\boldsymbol{u} + \nabla d\boldsymbol{u}^T\right), \qquad \text{and} \qquad d\boldsymbol{\omega} = \frac{1}{2}\left(\nabla d\boldsymbol{u} - \nabla d\boldsymbol{u}^T\right) \tag{3.6}$$

Now, after n time steps, the total deformation gradient will become

$$\mathbf{F} = \mathbf{I} + \sum_{i=1}^{n} d\varepsilon_i + \sum_{i=1}^{n} d\boldsymbol{\omega}_i \tag{3.7}$$

This result is acceptable as long as *both* total deformation and total rotation are small, but consider a problem with small strains but large rotations. Such a problem should still be fine in small deformation theory, but it is likely the tracked deformation gradient will be inaccurate when the rotations get large. An alternative approach is update deformation gradient by matrix multiplication rather than addition of strains and rotations or to always use:

$$\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1} \tag{3.8}$$

This matrix multiplication method improves deformation gradient tracking in small-strain materials.

A possible alternative is to continue with small strain increments, but evaluate rotations by polar decomposition. Writing $\mathbf{F}_n = \mathbf{R}_n\mathbf{U}_n^{(0)}$ and $\mathbf{F}_{n-1} = \mathbf{R}_{n-1}\mathbf{U}_{n-1}^{(0)}$ as polar decompositions of two deformation states, the *small strain/large rotation* increment in initial configuration between these two states is:

$$d\varepsilon_n^{(0)} = \mathbf{U}_n^{(0)} - \mathbf{U}_{n-1}^{(0)} = \mathbf{R}_n^T\mathbf{F}_n - \mathbf{R}_{n-1}^T\mathbf{F}_{n-1} \tag{3.9}$$

This subtraction of two non-incremental states might be ill advised numerically. Perhaps it is better to introduce incremental deformation and rotation using $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$ and $\mathbf{R}_n = \mathbf{dR}\mathbf{R}_{n-1}$ (or $\mathbf{dR} = \mathbf{R}_n\mathbf{R}_{n-1}^T$and note that $\mathbf{dR}$ is found from two decomposed rotation matrices and not from polar decomposition of $\mathbf{dF}$). The strain increment becomes:

$$d\varepsilon^{(0)} = \mathbf{U}_n^{(0)} - \mathbf{U}_{n-1}^{(0)} = \mathbf{R}_n^T\mathbf{dF}\mathbf{F}_{n-1} - \mathbf{R}_n^T\mathbf{dR}\mathbf{F}_{n-1} = \mathbf{R}_n^T(\mathbf{dF} - \mathbf{dR})\mathbf{F}_{n-1} \tag{3.10}$$

If this result is applied to case when *both* strain and rotation are small:

$$d\varepsilon_n^{(0)} = (\mathbf{I} - \boldsymbol{\omega}_n)(\mathbf{I} + d\varepsilon + d\boldsymbol{\omega} - \mathbf{I} - d\boldsymbol{\omega})(\mathbf{I} + \varepsilon_{n-1} + \boldsymbol{\omega}_{n-1}) \approx d\varepsilon \tag{3.11}$$

after ignoring all products of two small increments.

For isotropic materials, it might be more convenient to work in current configuration rather than initial configuration. The new strain increment in the current configuration is found by rotating $d\varepsilon$ from initial to current configuration using $\mathbf{R}_n$:

$$d\varepsilon_n^{(n)} = \mathbf{R}_n d\varepsilon_n^{(0)}\mathbf{R}_n^T = (\mathbf{dF} - \mathbf{dR})\mathbf{F}_{n-1}\mathbf{R}_n^T \tag{3.12}$$

When working with anisotropic materials, it might be convenient to work in material axes and those axes may not line up with analysis axes (which represent the initial configuration). If $\mathbf{R}_0$ is rotation *from* material axes *to* the initial configuration, we find strain increment in the material axes by rotating $d\varepsilon_n^{(0)}$ from initial configuration to the material axes:

$$d\varepsilon_n^{(m)} = \mathbf{R}_0^T d\varepsilon_n^{(0)}\mathbf{R}_0 = \mathbf{R}_0^T\left(\mathbf{R}_n^T(\mathbf{dF} - \mathbf{dR})\mathbf{F}_{n-1}\right)\mathbf{R}_0 \tag{3.13}$$

3.3 Small Strain, Large Rotation Algorithm

An algorithm for small strain materials but using polar decomposition to find rotations is as follows:

1. Calculate $\mathbf{dF} = \exp(\nabla v \Delta t)$, find $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$, and save new deformation on the particle (it is the tracked *total* deformation gradient).

2. Decompose both $\mathbf{F}_{n-1}$ and $\mathbf{F}_n$ to get $\mathbf{R}_{n-1}$, $\mathbf{R}_n$, and $\mathbf{dR} = \mathbf{R}_n\mathbf{R}_{n-1}^T$. Note that we do not need left or right stretch result from decompositions and therefore can use either left or right decomposition. A potential efficiency improvement would be to track rotation matrix on the particle. If that is done, this step only needs to find $\mathbf{R}_n$, retrieve $\mathbf{R}_{n-1}$, calculate $\mathbf{dR}$, and finally update rotation tracked on the particle.

3. Find incremental strain $d\varepsilon$ equal to $d\varepsilon_n^{(0)}$, $d\varepsilon_n^{(n)}$, or $d\varepsilon_n^{(m)}$ from $\mathbf{dF}$, $\mathbf{dR}$, $\mathbf{F}_{n-1}$, $\mathbf{R}_n$, and $\mathbf{R}_0$. Also find total rotation from axes for strain increment to the new current configuration. For $d\varepsilon_n^{(0)}$, $\mathbf{R}_{tot} = \mathbf{R}_n$; for $d\varepsilon_n^{(n)}$, $\mathbf{R}_{tot} = \mathbf{I}$; for $d\varepsilon_n^{(m)}$, $\mathbf{R}_{tot} = \mathbf{R}_n\mathbf{R}_0$.

4. Update stress on the particle using $\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + \mathbf{R}_{tot}\mathbf{C}(d\varepsilon - d\varepsilon_{res})\mathbf{R}_{tot}^T$. Note that residual strains, $d\varepsilon_{res}$, must be rotated into the same axes as the strain increment. Similarly, for anisotropic materials, $\mathbf{C}$ needs to be rotated into the same axes used for strain increment (thus if using material axes, no rotation is needed).

5. When tracking separate plastic strain (as an engineering Biot strain), the updated plastic strain is $\varepsilon_{p,n} = \mathbf{dR}\varepsilon_{p,n-1}\mathbf{dR}^T + \mathbf{R}_{tot}d\varepsilon_p\mathbf{R}_{tot}^T$ where $d\varepsilon_p$ is plastic strain increment found in the chosen axis system.

3.3.1 Traditional Hypoelastic Version

Assuming small incremental strain and rotation, the algorithm can be approximated as a *hypoelastic* material using following methods (which become the traditional hypoelastic methods described in text books):

1. Calculate $\nabla d\boldsymbol{u} = \mathbf{dF} - \mathbf{I}$, find $d\varepsilon = (1/2)\left(\nabla d\boldsymbol{u} + \nabla d\boldsymbol{u}^T\right)$ and $d\boldsymbol{\omega} = (1/2)\left(\nabla d\boldsymbol{u} - \nabla d\boldsymbol{u}^T\right)$, and update total deformation gradient to $\mathbf{F}_n = (\mathbf{I} + \nabla d\boldsymbol{u})\mathbf{F}_{n-1}$, and save new deformation on the particle (it is the tracked *total* deformation gradient). Note that using matrix multiplication instead of addition is because we may not have small *total* rotation. If rotational strains were just added, the analysis likely would not work well to large rotation.

2. This small strain increment is in the current configuration and needs to find rotation from material axes to the current configuration. For isotropic materials, $R_{tot} = \mathbf{I}$, but for anisotropic materials, $\mathbf{R}_{tot} = \mathbf{R}_n\mathbf{R}_0$ where $\mathbf{R}_n$ must come from polar decomposition of $\mathbf{F}_n$. Note that traditional analysis for anisotropic materials needs this one polar decomposition. Adding a second decomposition can update this method to larger rotation method in previous section.

3. Update stress in chosen axes system to $\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + \mathbf{R}_{tot}\mathbf{C}\mathbf{R}_{tot}^T(d\varepsilon - d\varepsilon_{res})$. Note that residual strains, $d\varepsilon_{res}$, must be rotated into current configuration. For anisotropic materials, the rotations applied to $\mathbf{C}$ rotates it to current configuration.

4. When tracking separate plastic strain (as a engineering Biot strain). The updated plastic strain is $\varepsilon_{p,n} = \mathbf{dR}\varepsilon_{p,n-1}\mathbf{dR}^T + d\varepsilon_p$ where $d\varepsilon_p$ is plastic strain increment found in the current configuration.

Notice that the incremental terms are ordinary elasticity updates that ignore rotations (except to rotate anisotropic properties to current configuration). The main task that converts this analysis to a hypoelastic material is to rotate previous state by **dR**. Hypoelastic methods in text books use first order approximation to **dR**:

$$d\boldsymbol{\omega} = \mathbf{dR} - \mathbf{I} = \begin{pmatrix} 0 & -\frac{d\omega_{xy}}{2} & -\frac{d\omega_{xz}}{2} \\ \frac{d\omega_{xy}}{2} & 0 & -\frac{d\omega_{yz}}{2} \\ \frac{d\omega_{xz}}{2} & \frac{d\omega_{yz}}{2} & 0 \end{pmatrix} \tag{3.14}$$

where $d\omega_{ij}$ is engineering rotational strain tracked in the code and equal to $2\Omega_{ji}$ where $2\Omega = \nabla \boldsymbol{u} - \nabla \boldsymbol{u}^T$ (note change in order of indices and resulting factors of 2 when forming $d\boldsymbol{\omega}$). The stress and plastic strain (accounting for engineering strain) become:

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \\ d\tau_{xz} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} d\sigma^{(0)}_{xx} - d\omega_{xy}\tau_{xy} - d\omega_{xz}\tau_{xz} \\ d\sigma^{(0)}_{yy} + d\omega_{xy}\tau_{xy} - d\omega_{yz}\tau_{yz} \\ d\sigma^{(0)}_{zz} + d\omega_{xz}\tau_{xz} + d\omega_{yz}\tau_{yz} \\ d\tau^{(0)}_{yz} + \frac{d\omega_{yz}}{2}(\sigma_{yy} - \sigma_{zz}) + \frac{d\omega_{xz}\tau_{xy}}{2} + \frac{d\omega_{xy}\tau_{xz}}{2} \\ d\tau^{(0)}_{xz} + \frac{d\omega_{xz}}{2}(\sigma_{xx} - \sigma_{zz}) + \frac{d\omega_{yz}\tau_{xy}}{2} - \frac{d\omega_{xy}\tau_{yz}}{2} \\ d\tau^{(0)}_{xy} + \frac{d\omega_{xy}}{2}(\sigma_{xx} - \sigma_{yy}) - \frac{d\omega_{yz}\tau_{xz}}{2} - \frac{d\omega_{xz}\tau_{yz}}{2} \end{pmatrix} \tag{3.15}$$

where $d\sigma^{(0)}_{ij}$ comes from $\mathbf{R}_{tot}\mathbf{C}\mathbf{R}^T_{tot}(d\varepsilon - d\varepsilon_{res})$. A similar update can be used to account for rotations of plastic strain (being sure to account for tracking of engineering plastic shear strain) as:

$$\begin{pmatrix} d\varepsilon_{xx,p} \\ d\varepsilon_{yy,p} \\ d\varepsilon_{zz,p} \\ d\gamma_{yz,p} \\ d\gamma_{xz,p} \\ d\gamma_{xy,p} \end{pmatrix} = \begin{pmatrix} d\varepsilon^{(0)}_{xx,p} - \frac{d\omega_{xy}\gamma_{xy,p}}{2} - \frac{d\omega_{xz}\gamma_{xz,p}}{2} \\ d\varepsilon^{(0)}_{yy,p} + \frac{d\omega_{xy}\gamma_{xy,p}}{2} - \frac{d\omega_{yz}\gamma_{yz,p}}{2} \\ d\varepsilon^{(0)}_{zz,p} + \frac{d\omega_{xz}\gamma_{xz,p}}{2} + \frac{d\omega_{yz}\gamma_{yz,p}}{2} \\ d\gamma^{(0)}_{yz,p} + d\omega_{yz}(\varepsilon_{yy,p} - \varepsilon_{zz,p}) + \frac{d\omega_{xz}\gamma_{xy}}{2} + \frac{d\omega_{xy}\gamma_{xz}}{2} \\ d\gamma^{(0)}_{xz,p} + d\omega_{xz}(\varepsilon_{xx,p} - \varepsilon_{zz,p}) + \frac{d\omega_{yz}\gamma_{xy}}{2} - \frac{d\omega_{xy}\gamma_{yz}}{2} \\ d\gamma^{(0)}_{xy,p} + d\omega_{xy}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) - \frac{d\omega_{yz}\gamma_{xz}}{2} - \frac{d\omega_{xz}\gamma_{yz}}{2} \end{pmatrix} \tag{3.16}$$

where $d\varepsilon^{(0)}_{ij,p}$ are calculated plastic strain increments (and may be zero when deformation is elastic). These equations appear with published hypoelasticity equation, but the derivation explicitly from polar decomposition is usually not given along with the equations.

Although most hypoelastic methods use the above first order method, in 2D, one can expand $\mathbf{dR} = \mathbf{R}(\theta + d\omega/2)\mathbf{R}^T(\theta)$ to second order in infinitesimal rotation terms:

$$d\boldsymbol{\omega} = \mathbf{dR} - \mathbf{I} = \begin{pmatrix} -\frac{d\omega^2_{xy}}{8} & -\frac{d\omega_{xy}}{2} \\ \frac{d\omega_{xy}}{2} & -\frac{d\omega^2_{xy}}{8} \end{pmatrix} \tag{3.17}$$

The stress and plastic strain (accounting for engineering strain) become:

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} d\sigma^{(0)}_{xx} - d\omega_{xy}\tau_{xy} - \frac{d\omega^2_{xy}}{4}(\sigma_{xx} - \sigma_{yy}) \\ d\sigma^{(0)}_{yy} + d\omega_{xy}\tau_{xy} + \frac{d\omega^2_{xy}}{4}(\sigma_{xx} - \sigma_{yy}) \\ d\tau^{(0)}_{xy} + \frac{d\omega_{xy}}{2}(\sigma_{xx} - \sigma_{yy}) - \frac{d\omega^2_{xy}}{2}\tau_{xy} \end{pmatrix} \tag{3.18}$$

and:

$$\begin{pmatrix} d\varepsilon_{xx,p} \\ d\varepsilon_{yy,p} \\ d\gamma_{xy,p} \end{pmatrix} = \begin{pmatrix} d\varepsilon^{(0)}_{xx,p} - \frac{1}{2} d\omega_{xy}\gamma_{xy,p} - \frac{d\omega^2_{xy}}{4}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) \\ d\varepsilon^{(0)}_{yy,p} + \frac{1}{2} d\omega_{xy}\gamma_{xy,p} + \frac{d\omega^2_{xy}}{4}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) \\ d\gamma^{(0)}_{xy,p} + d\omega_{xy}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) - \frac{d\omega^2_{xy}}{2}\gamma_{xy,p} \end{pmatrix} \tag{3.19}$$

But, it may be inconsistent to use second order incremental rotation when everything else in first order.

Chapter 4

Thermodynamics of Deformation

4.1 Introduction

In MPM, all thermodynamics quantities will vary with position by depending on particle state. Work is done on a particle by stresses and strains and a particle can exchange heat with neighboring particles by conduction or with exterior by thermal boundary conditions. `NairnMPM/OSParticulas` can run in two different modes labeled as "Adiabatic" or "Isothermal," but these modes refer to individual particles and not to global style of the simulation. The "Adiabatic" mode is essentially the correct physics for a dynamic problem where any mechanism that can cause particle temperature to change will change its temperature. The main mechanisms are coupling between volume change and heat (*e.g.*, compression heating) and dissipated energy (*e.g.*, plasticity, viscoelasticity, damage, *etc.*). This temperature change will remain on the particle but may transfer to other particles if conduction is activated. The "Isothermal" mode means those mechanisms will not change the particle temperature. Physcially, this mode corresponds to all energy that would cause temperature rise being converted to heat energy and exchanged with the exterior. Because heat conduction is normally slow, this mode is not physcially realistic, but it is useful when trying to get quasi-static results that are quasi-static for both mechanical and thermal effects. Most literature numerical and analytical results are isothermal, which makes the "isothermal" mode useful when running comparisons.

The thermodynamics of the global problems will depend on boundary conditions and conduction calculations. A given problem can model a global system that is described as "isolated" or "nonisolated" where an isolated system has no thermal boundary conditions that cause heat input or temperature changes on any particles. A nonisolated system has thermal boundary conditions. Similarly, the particles can be "isolated" or "nonisolated," which refer to conduction being off (isolated) or on (nonisolated).

First imagine each MPM particle as a "system" with all other particles and boundary conditions being the "exterior." The differential in particle internal energy per unit mass, U, with dissipative and irreversible processes is:

$$dU = dw + dq = \frac{1}{\rho}\boldsymbol{\sigma}\cdot\nabla\boldsymbol{u} + T\,d_eS \tag{4.1}$$

where dw is work and dq is heat exchanged with the particle's "exterior" (which includes conduction when activated). The second form associates work with stress power or work energy, where $\nabla\boldsymbol{u}$ is the deformation gradient, and heat flow with $dq = T\,d_eS$ where d_eS is the change in entropy (per unit mass) due to exchange of energy with the exterior. The full change in entropy per unit mass is

$$dS = \left(\frac{dS}{d\nabla\boldsymbol{u}}\right)_T\cdot\nabla\boldsymbol{u} + \frac{C_v dT}{T} \tag{4.2}$$

If we allow for irreversible increase in entropy of $d_i S = d\Phi/T$ due to dissipated energy, the entropy increment can be written as

$$dS = d_e S + d_i S = \left(\frac{dS}{d\nabla \boldsymbol{u}}\right)_T \cdot \nabla \boldsymbol{u} + \frac{C_v dT}{T} - \frac{d\Phi}{T} + \frac{d\Phi}{T} \tag{4.3}$$

or

$$d_e S = \left(\frac{dS}{d\nabla \boldsymbol{u}}\right)_T \cdot \nabla \boldsymbol{u} + \frac{C_v dT}{T} - \frac{d\Phi}{T} \tag{4.4}$$

Now define $dT_{dS=0}$ as the temperature change that would occur for an isoentropic process:

$$dT_{dS=0} = -\frac{T}{C_v}\left(\frac{dS}{d\nabla \boldsymbol{u}}\right)_T \cdot \nabla \boldsymbol{u} \tag{4.5}$$

and dT_{ad} as temperature increase due to isoentropic temperature change plus dissipated energy:

$$dT_{ad} = dT_{dS=0} + \frac{d\Phi}{C_v} \tag{4.6}$$

The entropy increments become

$$dS = \frac{C_v(dT - dT_{dS=0})}{T}, \quad d_e S = \frac{C_v(dT - dT_{ad})}{T}, \quad \text{and} \quad d_i S = \frac{d\Phi}{T} \tag{4.7}$$

For an elastic material

$$dT_{dS=0} = -\frac{\mathsf{M} \cdot \nabla \boldsymbol{u} T}{\rho C_v} \tag{4.8}$$

where M is the stress-temperature tensor:

$$\mathsf{M} = -\left(\frac{dS}{d\nabla \boldsymbol{u}}\right)_T = \left(\frac{\partial \boldsymbol{\sigma}}{\partial T}\right)_{\boldsymbol{u}} \tag{4.9}$$

For an isotropic, elastic material, $\mathsf{M} \cdot \nabla \boldsymbol{u} = -K\alpha_V \Delta V/V$ (here $\alpha_V \approx 3\alpha$ is the volumetric thermal expansion coefficient and should revisit this result for large deformation theory) leading to

$$\frac{dT_{dS=0}}{T} = -\frac{K\alpha_V}{\rho C_v}\frac{\Delta V}{V} = -J\frac{K}{K_0}\gamma_0\frac{\Delta V}{V} = -\frac{K}{K_0}\gamma_0\frac{\Delta V}{V_0} \tag{4.10}$$

where $J = V/V_0 = \rho_0/\rho$ and

$$\gamma_0 = \frac{K_0\alpha_V}{\rho_0 C_v} \tag{4.11}$$

Special cases of this analysis are given for an ideal gas (Eq. (8.166)) and for Mie-Grüniesen materials (Eq. (8.97)).

The goal of `NairnMPM/OSPartriculas` is to track heat, entropy and all other appropriate energies such as Internal energy and Helmholz energy:

$$A = U - TS \tag{4.12}$$

The challenge is dealing with material-specific dissipation or other isoentropic temperature changes while also allowing for external heating through thermal boundary conditions and heat conduction (*i.e.*, dealing with all simulation modes described above).

4.2 Adiabatic Mode

This mode is not really adiabatic, but rather corresponds to expected behavior for a full dynamic solution in that any material mechanism that causes temperature change will initially cause the particle temperature to rise by dT_{ad}. On subsequent time steps, the new temperature distribution and/or boundary conditions may cause heat flow that models general conditions of the problem. Examples of material specific mechanisms are volume change effects, plasticity, damage, *etc.*. In addition to this adiabatic processes, heat may flow through the system by conduction. The particle temperature update in the conduction code is

$$dT_p = dT_{cond} + dT_{ad} \tag{4.13}$$

The change in heat energy on a particle is only due to this conductive (or external) heating:

$$dq = C_v dT_{cond} \tag{4.14}$$

The particle updates become:

$$\begin{aligned} dT_p &= dT_{cond} + dT_{ad} && (4.15)\\ dq_p &= C_v dT_{cond} && (4.16)\\ dS_p &= \frac{C_v dT_{cond} + d\Phi}{T} = dS_{e,p} + dS_{i,p} && (4.17) \end{aligned}$$

where $d\Phi$ is dissipated energy. The entropy can separately track reversible and irreversible entropy, if ever useful, but currently only gets total entropy.

If a thermal ramp is used in conjunction with conduction and material temperature changes, the temperature added to each particle should increment heat energy and entropy as well using

$$dT_p = dT_{ramp}, \qquad dq_p = C_v dT_{ramp}, \qquad \text{and} \qquad dS_p = \frac{C_v dT_{ramp}}{T} \tag{4.18}$$

4.3 Isothermal Mode

For locally isothermal mode, it is assumed that all temperature increases in dT_{ad} are exchanged with the exterior through heat flow. This mode is an artificial mode in dynamic processes, but corresponds to bulk of literature computational mechanics and virtually all analytical solutions. It is therefore useful for comparison to other methods and verification of implemented constitutive laws. The particle updates become:

$$\begin{aligned} dT_p &= dT_{cond} && (4.19)\\ dq_p &= C_v(dT_{cond} - dT_{ad}) && (4.20)\\ dS_p &= \frac{C_v(dT_{cond} - dT_{ad}) + d\Phi}{T} = dS_{e,p} + dS_{i,p} && (4.21) \end{aligned}$$

If a thermal ramp is active, it adds to temperature, heat energy, and entropy as described in previous section. Note that if conduction is not activated causing $dT_{cond} = 0$, this mode has only non-zero q_p and S_p, and these terms do not affect any mechanics calculations (except for the Mie-Grüniesen materials). This mode thus corresponds to most mechanics models and solutions that are decoupled from heat equations.

4.4 Energy Tracking in `NairnMPM/OSParticulas`

Instead of tracking only total U (or any other state variable), a better approach is for each material type to track total work, w, heat energy, q, and entropy. The work update is:

$$dw = \frac{1}{\rho}\boldsymbol{\sigma}\cdot\nabla\boldsymbol{u} \tag{4.22}$$

It is also useful to track thermoelastic strain energy, W, whose increment is

$$dW = dw - dw_{res} \qquad \text{where} \qquad dw_{res} = \frac{1}{\rho}\boldsymbol{\sigma}\cdot d\boldsymbol{\varepsilon}_{res} \tag{4.23}$$

and $d\boldsymbol{\varepsilon}_{res}$ is the free residual strain for the current time step.

Particle temperature, heat, and entropy can incrementally be tracked in each strain update, in the particle update, and in thermal ramp (if used). In each strain update, the updates are:

$$\sum dT_{ad} \quad += \quad \begin{cases} dT_{ad} & \text{adiabatic} \\ 0 & \text{isothermal} \end{cases} \tag{4.24}$$

$$dq_p \quad = \quad \begin{cases} 0 & \text{adiabatic} \\ -C_v dT_{ad} & \text{isothermal} \end{cases} \tag{4.25}$$

$$dS_p \quad = \quad \begin{cases} \dfrac{d\Phi^{(n)}}{T_{g\to p}} & \text{adiabatic} \\ \dfrac{-C_v dT_{ad} + d\Phi}{T_{g\to p}} = \dfrac{-C_v dT_{dS=0}}{T_{g\to p}} & \text{isothermal} \end{cases} \tag{4.26}$$

Note that the particle temperature is not incremented by dT_{ad} in the strain update because that approach causes minor inconsistencies between various strain update modes (`USF`, `USAVG±`, and `USL±`). Instead, dT_{ad} is added to a buffer, which is used in the particle updates. In particle updates:

$$dT_p = dT_{cond} + \sum dT_{ad} \tag{4.27}$$

$$dq_p = C_v dT_{cond} \tag{4.28}$$

$$dS_p = \frac{C_v dT_{cond}}{T_{g\to p}} \tag{4.29}$$

Note that the buffer, $\sum dT_{ad}$ will be zero in isothermal mode or only added in the adiabatic mode. Likewise, the updates in a thermal ramp are same in both modes:

$$dT_p = dT_{ramp}, \qquad dq_p = C_v dT_{ramp}, \qquad \text{and} \qquad dS_p = \frac{C_v dT_{ramp}}{T} \tag{4.30}$$

Note that the $d\Phi$ terms are irreversible entropy production. These results could be used to separately track reversible and irreversible entropy if that ever becomes useful (maybe in plasticity, in damage, or in cracks? But, cracks would require dealing with way they are added not through a conduction source?)

Each material model's constitutive law in `NairnMPM/OSParticulas` is responsible for tracking w and w_{res} using the above updates. Material constitutive laws, however, should not update particle T, q, or S on their own. Instead, all temperature and heat updates should be done by the constitutive law calling `IncrementHeatEnergy(mptr,dT`$_{dS=0}$`,dΦ)` where `mptr` is pointer to the material point, `dT`$_{dS=0}$ is isoentropic temperature change on the particle, and $d\Phi \ge 0$ is dissipated heat in the time step.

Table 4.1: The changes in particle heat (dq), global heat (dQ), global entropy (dS), and average temperature (dT) for each `NairnMPM/OSParticulas` thermodynamics mode. For entropy, all processes other than heat conduction are assumed reversible.

		Adiabatic				Isothermal			
System	Particles	dq	dQ	dS	dT	dq	dQ	dS	dT
Isolated	Isolated	0[1]	0	0	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$	0
Isolated	Nonsolated	$\neq 0$[2]	0	≥ 0[2]	$\neq 0$	$\neq 0$[3]	$\neq 0$[3]	$\neq 0$[3]	0[3]
Nonsolated	Isolated	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$[4]	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$[4]
Nonsolated	Nonsolated								

1. If any particles start with a temperature that is different then the stress free temperature, the first time step will add $dq = C_v(dT_i - dT_0)$ to the particle heat energy. The above conditions will hold thereafter, but a constant will be added to dS and dQ.
2. The dq will be due to conduction only and total entropy will increase because conduction is irreversible.
3. This mode is identical to system and particles isolated if the initial temperature of all particles is equal to the stress-free temperature. Thus, a simulation in this mode should turn off conduction for efficiency when all particles are at the stress free temperature.
4. When particles are isolated, the only possible thermal boundary condition is a thermal ramp that applies uniform temperature change to all particles. If there is no thermal ramp, then the system is isolated and refer to first mode instead.

This function automatically updates correctly depending on the current thermodynamics mode being used and takes care of particle temperature update (which is zero if isothermal).

If w, w_{res}, q, S, T, $\boldsymbol{\sigma}$, and ε are tracked than other thermodynamic state functions can be found:

$$U = w + q \tag{4.31}$$

$$A = U - TS = w + q - TS \tag{4.32}$$

$$H = U + \frac{1}{\rho}\boldsymbol{\sigma}\cdot\varepsilon = w + q + \frac{1}{\rho}\boldsymbol{\sigma}\cdot\varepsilon \tag{4.33}$$

$$G = H - TS = w + q + \frac{1}{\rho}\boldsymbol{\sigma}\cdot\varepsilon - TS \tag{4.34}$$

$$W = w - w_{res} \tag{4.35}$$

Finally, table 4.1 summarizes thermodynamics properties of the various system/particle states in the two `NairnMPM/OSParticulas` modes — "Adiabatic" and "Isothermal." The term dq is heat change on a single particle. The global terms are defined by:

$$dQ = \sum_p dq, \quad dS = \sum_p dS_p, \quad \text{and} \quad T = \frac{1}{n_p}\sum_p T_p \tag{4.36}$$

An "isolated" system means no thermal boundary conditions are being used, while a "nonisolated" system has thermal boundary conditions. "Isolated" particles means conduction is turned off, while "nonisolated" particles means conduction is on.

4.5 Alternate Approach Based on Incremental Temperature Change

An alternate approach to heat and entropy calculations is to do them all in the constitutive law based on dT or the incremental temperature change in the current time step. The problem is this dT includes

both heat flow due to conduction and boundary conditions and temperature change due to isoentropic material processes in previous steps. Those two terms have to be separated. This approach is no longer an option in the code.

4.5.1 Adiabatic Mode From Temperature Increment

in adiabatic mode, the instantaneous temperature on the particle will rise by dT_{ad}. This state corresponds to instantaneous confinement of heat on the particle or the particle's $dq = 0$ due to material-specific mechanisms (*e.g.*, due to volume change, plasticity, damage, *etc.*). If conduction is not modeled, the temperature rise will remain on the particle. But in full-physics simulations with conduction, heat generated on the particle will conduct to other particles in later time steps and T on a particle in any time step might also increase due to exchange of heat with the exterior (conduction between particles or thermal input at boundary conditions). Let those temperature changes be dT_{cond} to indicate heat exchange by conduction. For simulations with conduction not modeled, dT_{cond} is replaced by any imposed temperature change (such as a thermal ramp to change all particle temperatures). The change in heat energy on a particle is only due to this conductive (or external) heating:

$$dq = C_v dT_{cond} \tag{4.37}$$

Any adiabatic processes causing dT_{ad} should not contribute to particle heat energy.

In `OSParticulas`, we have to consider three different update modes — `USF`, `USL`, and `USAVG`. All three methods have a single particle update, which includes the single transport property update, but they have one or two strain updates, which is where dT_{ad} is calculated, and strain updates come before and/or after the single particle update. Let subscripts 1 and 2 refer to strain update before and after the particle update. In strain updates, the temperature change provided to the constitutive law is found be extrapolating temperature from the grid (because the method is more reliable than looking at change on the particle). For `USF`:

$$dT_1^{(n)} = T_{g\to p}^{(n)} - T_{g\to p}^{(n-1)} \approx T_p^{(n)} - T_p^{(n-1)} = dT_{cond}^{(n-1)} + dT_{ad,1}^{(n-1)} \qquad dT_2^{(n)} = dT_{ad,2}^{(n)} = 0 \tag{4.38}$$

where $g \to p$ means extrapolation of grid temperature to the particle. This difference is only approximately equal to particle temperature increase that occurred on the previous time step where $dT_{ad}^{(n-1)}$ is done in strain update in the prior time step. The relation is approximate because the first finds $dT_1^{(n)}$ from smoothing of a grid extrapolation while second is particle change from a FLIP update. They should be close is well-behaved and resolved problems. For `USL`

$$\begin{aligned} dT_1^{(n)} &= dT_{ad,1}^{(n)} = 0 && (4.39)\\ dT_2^{(n)} &= T_{g\to p}^{(n)\prime} - T_{g\to p}^{(n-1)\prime} = T_{g\to p}^{(n)} + dT_{cond}^{(n)} - T_{g\to p}^{(n-1)} - dT_{cond}^{(n-1)} && (4.40)\\ &\approx T_p^{(n)} - T_p^{(n-1)} + dT_{cond}^{(n)} - dT_{cond}^{(n-1)} = dT_{cond}^{(n)} + dT_{ad,2}^{(n-2)} && (4.41) \end{aligned}$$

where superscript $(n)'$ means temperature update on the grid due to conduction term only (and calculated before the second strain update). Finally for `USAVG`, $dT^{(n)}$ is found from new extrapolation compared the previous extrapolation used to find $dT^{(n)}$ or:

$$\begin{aligned} dT_1^{(n)} &= T_{g\to p}^{(n)} - T_{g\to p}^{(n-1)\prime} = T_{g\to p}^{(n)} - T_{g\to p}^{(n-1)} - dT_{cond}^{(n-1)} && (4.42)\\ &\approx T_p^{(n)} - T_p^{(n-1)} - dT_{cond}^{(n-1)} = dT_{ad,2}^{(n-2)} + dT_{ad,1}^{(n-1)} && (4.43)\\ dT_2^{(n)} &= T_{g\to p}^{(n)\prime} - T_{g\to p}^{(n)} = T_{g\to p}^{(n)} + dT_{cond}^{(n)} - T_{g\to p}^{(n)} = dT_{cond}^{(n)} && (4.44) \end{aligned}$$

For a general heat flow scheme, we introduce $dT_{q,buf}$ and $dT_{ad,buf}$ to buffer temperature change used in heat energy calculations and temperature change used in particle temperature update. We calculate heat energy in each strain update using

$$dq = C_v(dT - dT_{q,buf}) \quad \text{and clear buffer to} \quad dT_{q,buf} = 0 \tag{4.45}$$

This equation is approximating finding $C_v dT_{cond}$ by removing adiabatic changes from previous steps. The strain update also adds dT_{ad} to $dT_{ad,buf}$. In particle update, the particle temperature update is

$$dT_p = dT_{cond} + dT_{ad,buf} \quad \text{and reset buffers to} \quad dT_{q,buf} = dT_{ad,buf} \quad \text{and} \quad dT_{ad,buf} = 0 \tag{4.46}$$

For USF, step $(n-1)$ will have ended with a particle update that resets buffers to $dT_{q,buf} = dT_{ad,1}^{(n-1)}$ and $dT_{ad,buf} = 0$. The next step will have:

$$\text{Strain Update :} \qquad dq_1 = C_v(dT_1 - dT_{ad,1}^{(n-1)}) \tag{4.47}$$

$$dT_{q,buf} = 0,\ dT_{ad,buf} = dT_{ad,1}^{(n)} \tag{4.48}$$

$$\text{Particle Update :} \qquad dT_p = dT_{cond}^{(n)} + dT_{ad,1}^{(n)} \tag{4.49}$$

$$dT_{q,buf} = dT_{ad,1}^{(n)},\ dT_{ad,buf} = 0 \tag{4.50}$$

$$\text{Net Heat} \qquad dq^{(n)} = C_v(dT_{cond}^{(n-1)} + dT_{ad,1}^{(n-1)} - dT_{ad,1}^{(n-1)}) = C_v dT_{cond}^{(n-1)} \tag{4.51}$$

The final states matches the starting step and therefore repeats on subsequent time steps. For USL, step $(n-1)$ will have ended with a strain update that resets buffers to $dT_{q,buf} = 0$ and $dT_{ad,buf} = dT_{ad,2}^{(n-1)}$. The next step will have:

$$\text{Particle Update :} \qquad dT_p = dT_{cond}^{(n)} + dT_{ad,2}^{(n-1)} \tag{4.52}$$

$$dT_{q,buf} = dT_{ad,2}^{(n-1)},\ dT_{ad,buf} = 0 \tag{4.53}$$

$$\text{Strain Update :} \qquad dq_2 = C_v(dT_2 - dT_{ad,2}^{(n-1)}) \tag{4.54}$$

$$dT_{q,buf} = 0,\ dT_{ad,buf} = dT_{ad,2}^{(n)} \tag{4.55}$$

$$\text{Net Heat} \qquad dq^{(n)} = C_v(dT_{cond}^{(n)} + dT_{ad,2}^{(n-2)} - dT_{ad,2}^{(n-1)}) \tag{4.56}$$

The final states matches the starting step and therefore repeats on subsequent time steps. Summing all steps, the net heat will correctly equal $C_v dT_{cond}$ with adiabatic terms form previous steps canceling out. For USAVG, step $(n-1)$ will have ended with a strain update that resets buffers to $dT_{q,buf} = 0$ and $dT_{ad,buf} = dT_{ad,2}^{(n-1)}$. The next step will have:

$$\text{Strain Update :} \qquad dq_1 = C_v dT_1 \tag{4.57}$$

$$dT_{q,buf} = 0,\ dT_{ad,buf} = dT_{ad,2}^{(n-1)} + dT_{ad,1}^{(n)} \tag{4.58}$$

$$\text{Particle Update :} \qquad dT_p = dT_{cond}^{(n)} + dT_{ad,2}^{(n-1)} + dT_{ad,1}^{(n)} \tag{4.59}$$

$$dT_{q,buf} = dT_{ad,2}^{(n-1)} + dT_{ad,1}^{(n)},\ dT_{ad,buf} = 0 \tag{4.60}$$

$$\text{Strain Update :} \qquad dq_2 = C_v(dT_2 - dT_{ad,2}^{(n-1)} - dT_{ad,1}^{(n)}) \tag{4.61}$$

$$dT_{q,buf} = 0,\ dT_{ad,buf} = dT_{ad,2}^{(n)} \tag{4.62}$$

$$\text{Net Heat} \qquad dq^{(n)} = C_v(dT_{cond}^{(n)} + dT_{ad,2}^{(n-2)} + dT_{ad,1}^{(n-1)} - dT_{ad,2}^{(n-1)} - dT_{ad,1}^{(n)}) \tag{4.63}$$

The final states matches the starting step and therefore repeats on subsequent time steps. Summing all steps, the net heat will correctly equal $C_v dT_{cond}$ with adiabatic terms form previous steps canceling out.

For entropy update in adiabatic mode, the entropy update is

$$dS^{(n)} = \frac{C_v dT^{(n)}_{cond} + d\Phi^{(n)}}{T^{(n-1)}} = \frac{dq^{(n)} + d\Phi^{(n)}}{T^{(n-1)}} \tag{4.64}$$

The first term in the numerator is reversible entropy exchanged with the exterior. The second terms is irreversible entropy (and it must always be positive or $d\Phi^{(n)} \geq 0$).

4.5.2 Isothermal Mode From Temperature Increment

For a locally isothermal process, $dT = 0$ due to material processes, although dT_{cond} may still be nonzero if the system is nonisolated. In fact, conduction and boundary conditions are the only mechanisms to increase particle temperature meaning that $dT = dT_{cond}$. We assume (perhaps inconsistently with a dynamic analysis, but still useful mode), that all heat generated by the particle that would cause a temperature rise in an adiabatic process (dT_{ad}) is expelled to the exterior. An isothermal mode is approximation to quasi-static thermal condition. It is inconsistent for use in dynamic mechanical problems, but useful when ignoring temperature as done in most of the literature. The change in particle heat energy therefore becomes:

$$dq^{(n)} = C_v(dT^{(n)}_{cond} - dT^{(n)}_{ad}) = C_v(dT^{(n)} - dT^{(n)}_{ad}) \tag{4.65}$$

The change in entropy is this heat (which is exchanged with the exterior) and irreversible dissipated energy:

$$dS^{(n)} = \frac{C_v(dT^{(n)} - dT^{(n)}_{ad}) + d\Phi^{(n)}}{T} = \frac{C_v(dT^{(n)} - dT^{(n)}_{dS=0})}{T} \tag{4.66}$$

where $C_v dT^{(n)}_{dS=0} = C_v dT^{(n)}_{ad} - d\Phi$. This update is similar to adiabatic one in previous section, with the simplification that the $dT^{(n)}$ seen on each time step is always equal $dT^{(n)}_{cond}$ (*i.e.*, $dT^{(n)}_{ad}$ is not buffered because it is not needed to separate $dT^{(n)}_{cond}$ from $dT^{(n)}$).

4.5.3 Energy Tracking in `NairnMPM/OSParticulas` From Temperature Increment

Tracking of heat and entropy can be done in universal updates that apply with or without thermal boundary conditions and with or without conduction activated. Those updates are:

$$dq^{(n)} = \begin{cases} C_v(dT^{(n)} - dT_{q,buf}) & \text{adiabatic} \\ C_v(dT^{(n)} - dT^{(n)}_{ad}) & \text{isothermal} \end{cases} \tag{4.67}$$

$$dS^{(n)} = \begin{cases} \dfrac{C_v(dT^{(n)} - dT_{q,buf}) + d\Phi^{(n)}}{T^{(n-1)}} & \text{adiabatic} \\ \dfrac{C_v(dT^{(n)} - dT^{(n)}_{dS=0})}{T^{(n-1)}} & \text{isothermal} \end{cases} \tag{4.68}$$

$$dT^{(n)}_{p,ad} = \begin{cases} dT_{ad,buf} & \text{adiabatic} \\ 0 & \text{isothermal} \end{cases} \tag{4.69}$$

Although these updates are general, simplified equations can be derived for the special case of isolated system and particles (*i.e.* no thermal boundary conditions and no conduction). In this type

of simulation $dT_{ext}^{(n)} = 0$, which implies that for adiabatic mode that $(dT^{(n)} - dT_{ad}^{(n-1)}) = 0$ and for isothermal mode that $dT^{(n)} = 0$. Substitution into the above update gives:

$$dq^{(n)} = \begin{cases} 0 & \text{adiabatic} \\ -C_v dT_{ad}^{(n)} & \text{isothermal} \end{cases} \tag{4.70}$$

$$dS^{(n)} = \begin{cases} \dfrac{d\Phi^{(n)}}{T^{(n-1)}} & \text{adiabatic} \\ -\dfrac{C_v dT_{dS=0}^{(n)}}{T^{(n-1)}} & \text{isothermal} \end{cases} \tag{4.71}$$

$$dT_{p,ad}^{(n)} = \begin{cases} dT_{ad,buf} & \text{adiabatic} \\ 0 & \text{isothermal} \end{cases} \tag{4.72}$$

Note that only one of the buffers is needed.

`NairnMPM/OSParticulas` uses the isolated system and particles special case when possible to avoid needlessly calculating and adding zero. Also note that because $C_v dT_{ad}^{(n)} = C_v dT_{dS=0}^{(n)} + d\Phi^{(n)}$, that all updates have $dS^{(n)} = (dq^{(n)} + d\Phi^{(n)})/T^{(n-1)}$, which follows because $dq^{(n)}$ is reversible heat and $d\Phi^{(n)}/T^{(n-1)}$ is irreversible entropy production. This result could be used to separately track reversible and irreversible entropy if that ever becomes useful (maybe in plasticity, in damage, or in cracks?)

Each material model's constitutive law in `NairnMPM/OSParticulas` is responsible for tracking w and w_{res} using the above updates. Material constitutive laws, however, should not update particle T, q, or S on their own. Instead, all temperature and heat updates should be done by the constitutive law calling `IncrementHeatEnergy(mptr,dT,dT`$_{dS=0}$`,dΦ)` where `mptr` is pointer to the material point, `dT` is total temperature change in the time step, `dT`$_{dS=0}$ is isoentropic temperature change on the particle, and $d\Phi \geq 0$ is dissipated heat in the time step. This function automatically updates correctly depending on the current thermodynamics mode being used and takes care of particle temperature update (which is zero if isothermal). This version of `IncrementHeatEnergy(mptr,dT,dT`$_{dS=0}$`,dΦ)` is no longer in the code.

Chapter 5

Anisotropic Damage Mechanics Materials

5.1 Introduction

This chapter describes softening materials based on anisotropic damage mechanics (ADaM) methods. In ADaM, which are based on small-strain elastic materials, the material's constitutive law is

$$\boldsymbol{\sigma} = \mathbf{C}(\mathbf{I}-\mathbf{D})(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_{res}) \tag{5.1}$$

where $\mathbf{C}$ is undamaged compliance tensor, where $\mathbf{D}$ is a fouth-order damage tensor (note that putting $\mathbf{D}$ after $\mathbf{C}$ differs from other literature with net effect that $\mathbf{D}$ here is transpose or other $\mathbf{D}$ tensors), and $\boldsymbol{\varepsilon}_{res}$ is residual stress (such as $\boldsymbol{\varepsilon}_{res} = \boldsymbol{\alpha} dT + \boldsymbol{\beta} dc$ for residual thermal and moisture stresses). This law is supplemented with an initiation criterion, which starts the damage process, and softening laws/strength models that control damage evolution.

This damage stress is a state function of $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_{res}$, and $\mathbf{D}$. A thermodynamic increment in stress becomes

$$d\boldsymbol{\sigma} = \mathbf{C}(\mathbf{I}-\mathbf{D})(d\boldsymbol{\varepsilon}-d\boldsymbol{\varepsilon}_{res}) - \mathbf{C}d\mathbf{D}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_{res})$$

First, note that strain always appears a $(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_{res})$, which means we can replace that strain by just $\boldsymbol{\varepsilon}$, which is understood to be an effective strain (and effective strain increment) found by subtracting the residual strain (and residual strain increment). The stress update becomes

$$d\boldsymbol{\sigma} = \mathbf{C}\big((\mathbf{I}-\mathbf{D})d\boldsymbol{\varepsilon} - d\mathbf{D}\boldsymbol{\varepsilon}\big)$$

The tensor $\mathbf{D}$ is a state variable describing the current state of damage. Whenever $\mathbf{D}$ is constant, the stress increment describes a material with reduced stiffness $\mathbf{C}_{eff} = \mathbf{C}(\mathbf{I}-\mathbf{D})$. The elastic potential energy of the damaged material is

$$\Psi = \frac{1}{2}\mathbf{C}(\mathbf{I}-\mathbf{D})\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}$$

Note: some papers call it Helmholz energy, but that would need $-ST$ as well and would need to account for heat caused by energy dissipation. Whenever $\mathbf{D}$ changes, the material dissipates energy. The energy dissipation rate is

$$d\Omega = \boldsymbol{\sigma}\cdot d\boldsymbol{\varepsilon} - d\Psi = \frac{1}{2}\mathbf{C}d\mathbf{D}\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \tag{5.2}$$

This energy increment must be zero during elastic deformation and always positive during damage evolution.

5.2 One Dimensional Damage Mechanics

We start with one dimensional damage mechanics, because it lays out the principles and helps to guide the proper approach of extending to 3D damage mechanics. The 1D stress and stress update are

$$\sigma = E(1-D)\varepsilon \qquad \text{and} \qquad d\sigma = E(1-D)d\varepsilon - E\varepsilon dD \tag{5.3}$$

where modulus E replaces $\mathbf{C}$, scalar D replaces tensor $\mathbf{D}$, and scalar ε replaces tensor $\boldsymbol{\varepsilon}$. First, we define a cracking strain such that total strain is partitioned into elastic and cracking strain ($\varepsilon = \varepsilon_e + \varepsilon_c$) and stress is due solely to the elastic strain:

$$\sigma = E\varepsilon_e = E(\varepsilon - \varepsilon_c) \qquad \text{and} \qquad d\sigma = E(d\varepsilon - d\varepsilon_c)$$

The cracking strain characterizes the opening of a crack or a "strong discontinuity." Comparing to Eq. (5.3), cracking strain is related to D by

$$\varepsilon_c = D\varepsilon \qquad \text{and} \qquad d\varepsilon_c = Dd\varepsilon - \varepsilon dD$$

In other words, a physical interpretation of D is as the ratio of cracking strain to total strain ($D = \varepsilon_c/\varepsilon$) and this interpretation applies during both elastic loading (D constant) and damage evolution ($dD \neq 0$). This interpretation of D differs from the conventional interpretation that D corresponds to an effective modulus $E_{eff} = E(1-D)$. These two interpretations give identical results in 1D damage mechanics, but the strain-ratio view is preferred when extending to 3D.

To complete the 1D analysis, we postulate the existence of a material property, $F(\delta)$, that gives the material's strength as a function of a second damage state variable, δ. $F(\delta)$ is often referred to as the material's softening law. Perhaps a better term for $F(\delta)$ is a 1D strength model for the material. The definition of δ is as the *critical cracking strain* at which the stress reaches $F(\delta)$ in the current state of damage. A relation between D and δ is derived by solving for the strain to initiate damage, ε_i, and then expressing D using its ratio interpretation or $D = \delta/\varepsilon_i$:

$$\sigma = E(\varepsilon_i - \delta) = F(\delta) \quad \Longrightarrow \quad \varepsilon_i = \delta + \frac{F(\delta)}{E} \quad \Longrightarrow \quad D = \frac{\delta}{\varepsilon_i} = \frac{\delta}{\delta + \frac{F(\delta)}{E}} \tag{5.4}$$

Equation (5.4) shows that damage evolution can be tracked using either D or δ. The traditional approach in the literature is to track D. This parameter goes from 0 to 1 and directly describes evolving elastic properties and is directly related to energy dissipation (see Energy Dissipation). In contrast, δ goes from 0 to δ_{max} and it describes crack opening displacement of the displacement discontinuity.

For general softening laws, the relations in Eq. (5.4) require numerical inversion to get D from δ. But for linear softening law ($F(\delta) = \sigma_I(1-\delta_n/\delta_{max})$), analytical inversion is possible:

$$D = \frac{\delta}{\delta + \varepsilon_0\left(1 - \frac{\delta}{\delta_{max}}\right)} \quad \text{and} \quad \delta = \frac{\delta_{max} D\varepsilon_0}{\delta_{max}(1-D) + D\varepsilon_0} \tag{5.5}$$

where $\varepsilon_0 = \sigma_I/E = F(0)/E$ is strain to initiate damage. Linear softening in terms of cracking strain translates to nonlinear softening as a function of D:

$$F(D) = \frac{\sigma_I}{1 + \frac{\varepsilon_0}{\delta_{max}}\frac{D}{1-D}} \tag{5.6}$$

These two softening laws are plotted in Fig. 5.1 and compared to exponential and smooth-step softening laws (see Section 5.7). What might ask why use δ in the strength model instead of D? If one plots stress as a function fo strain for a softening the material, the softening *vs.* strain is described better by $F(\delta)$. In other words, selecting $F(\delta)$ is more intuitive than selecting $F(D)$. The shape of the $F(D)$ curves corresponding to linear softening emphasizes this comment.

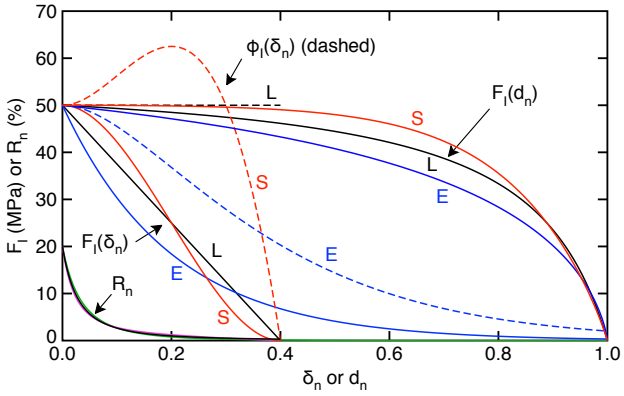

Figure 5.1: Plots for $F(\delta)$, $F(D)$, $\mathbb{R}(\delta)$, and $\varphi(\delta)$ for linear (L), exponential (E), and smooth-step (S) strength models. The plots used properties $E = 1000$ MPa, $G_c = 1000$ J/m^2, $\sigma_I = 50$ MPa, and $\varepsilon_0 = 0.05$. Assuming particle size of $\Delta x_p = 0.1$ mm, these properties give $\delta_{max} = 0.4$. The limiting values for linear softening are $\mathbb{R}(0) = 20$ and $\mathbb{R}(\delta_{max}) = 0.3125$.

1D Numerical Implementation

Numerical implementation has an initiation phase and damage evolution phases. The follow steps describe 1D numerical implementation in terms that facilitate extending it to 3D:

Initiation Phase: At the start of a simulation, $\delta = D = 0$ and the material evolves until stress reaches the initiation stress state. In 1D, the initiation stress is the strength model or $\sigma_i = F(0)$. Prior to initiation, the material evolves as an undamaged material. Once damage initiates, the material point is marked as damaged and subsequent steps may involve damage evolution. The initiation process also requires finding normal to an initiated crack. In 1D, the normal is in the one direction (3D modeling will need more work on initiation).

Damage Evolution: Once a material point is damaged, each increment starts by evaluating a trial stress that assumes no change in damage.

$$\sigma^{(trial)} = E(1-D)d\varepsilon$$

If $\sigma^{(trial)} \le F(\delta)$, the update is elastic. The trial stress is accepted, no changes are made to d or D, but after initiation one should track and update cracking strain — it updates by $d\varepsilon_c = Dd\varepsilon$.

If $\sigma^{(trial)} > F(\delta)$, the damage state has to evolve. For small inrements, all damage evolution steps will start with $\sigma = F(\delta)$ and damage evolution corresponds to moving on the failure surface of the material. The stress increment must therefore match the damage surface evolution or:

$$\nabla\sigma \cdot (d\varepsilon, dD) = F'(\delta)d\delta$$
$$E(1-D)d\varepsilon = E\varepsilon dD + F'(\delta)d\delta$$

To solve for increment in δ, we express increment in D by

$$\mathbb{R}(\delta) = \frac{dD}{d\delta} = \frac{\varphi(\delta)}{E\left(\delta + \frac{F(\delta)}{E}\right)^2} \quad \text{where} \quad \varphi(\delta) = F(\delta) - \delta F'(\delta)$$

Other useful forms for $\mathbb{R}(\delta)$ are

$$\mathbb{R}(\delta) = \frac{E(1-D)^2\varphi(\delta)}{F(\delta)^2} = \frac{(1-D)D\varphi(\delta)}{\delta F(\delta)} = \frac{D^2\varphi(\delta)}{E\delta^2} = \frac{\sigma D\varphi(\delta)}{\varepsilon E\delta F(\delta)} \tag{5.7}$$

These results are general (depending only of relation between D and δ).

For an example of this new function, the $\mathbb{R}(\delta)$ function for linear softening becomes:

$$\mathbb{R}(\delta) = \frac{\varepsilon_0}{\left(\delta + \varepsilon_0\left(1 - \frac{\delta}{\delta_{max}}\right)\right)^2}$$

Example plots for $\mathbb{R}(\delta)$ and $\varphi(\delta)$ are given in Fig. 5.1. Note that for linear softening than $\mathbb{R}(0) = 1/\varepsilon_0$ and $\mathbb{R}(\delta_{max}) = \varepsilon_0/\delta_{max}^2$. Figure 5.1 also plots exponential and smooth-step softening laws along with their $\mathbb{R}(\delta)$ and $\varphi(\delta)$ curves (see Section 5.7). Although softening laws look different, their $\mathbb{R}(\delta)$ are nearly identical. Also note that the smooth-step $\mathbb{R}(\delta_{max}) \to 0$, which may be a preferred behavior, but $\varphi(\delta)$ is constant for linear softening, which may also be preferred.

Using the $\mathbb{R}(\delta)$ function and noting that $\varepsilon = \delta/D$ during 1D damage evolution, the increment in δ simplifies to

$$d\delta = \frac{E(1-D)d\varepsilon}{F'(\delta) + E\varepsilon\mathbb{R}(\delta)} = \frac{E(1-D)d\varepsilon}{F'(\delta) + E(1-D)\frac{\varphi(\delta)}{F(\delta)}} = \frac{d\varepsilon}{(1 + \frac{E\delta}{F(\delta)})\frac{F'(\delta)}{E} + 1 - \frac{\delta F'(\delta)}{F(\delta)}} = \frac{d\varepsilon}{1 + \frac{F'(\delta)}{E}} \tag{5.8}$$

The increment in cracking strain during 1D damage evolution ($d\varepsilon_c = Dd\varepsilon + \varepsilon\mathbb{R}d\delta$) is

$$d\varepsilon_c = Dd\varepsilon + \frac{\sigma D\varphi(\delta)}{E\delta F(\delta)}d\delta$$

Using the identity:

$$1 + \frac{F'(\delta)}{E} = \frac{1}{D} - \frac{\varphi(\delta)}{E\delta} \qquad \text{or} \qquad \frac{D\varphi(\delta)}{E\delta} = 1 - D\left(1 + \frac{F'(\delta)}{E}\right)$$

this form transforms to

$$d\varepsilon_c = D\left[d\varepsilon - \frac{\sigma}{F(\delta)}\left(1 + \frac{F'(\delta)}{E}\right)d\delta\right] + \frac{\sigma}{F(\delta)}d\delta \tag{5.9}$$

Finally, using 1D evolution equation and noting that $\delta = F(\delta)$, this results reduces to $d\varepsilon_c = d\delta$. In other words, cracking strain is equal to δ during damage evolution or δ is physically equal to the maximum value of cracking strain seen during a simulation: $\delta = \max(\varepsilon_c)$. This interpretation does not hold in 3D.

An alternate solution to damage evolution is to imagine $F(\delta)$ as a failure surface. If a trial state exceeds this 1D surface, we evaluate damage increment with a "return" vector r that moves to the evolved fracture surface

$$\sigma = \sigma^{(trial)} - E\varepsilon dD = \sigma^{(trial)} - r = F(\delta + d\delta)$$

Expanding all terms in a Taylor series to first order gives

$$\sigma_0 + E(1-D)d\varepsilon - E\varepsilon dD = F(\delta) + F'(\delta)d\delta$$

Noting that $\sigma_0 = F(\delta)$ at the start of the step, this geometric approach is identical to the gradient equation. In 3D, the surface interpretation is sometimes easier, albeit equivalent, to the gradient equation approach.

Energy Dissipation

In one-dimensional loading, the energy dissipation rate is

$$d\Omega = \frac{1}{2}E\varepsilon^2 dD = \frac{1}{2}E\varepsilon^2 \mathbb{R}(\delta)d\delta = \frac{1}{2}\frac{\sigma D\varepsilon\varphi(\delta)}{\delta F(\delta)}d\delta = \frac{1}{2}\varphi(\delta)d\delta$$

The last step recognized that $\sigma = F(\delta)$ and $\delta = D\varepsilon$ during 1D damage evolution (this result will have to change in 3D). During uniaxial damage loading, the energy dissipation per unit volume has three equivalent forms:

$$d\Omega = \frac{d\overline{G}}{d\varepsilon}d\varepsilon = \frac{1}{2}\left(\frac{\varphi(\delta)}{1+\frac{F'(\delta)}{E}}\right)d\varepsilon = \frac{1}{2}\left(F(\delta) - \frac{\varepsilon F'(\delta)}{1+\frac{F'(\delta)}{E}}\right)d\varepsilon$$

where $\overline{G}$ is the energy released per unit volume.

The total energy dissipated up to current crack opening strain during uniaxial loading can be found by integration:

$$\overline{G} = \frac{1}{2}\int_{\varepsilon_0}^{\varepsilon}\left(F(\delta) - \varepsilon F'(\delta)\frac{d\delta}{d\varepsilon}\right)d\varepsilon$$

The initial limit is ε_0 because the dissipated energy only occurs during damage loading. Integrating the second term by parts gives

$$\overline{G} = \int_{\varepsilon_0}^{\varepsilon} F(\delta)d\varepsilon - \frac{1}{2}\varepsilon F(\delta)|_{\varepsilon_0}^{\varepsilon_n} \tag{5.10}$$

$$= \int_{\varepsilon_0}^{\varepsilon} F(\delta)d\varepsilon + \frac{\sigma_I\varepsilon_0}{2} - \frac{\varepsilon_n F(\delta_n)}{2} \tag{5.11}$$

Integrating instead over δ (the second term integrated by parts) gives

$$\overline{G} = \frac{1}{2}\int_0^{\delta}(F(\delta) - \delta F'(\delta))d\delta = \int_0^{\delta} F(\delta)d\delta - \frac{1}{2}\delta F(\delta)|_0^{\delta} = \int_0^{\delta} F(\delta)d\delta - \frac{\delta F(\delta)}{2} \tag{5.12}$$

The second term is energy released on unloading elastically from $F(\delta)$ to zero load over total cracking strain of δ. At failure, $F(\delta_{max}) = 0$ leading to the expected result for total energy released up to failure of:

$$\overline{G} = \int_0^{\delta_{max}} F(\delta)d\delta \tag{5.13}$$

This result ties total dissipated energy to area under the strength model.

To connect to critical energy release rate per unit area, multiply by particle volume (V_p) and then divide by crack surface area across the particle (A_c accounting for orientation) to get toughness:

$$G_{Ic} = \frac{V_p\rho\overline{\sigma}_I}{A_c}\int_0^{\delta_{max}}\frac{F(\delta)}{\sigma_I}d\delta \tag{5.14}$$

where $\overline{\sigma}_I$ is a specific stress at initiation Given toughness, V_p, and A_c, this equation can be solved to find the appropriate δ_{max} (see Examples of Softening Laws for δ_{max} solutions).

5.3 Three Dimensional Damage Mechanics

This section considers extension to 3D in general terms (*e.g.*, for initially isotropic or anisotropic materials) and makes no assumptions about how damage variables in different directions are coupled (until those assumptions are needed).

5.3.1 Damage Initiation

This material evolves as a standard, small strain material until the stress state reaches some initiation condition or "strength model." Once strength is reached, damage is initiated and the following sections describe subsequent constitutive law modeling with damage evolution. Beside marking a material point as damaged, a second task of damage initiation is to define normal vector to an initiated crack or discontinuity — $\hat{\boldsymbol{n}}$. This tasks is trivial in 1D, but requires more work in 3D and will depend on the stress state at damage initiation.

An essential property of damage initiation and normal criteria is that they are consistent with subsequent strength models used for damage evolution. In other words, when damage initiates, the crack traction on the initiated crack surface must result in damage evolution on the same time step that initiated the damage. The consequences of this criterion are discussed in the **??** section.

5.3.2 Post Damage Initiation Constitutive Law

Damage evolution modeling is best done in an axis system with the crack normal in the $\hat{\boldsymbol{x}}$ direction, which is denoted as the *crack axis system* (CAS). The first step in 3D define the form of the fourth-rank damage tensor $\mathbf{D}$. That form is best found by the strain-ratio concept for $\mathbf{D}$. In other words, we define a 3D cracking strain as

$$\boldsymbol{\varepsilon}_c = \mathbf{D}\boldsymbol{\varepsilon}$$

Over the volume of a material point (or a finite element), this crack strain corresponds to a cracking opening displacement in the CAS of:

$$COD = \boldsymbol{u} = \Delta x \boldsymbol{\varepsilon}_c \hat{\boldsymbol{n}}$$

where Δx is length of material point in the x direction. By this equation, the only acceptable components of $\boldsymbol{\varepsilon}_c$ in the CAS are $\varepsilon_{c,xx}$, $\gamma_{c,xy}$, γ_{c_xz}. Any other components would correspond to non-physical response that strain parallel to a crack causes it to open. This observation means rows 2, 3, and 4 of $\mathbf{D}$ must be zero (when expressing $\mathbf{D}$ using Voight notation in CAS). Combining this criterion with the requirement that stress be symmetric, the only allowable $\mathbf{D}$ in 3D is:

$$\mathbf{D} = \begin{bmatrix} H(\sigma_{xx})d_n & \frac{H(\sigma_{xx})C_{12}}{C_{11}}d_n & \frac{H(\sigma_{xx})C_{13}}{C_{11}}d_n & \frac{H(\sigma_{xx})C_{14}}{C_{11}}d_n & \frac{H(\sigma_{xx})C_{15}}{C_{11}}d_n & \frac{H(\sigma_{xx})C_{16}}{C_{11}}d_n \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{C_{15}}{C_{55}}d_{xz} & \frac{C_{25}}{C_{55}}d_{xz} & \frac{C_{35}}{C_{55}}d_{xz} & \frac{C_{45}}{C_{55}}d_{xz} & d_{xz} & \frac{C_{56}}{C_{55}}d_{xz} \\ \frac{C_{16}}{C_{66}}d_{xy} & \frac{C_{26}}{C_{66}}d_{xy} & \frac{C_{36}}{C_{66}}d_{xy} & \frac{C_{46}}{C_{66}}d_{xy} & \frac{C_{56}}{C_{66}}d_{xz} & d_{xy} \end{bmatrix} \tag{5.15}$$

where d_n, d_{xy}, and d_{xz} are normal and two shear damage parameters and $H(\sigma_{xx})$ is Heaviside function to distinguish tension and compression on the crack surface. Furthermore, this is not an *optional* form for $\mathbf{D}$ — it is the only form consistent with damage mechanics modeling a crack or a strong discontinuity.

This form is also general for any anisotropic material. For an isotropic material, $\mathbf{D}$ simplifies to

$$\mathbf{D} = \begin{bmatrix} H(\sigma_{xx})d_n & \frac{H(\sigma_{xx})\nu}{1-\nu}d_n & \frac{H(\sigma_{xx})\nu}{1-\nu}d_n & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{xz} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{xy} \end{bmatrix} \tag{5.16}$$

This isotropic form matches the damage tensor first proposed by Chaboche (but transposed and with a modification to account for tension and compression). A key difference is that he derived it as a *specific* $\mathbf{D}$ based on a model for stiffness reduction due to an array of aligned microcracks. The strain-ratio interpretation of $\mathbf{D}$ recommends it as the only damage mechanics tensor and shows that $\mathbf{D}$ can derived without a separate model for stiffness reduction. As a consequence, the large field of fracture mechanics known as "isotropic" or "scalar" damage mechanics that simplifies the analysis by setting $\mathbf{D} = d\mathbf{I}$ (or a diagonal tensor with d on the diagonals) is not a valid extension of damage mechanics to 3D. It is closer to plasticity modeling with softening instead of harding and with unloading using a reduced modulus rather than the initial modulus. It should not be called "damage mechanics."

Elastic Update

An elastic update is an update when $d\mathbf{D} = 0$ or when there is no damage evolution (and energy is conserved). In 3D damage mechanics, a material simply updates by constitutive law at constant $\mathbf{D}$. The only new tasks is to update cracking strain. The full update becomes:

$$d\boldsymbol{\sigma} = \mathsf{C}(\mathbf{I}-\mathbf{D})d\boldsymbol{\varepsilon} \qquad d\boldsymbol{\varepsilon}_c = \mathbf{D}d\boldsymbol{\varepsilon} \qquad d\boldsymbol{\varepsilon}_e = (\mathbf{I}-\mathbf{D})d\boldsymbol{\varepsilon} \qquad d\mathbf{D} = 0$$

Recall that strain here is because an *effective* strain in the present of residual strains or $\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{res}$.

Damage Evolution Update

During damage evolution, $\mathbf{D}$ will change and the full update changes to:

$$d\boldsymbol{\sigma} = \nabla\boldsymbol{\sigma} \cdot (d\boldsymbol{\varepsilon}, d\mathbf{D}) = \mathbf{C}(\mathbf{I}-\mathbf{D})d\boldsymbol{\varepsilon} - \mathbf{C}d\mathbf{D}\boldsymbol{\varepsilon} \tag{5.17}$$

Because of the specific form derived for $\mathbf{D}$ and by doing calculations in the crack axis system, the updates for the three crack tractions are:

$$d\boldsymbol{T} = d\boldsymbol{\sigma} \cdot \hat{\mathbf{n}} = (d\sigma_{xx}, d\tau_{xy}, d\tau_{xz}) \tag{5.18}$$

where stress component increments are analgous to 1D updates or:

$$\begin{pmatrix} d\sigma_{xx} \\ d\tau_{xy} \\ d\tau_{xz} \end{pmatrix} = \begin{pmatrix} C_{11}(d\varepsilon_n - H(\sigma_{xx})d(d_n\varepsilon_n)) \\ C_{55}\big(d\gamma_y - d\big(d_{xy}\gamma_y\big)\big) \\ C_{66}\big(d\gamma_z - d\big(d_{xz}\gamma_z\big)\big) \end{pmatrix} \tag{5.19}$$

where

$$\varepsilon_n = \sum_{i=1}^{6} \frac{C_{1i}}{C_{11}}\varepsilon_i \qquad \gamma_z = \sum_{i=1}^{6} \frac{C_{5i}}{C_{55}}\varepsilon_i \qquad \gamma_y = \sum_{i=1}^{6} \frac{C_{6i}}{C_{66}}\varepsilon_i$$

are effective strains associated with normal and shear crack opening deformations and ε_i are components of the usual Voight ordering of strains $\boldsymbol{\varepsilon} = (\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \gamma_{yz}, \gamma_{xz}, \gamma_{xy})$. The cracking strain increments (as full differentials) in the crack axis system are:

$$d\varepsilon_{c,xx} = H(\sigma_{xx}) d(d_n \varepsilon_n), \quad d\gamma_{c,xz} = d(d_{xz}\gamma_z), \quad \text{and} \quad d\gamma_{c,xy} = d(d_{xy}\gamma_y) \tag{5.20}$$

Notice that this update reduces to the elastic case when the damage parameters are constant.

To evolve damage, we have to postulate a traction failure surface that gives maximum magnitude as function of damage paramaters and possible strain directions. We denote the strength model as

$$S(\boldsymbol{c}) \quad \text{where} \quad \boldsymbol{c} = (\varepsilon_n, \gamma_y, \gamma_z, \delta_n, \delta_{xy}, \delta_{xz})$$

is a vector of effective strains on the crack and the current damage state of the material. $S(\boldsymbol{c})$ must be a state function of damage, which is best achieved by defining it terms of three unidirectional strength models — $F_n(\delta_n)$, $F_{xy}(\delta_{xy})$, and $F_{xz}(\delta_{xz})$. Because ε_n, γ_y, and γ_z may change during elastic loading that does not change the damage state, $S(\boldsymbol{c})$ can only depend on ratios of these strains (*i.e*, current mode mixity of the deformation) In 3D, the damage parameters, δ_n, δ_{xy} and δ_{xz}, are not maximum cracking strains, but rather correspond to the cracking strain required to initiate damage in the current state of damage if unloaded and then reloaded by uniaxial effective normal or shear strain. Their relations to d_n, d_{xy}, and d_{xz} are identical to the 1D relations:

$$d_n = \frac{\delta_n}{\delta_n + \frac{F_n)}{C_{11}}} \qquad d_{xy} = \frac{\delta_{xy}}{\delta_{xy} + \frac{F_{xy}}{C_{66}}} \qquad d_{xy} = \frac{\delta_{xz}}{\delta_{xz} + \frac{F_{xz}}{C_{55}}} \tag{5.21}$$

Note that the F functions (and subsequent used $\mathbb{R}$ and φ functions) implicitly depend on δ_n, δ_{xy} and δ_{xz} as indicated by their subscript.

Once a strength model is defined, update of the damage parameters can proceed to by two equivalent methods (whichever is easier). The first to equate crack traction increment to change in strength:

$$\nabla \|\boldsymbol{T}\| \cdot d\boldsymbol{c} = \nabla S(\boldsymbol{c}) \cdot d\boldsymbol{c} \quad \text{where} \quad \boldsymbol{T} = (\tau_{xy}, \tau_{xz}, \sigma_{xx})$$

and solve for $d\delta_n$, $d\delta_{xy}$ and $d\delta_{xz}$. The second is move to a trial traction and then if that update is beyond the traction surface, return to the evolved surface. Note that these two approaches will get *only* one equation to update three damage variables. This equation thus must be supplemented by additional assumptions. These assumptions are what will lead to couplings (or lack of couplings) between the damage variables.

Energy Dissipation

3D damage evolution is found by evaluating $\mathbf{C}d\mathbf{D}\boldsymbol{\varepsilon}$ in Eq. (5.2) in the crack axis system leading to

$$\begin{aligned} d\Omega &= \frac{1}{2} \begin{bmatrix} H(\sigma_{xx})C_{11}\varepsilon_n\, dd_n + C_{15}\gamma_z\, dd_{xz} + C_{16}\gamma_y\, dd_{xy} \\ H(\sigma_{xx})C_{12}\varepsilon_n\, dd_n + C_{25}\gamma_z\, dd_{xz} + C_{26}\gamma_y\, dd_{xy} \\ H(\sigma_{xx})C_{13}\varepsilon_n\, dd_n + C_{35}\gamma_z\, dd_{xz} + C_{36}\gamma_y\, dd_{xy} \\ H(\sigma_{xx})C_{14}\varepsilon_n\, dd_n + C_{45}\gamma_z\, dd_{xz} + C_{46}\gamma_y\, dd_{xy} \\ H(\sigma_{xx})C_{15}\varepsilon_n\, dd_n + C_{55}\gamma_z\, dd_{xz} + C_{56}\gamma_y\, dd_{xy} \\ H(\sigma_{xx})C_{16}\varepsilon_n\, dd_n + C_{65}\gamma_z\, dd_{xz} + C_{66}\gamma_y\, dd_{xy} \end{bmatrix} \cdot \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{bmatrix} \\ &= \frac{1}{2} H(\sigma_{xx}) C_{11} \varepsilon_n^2 dd_n + \frac{1}{2} C_{55} \gamma_z^2 dd_{xz} + \frac{1}{2} C_{66} \gamma_y^2 dd_{xy} \end{aligned} \tag{5.22}$$

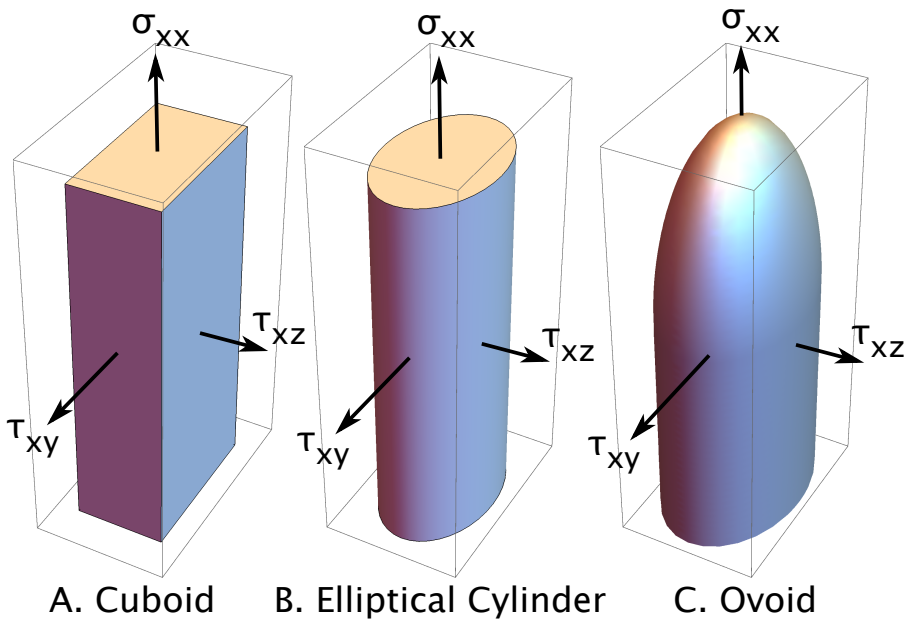

Figure 5.2: Three surface plots illustrating a strength mode, $S(\boldsymbol{c})$ based on a A. cuboid surface, B. elliptical cylinder surfaces, and a C. ovoid surface.

Using Eq. (5.7), energy dissipation can be written in terms of critical cracking strain increments:

$$\begin{aligned} d\Omega &= \frac{H(\sigma_{xx})}{2C_{11}}\left(\frac{\sigma_{xx}}{1-d_n}\right)^2 \mathbb{R}_n\, d\delta_n + \frac{1}{2C_{66}}\left(\frac{\tau_{xy}}{1-d_{xy}}\right)^2 \mathbb{R}_{xy}\, d\delta_{xy} + \frac{1}{2C_{55}}\left(\frac{\tau_{xz}}{1-d_{xz}}\right)^2 \mathbb{R}_{xz}\, d\delta_{xz} \\ &= \frac{H(\sigma_{xx})}{2}\left(\frac{\sigma_{xx}}{F_n}\right)^2 \varphi_n\, d\delta_n + \frac{1}{2}\left(\frac{\tau_{xy}}{F_{xy}}\right)^2 \varphi_{xy}\, d\delta_{xy} + \frac{1}{2}\left(\frac{\tau_{xz}}{F_{xz}}\right)^2 \varphi_{xz}\, d\delta_{xz} \end{aligned} \tag{5.23}$$

Strength Models or Damage Surfaces

Finding damage increments and their energy dissipation requires some traction failure surface and its associated strength model. This section considers the three rational surfaces in Fig. 5.2.

Cuboid Surface

The simplest model is a cuboid with edges of length F_n (in tension), F_{xy}), and F_{xz}; the compression end is unbounded for normal stresses. Assuming this shape, the three components evolve damage independently. This surface thus leads to three decoupled 1D evolutions and explained in 1D Numerical Implementation. The normal evolutions from Eq. (5.8) is:

$$d\delta_n = \frac{d\varepsilon_n}{1+\frac{F_n'}{C_{11}}}$$

The shear evolutions are:

$$d\delta_{xy} = \frac{\text{sign}(\tau_{xy})d\gamma_y}{1+\frac{F_{xy}'}{C_{66}}} \quad d\delta_{xz} = \frac{\text{sign}(\tau_{xz})d\gamma_z}{1+\frac{F_{xz}'}{C_{55}}} \quad \text{where} \quad \text{sign}(\tau_{ij}) = \frac{\tau_{ij}}{|\tau_{ij}|} \tag{5.24}$$

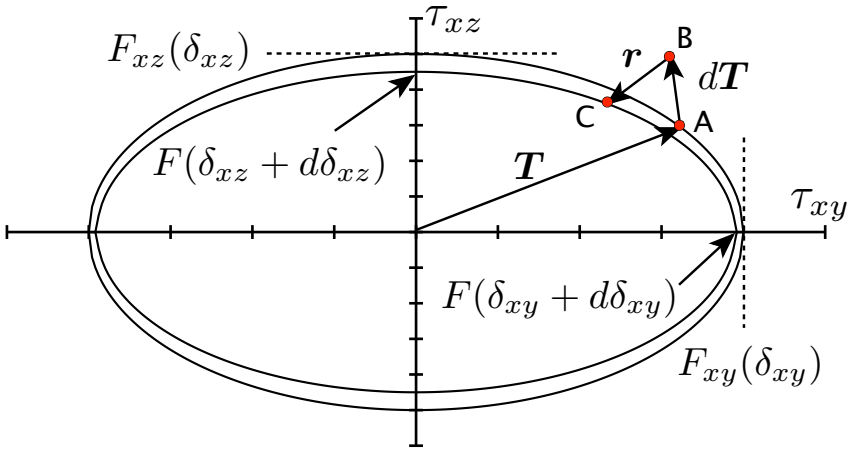

Figure 5.3: Decoupled shear. Point A is previous stress state on the surface. Point B is trial elastic update. Point C is final updated stress state.

where the sign(τ_{ij}) function allow damage to happen by either positive or or negative shear beyond the shear strength. Energy dissipation follows 1D methods in Energy Dissipation.

Cylindrical Surface

This approach still decouples tension and shear. The tension evolves by the Cuboid Surface method while the shear stresses evolve to an ellipse with axes F_{xy} and F_{xz} in 2D plot with shear stress on the axes (see Fig. 5.3). In 2D with only one shear axis, the method reverts to a Cuboid method. For 3D, a coupled analysis is needed.

For a strength model, we write the shear traction vector in terms of shear strains and either d or δ damage paramters:

$$\boldsymbol{T} = \left(C_{66}(1-d_{xy})\gamma_y, C_{55}(1-d_{xz})\gamma_z\right) = \left(\frac{F_{xy}\gamma_y}{\delta_{xy}+\frac{F_{xy}}{C_{66}}}, \frac{F_{xz}\gamma_z}{\delta_{xz}+\frac{F_{xz}}{C_{66}}}\right)$$

Writing shear strains as a vector, $\boldsymbol{\gamma} = (\gamma_y, \gamma_z)$ and its components using polar coordinates as $\gamma_y = \|\boldsymbol{\gamma}\|\sin\theta$ and $\gamma_z = \|\boldsymbol{\gamma}\|\cos\theta$ where $\|\boldsymbol{\gamma}\| = \sqrt{\gamma_y^2+\gamma_z^2}$, the traction magnitude/strain magnitude relation is

$$\|\boldsymbol{T}\| = \|\boldsymbol{\gamma}\|\sqrt{C_{66}^2(1-d_{xy})^2\sin^2\theta + C_{55}^2(1-d_{xz})^2\cos^2\theta} = k_s\|\boldsymbol{\gamma}\|$$

where

$$k_s = \sqrt{C_{66}^2(1-d_{xy})^2\sin^2\theta + C_{55}^2(1-d_{xz})^2\cos^2\theta}$$

where k_s is effective shear stiffness or slope of $\|\boldsymbol{T}\|$ *vs.* $\|\boldsymbol{u}\|$. This traction magnitude causes damage when the elliptical surface is reached and that happens when

$$1 = \left(\frac{T_{xy}}{F_{xy}}\right)^2 + \left(\frac{T_{xz}}{F_{xz}}\right)^2 = \gamma_d^2\left(\frac{C_{66}^2(1-d_{xy})^2\sin^2\theta}{F_{xy}^2} + \frac{C_{55}^2(1-d_{xz})^2\cos^2\theta}{F_{xz})^2}\right) \tag{5.25}$$

where γ_d is the magnitude of the shear strain vector when the traction vector is on the traction failure surface:

$$\gamma_d = \frac{1}{\sqrt{\frac{C_{66}^2(1-d_{xy})^2\sin^2\theta}{F_{xy}^2} + \frac{C_{55}^2(1-d_{xz})^2\cos^2\theta}{F_{xz}^2}}}$$

The strength model can now be represented by a 4D surface given by traction when $\|\boldsymbol{\gamma}\| = \gamma_d$:

$$F(\delta_{xy},\delta_{xz},\theta) = k_s\gamma_d = \sqrt{\frac{C_{66}^2(1-d_{xy})^2\sin^2\theta + C_{55}^2(1-d_{xz})^2\cos^2\theta}{\frac{C_{66}^2(1-d_{xy})^2\sin^2\theta}{F_{xy}^2} + \frac{C_{55}^2(1-d_{xz})^2\cos^2\theta}{F_{xz}^2}}} \tag{5.26}$$

Damage evolution occurs when $\|\boldsymbol{T}\| = k_s\gamma_d$ and $\|\boldsymbol{u}\| = \gamma_d$. It is more conventient to use γ_y and γ_z as the key variables rather then $\|\boldsymbol{u}\|$ and θ. To use them we write

$$\|\boldsymbol{T}\| = \sqrt{C_{66}^2(1-d_{xy})^2\gamma_y^2 + C_{55}^2(1-d_{xz})^2\gamma_z^2}$$

$$F(\gamma_y,\gamma_z,\delta_{xy},\delta_{xz}) = \sqrt{\frac{C_{66}^2(1-d_{xy})^2\gamma_y^2 + C_{55}^2(1-d_{xz})^2\gamma_z^2}{\frac{C_{66}^2(1-d_{xy})^2\gamma_y^2}{F_{xy}^2} + \frac{C_{55}^2(1-d_{xz})^2\gamma_z^2}{F_{xz}^2}}}$$

a. Gradient Equation Solution

The damage evolution equation is then

$$\nabla\big(\|\boldsymbol{T}\| - F(d\gamma_y, d\gamma_z, d\delta_{xy}, d\delta_{xz})\big)\cdot(d\gamma_y, d\gamma_z, d\delta_{xy}, d\delta_{xz}) = 0$$

The gradient in this equation evaluates to

$$\begin{aligned}
\nabla(\|\boldsymbol{T}\| - F) = \Bigg\{ & \frac{C_{66}^2(1-d_{xy})^2\gamma_y}{\|\boldsymbol{T}\|}\left[1 - \overline{\gamma_d}^3 C_{55}^2(1-d_{xz}^2)\gamma_z^2\left(\frac{1}{F_{xz}^2} - \frac{1}{F_{xy}^2}\right)\right], \\
& \frac{C_{55}^2(1-d_{xz})^2\gamma_z}{\|\boldsymbol{T}\|}\left[1 - \overline{\gamma_d}^3 C_{66}^2(1-d_{xy}^2)\gamma_y^2\left(\frac{1}{F_{xy}^2} - \frac{1}{F_{xy}^2}\right)\right], \\
& -\frac{C_{66}^2(1-d_{xy})^2\gamma_y^2}{\|\boldsymbol{T}\|}\left(\left[1 - \overline{\gamma_d}^3 C_{55}^2(1-d_{xz}^2)\gamma_z^2\left(\frac{1}{F_{xz}^2} - \frac{1}{F_{xy}^2}\right)\right]\frac{\mathbb{R}_{xy}(\delta_{xy})}{1-d_{xy}} + \overline{\gamma_d}^3\|\boldsymbol{T}\|^2\frac{F'_{xy}(\delta_{xy})}{F_{xy}^3}\right), \\
& -\frac{C_{55}^2(1-d_{xz})^2\gamma_z^2}{\|\boldsymbol{T}\|}\left(\left[1 - \overline{\gamma_d}^3 C_{66}^2(1-d_{xy}^2)\gamma_y^2\left(\frac{1}{F_{xy}^2} - \frac{1}{F_{xz}^2}\right)\right]\frac{\mathbb{R}_{xz}(\delta_{xz})}{1-d_{xz}} + \overline{\gamma_d}^3\|\boldsymbol{T}\|^2\frac{F'_{xz}(\delta_{xz})}{F_{xz}^3}\right)\Bigg\}
\end{aligned}$$

where

$$\overline{\gamma_d} = \frac{1}{\sqrt{\frac{C_{66}^2(1-d_{xy})^2\gamma_y^2}{F_{xy}^2} + \frac{C_{55}^2(1-d_{xz})^2\gamma_z^2}{F_{xz}^2}}} = \frac{\gamma_d}{\|\boldsymbol{\gamma}\|} \tag{5.27}$$

During damage evolution $\|\boldsymbol{\gamma}\| = \gamma_d$ and therefore $\overline{\gamma_d} = 1$. This result simplifies by replacing $\overline{\gamma_d}^3$ with $\overline{\gamma_d}^2$ (which are both one) and using Eq. (5.27). Two terms then reduce to

$$1 - \overline{\gamma_d}^3 C_{55}^2(1-d_{xz}^2)\gamma_z^2\left(\frac{1}{F_{xz}^2} - \frac{1}{F_{xy}^2}\right) = \frac{\|\boldsymbol{T}\|^2}{F_{xy}^2}$$

$$1 - \overline{\gamma_d}^3 C_{66}^2(1-d_{xy}^2)\gamma_y^2\left(\frac{1}{F_{xy}^2} - \frac{1}{F_{xy}^2}\right) = \frac{\|\boldsymbol{T}\|^2}{F_{xz}^2}$$

Using this result, taking the dot product with increments, and removing constant, non-zero terms leads to

$$\frac{\tau_{xy}^2}{F_{xy}^3}\left(\frac{F_{xy}\mathbb{R}_{xy}}{1-d_{xy}}+F'_{xy}\right)+\frac{\tau_{xz}^2}{F_{xz}^3}\left(\frac{F_{xz}\mathbb{R}_{xz}}{1-d_{xz}}+F'_{xz}\right)=\frac{\tau_{xy}C_{66}(1-d_{xy})}{F_{xy}^2}+\frac{\tau_{xz}C_{55}(1-d_{xz})}{F_{xz}^2}$$

where

$$\tau_{xy}=C_{66}(1-d_{xy})\gamma_y \quad \text{and} \quad \tau_{xz}=C_{65}(1-d_{xz})\gamma_z$$

are the initial shear stresses (which are assumed to fall on the failure surface). Finally, using Eq. (5.7):

$$\frac{F_{xy}\mathbb{R}_{xy}}{1-d_{xy}}+F'_{xy}=\frac{F_{xy}\left(1+\frac{F'_{xy}}{C_{66}}\right)}{\delta_{xy}+\frac{F_{xy}}{C_{66}}}=C_{66}(1-d_{xy})\left(1+\frac{F'_{xy}}{C_{66}}\right) \tag{5.28}$$

with analogous result for xz terms. The damage evolution equation becomes

$$\frac{\tau_{xy}^2C_{66}(1-d_{xy})}{F_{xy}^3}\left(1+\frac{F'_{xy}}{C_{66}}\right)+\frac{\tau_{xz}^2C_{55}(1-d_{xz})}{F_{xz}^3}\left(1+\frac{F'_{xz}}{C_{55}}\right)=\frac{\tau_{xy}C_{66}(1-d_{xy})}{F_{xy}^2}+\frac{\tau_{xz}C_{55}(1-d_{xz})}{F_{xz}^2}$$

c. Return to Fracture Surface Analysis

In Fig. 5.3, point A is the initial stress, which is assumed to start on the current failure surface. Point B is the trial stress update assuming no damage evolution given by:

$$\begin{aligned}\left(\tau_{xy}^{(trial)},\tau_{xz}^{(trial)}\right)&=\left(C_{66}(1-d_{xy})(\gamma_y+d\gamma_y),C_{55}(1-d_{xz})(\gamma_z+d\gamma_z)\right)\\&=\left(\tau_{xy}^{(0)}+C_{66}(1-d_{xy})d\gamma_y,\tau_{xz}^{(0)}+C_{55}(1-d_{xz})d\gamma_z\right)\end{aligned}$$

When point B is outside the envelop, we must return to the evolved envelop or point C, which is given by generalized update with as-yet-unknown increments $d\delta_{xy}$ and $d\delta_{xz}$:

$$\boldsymbol{C}=\left(\tau_{xy}^{(trial)}-C_{66}\gamma_y\mathbb{R}_{xy}d\delta_{xy},\tau_{xz}^{(trial)}-C_{55}\gamma_z\mathbb{R}_{xz}d\delta_{xz}\right)$$

Note that the "return" vector (see Fig. 5.3) is:

$$\boldsymbol{r}=\left(C_{66}\gamma_y\mathbb{R}_{xy}d\delta_{xy},C_{55}\gamma_z\mathbb{R}_{xz}d\delta_{xz}\right)=\left(C_{66}\gamma_y dd_{xy},C_{55}\gamma_z dd_{xz}\right)$$

The damage evolution equation can be derived by finding increments such that updated state falls on the update failure surface:

$$\left(\frac{\tau_{xy}^{(trial)}-C_{66}\gamma_y\mathbb{R}_{xy}d\delta_{xy}}{F_{xy}(\delta_{xy}+d\delta_{xy})}\right)^2+\left(\frac{\tau_{xz}^{(trial)}-C_{55}\gamma_z\mathbb{R}_{xz}d\delta_{xz}}{F_{xz}(\delta_{xz}+d\delta_{xz})}\right)^2=1 \tag{5.29}$$

Expanding and keeping only first-order terms in incremental strain or cracking strain leads to:

$$\frac{\tau_{xy}^2\left(\frac{F_{xy}\mathbb{R}_{xy}}{1-d_{xy}}+F'_{xy}\right)}{F_{xy}^3}d\delta_{xy}+\frac{\tau_{xz}^2\left(\frac{F_{xz}\mathbb{R}_{xz}}{1-d_{xz}}+F'_{xz}\right)}{F_{xz}^3}d\delta_{xz}=\frac{C_{66}\tau_{xy}(1-d_{xy})}{F_{xy}^2}d\gamma_y+\frac{C_{55}\tau_{xz}(1-d_{xz})}{F_{xz}^2}d\gamma_z$$

Using Eq. (5.28) simplifies the evolution equation to:

$$\frac{\tau_{xy}^2 C_{66}(1-d_{xy})\left(1+\frac{F'_{xy}}{C_{66}}\right)}{F_{xy}^3}d\delta_{xy}+\frac{\tau_{xz}^2 C_{55}(1-d_{xz})\left(1+\frac{F'_{xz}}{C_{55}}\right)}{F_{xz}^3}d\delta_{xz} = \frac{\tau_{xy}C_{66}(1-d_{xy})}{F_{xy}^2}d\gamma_y+\frac{\tau_{xz}C_{55}(1-d_{xz})}{F_{xz}^2}d\gamma_z \tag{5.30}$$

or can be expressed in terms of $\mathbb{R}$ functions:

$$\frac{\tau_{xy}^2\left(1+\frac{F'_{xy}}{C_{66}}\right)\mathbb{R}_{xy}d\delta_{xy}}{(1-d_{xy})F_{xy}\varphi_{xy}}+\frac{\tau_{xz}^2\left(1+\frac{F'_{xz}}{C_{55}}\right)\mathbb{R}_{xz}d\delta_{xz}}{(1-d_{xz})F_{xz}\varphi_{xz}}=\frac{\tau_{xy}\mathbb{R}_{xy}d\gamma_y}{(1-d_{xy})\varphi_{xy}}+\frac{\tau_{xz}\mathbb{R}_{xz}d\gamma_z}{(1-d_{xz})\varphi_{xz}} \tag{5.31}$$

d. Coupling Options

The two previous sections gave the same equation, which is one equation in two unknowns. To solve for the upgrade requires a second equation, the consequence of which is to couple the two damage parameters. The following sections summarize some coupling options.

d.1 Linked d Parameters

A desirable result at failure is that all components of crack tracking simultaneously. This goal is achieved by linking the damage parameters or $d_{xy}=d_{xz}$. The second equation for δ's is then

$$\mathbb{R}_{xy}d\delta_{xy}=\mathbb{R}_{xz}d\delta_{xz}$$

d.2 Return From Trial Traction to the Origin

Another way for all components of traction to approach zero simultaneously is for the return vector $\boldsymbol{r}$ to be parallel to the traction vector (or the incrementally different trial traction vector). The second equation is then

$$0=\|\boldsymbol{r}\times\boldsymbol{T}^{(trial)}\|=(1-d_{xy})(\gamma_y+d\gamma_y)\gamma_z\mathbb{R}_{xz}d\delta_{xz}-(1-d_{xz})(\gamma_z+d\gamma_z)\gamma_y\mathbb{R}_{xy}d\delta_{xy}$$

Keeping just first order terms

$$\frac{\mathbb{R}_{xz}d\delta_{xz}}{1-d_{xz}}=\frac{\mathbb{R}_{xy}d\delta_{xy}}{1-d_{xy}}\quad\text{or}\quad\frac{dd_{xz}}{1-d_{xz}}=\frac{dd_{xy}}{1-d_{xy}}$$

At the start of damage, $d_{xy}=d_{xz}=0$ and the update becomes $dd_{xy}=dd_{xz}$. On the next step, the d's will be equal as well as all subsequent steps. In other words this return is identical to synching the d parameters.

d.3. Return Normal to the Failure Surface

One is tempted to adopt methods from plasticity theory (but being careful to recognize that damage mechanics and plasticity are physically different) and derive second equation by returning normal to the failure surface. The normal to the updated failure surface is:

$$\hat{\boldsymbol{n}}\|\hat{\boldsymbol{n}}\|=\left(\frac{\tau_{xy}^{(trial)}-C_{66}\gamma_y\mathbb{R}_{xy}d\delta_{xy}}{F_{xy}^2(\delta_{xy}+d\delta_{xy})},\frac{\tau_{xz}^{(trial)}-C_{55}\gamma_z\mathbb{R}_{xz}d\delta_{xz}}{F_{xz}^2(\delta_{xz}+d\delta_{xz})}\right)$$

For this vector to be parallel to $\boldsymbol{r}$, the coupling equation is

$$\|\boldsymbol{r} \times \boldsymbol{n}\| = 0$$

which explicitly evaluates to:

$$0 = \frac{C_{55}\gamma_z \mathbb{R}_{xz} d\delta_{xz}(\tau_{xy}^{(trial)} - C_{66}\gamma_y \mathbb{R}_{xy} d\delta_{xy})}{F_{xy}^2(\delta_{xy} + d\delta_{xy})} - \frac{C_{66}\gamma_y \mathbb{R}_{xy} d\delta_{xy}(\tau_{xz}^{(trial)} - C_{55}\gamma_z \mathbb{R}_{xz} d\delta_{xz})}{F_{xz}^2(\delta_{xz} + d\delta_{xz})}$$

Expanding and keeping only first order terms in strain or cracking strain increments leads to

$$0 = \frac{\mathbb{R}_{xz}}{(1-d_{xz})F_{xy}^2} d\delta_{xz} - \frac{\mathbb{R}_{xy}}{(1-d_{xy})F_{xz}^2} d\delta_{xy} \tag{5.32}$$

or substituting for $\mathbb{R}$ functions and remove constant terms:

$$C_{66}(1-d_{xy})\varphi_{xy} d\delta_{xy} = C_{55}(1-d_{xz})\varphi_{xz} d\delta_{xz} \tag{5.33}$$

Note that one simplification divided through by $\tau_{xy}^0 \tau_{xz}^0$. Thus formally, these relations apply only when $\tau_{xy}^0 \tau_{xz}^0 \neq 0$, but because the final result is independent of initial stress, we can assume it also for uniaxial shear loading.

Unlike the previous two methods, this method does not reduce to a single d parameter. Thus, the two directions will not simultaneously reach zero at the same time. Perhaps even less realistic, it is possible that uniaxial γ_y loading by τ_{xy} alone could fail first in the zero τ_{xz} direction (depending on relative strength models). Note, however, that if the material is isotropic and $C_{66} = C_{55} = G$, this coupling will result in $d_{xy} = d_{xz}$. Physically, the failure surface becomes a circle that make returning to the origin the same a returning normal to the failure surface. For anisotropic materials, the return to the origin appears to be the better coupling method.

d.4. Energy Minimization or Maximization for Cylindrical Surface

Some damage and fracture principles are based on energy, which could be either to minimize of maximize dissipated energy. For example, mixed-mode crack growth is based on finding the direction that maximizes the energy release rate. For a given return vector, a coupling equation based on energy (from shear energy in Eq. (5.23)) minimization or maximization would be to find

$$\min\big(\boldsymbol{r} \cdot (\gamma_y, \gamma_z)\big) \qquad \text{or} \qquad \max\big(\boldsymbol{r} \cdot (\gamma_y, \gamma_z)\big)$$

Solving Eq. (5.31) for $d\delta_{xz}$ gives

$$\mathbb{R}_{xz} d\delta_{xz} = \frac{\frac{\tau_{xy}^0 \mathbb{R}_{xy} d\gamma_y}{(1-d_{xy})\varphi_{xy}} + \frac{\tau_{xz}^0 \mathbb{R}_{xz} d\gamma_z}{(1-d_{xz})\varphi_{xz}} - \frac{(\tau_{xy}^0)^2\left(1+\frac{F'_{xy}}{C_{66}}\right)\mathbb{R}_{xy} d\delta_{xy}}{(1-d_{xy})F_{xy}\varphi_{xy}}}{\frac{(\tau_{xz}^0)^2\left(1+\frac{F'_{xz}}{G_{zx}}\right)}{(1-d_{xz})F_{xz}\varphi_{xz}}}$$

The shear energy increment (from Eq. (5.23)) becomes

$$2d\Omega = \left[\frac{1}{C_{66}}\left(\frac{\tau_{xy}^0}{1-d_{xy}}\right)^2 - \frac{1}{C_{55}}\left(\frac{\tau_{xz}^0}{1-d_{xz}}\right)^2 \frac{\frac{(\tau_{xy}^0)^2\left(1+\frac{F'_{xy}}{C_{66}}\right)}{(1-d_{xy})F_{xy}\varphi_{xy}}}{\frac{(\tau_{xz}^0)^2\left(1+\frac{F'_{xz}}{G_{zx}}\right)}{(1-d_{xz})F_{xz}\varphi_{xz}}} \right] \mathbb{R}_{xy}\, d\delta_{xy} + (\text{constant})$$

If the term in brackets is non-zero, minimized or maximized energy would require $d\delta_{xy} \to 0$ or $d\delta_{xy} \to \delta_{xy,max}$ depending on sign of that term. In other words, the energy minimum is on the boundary for acceptable values of $d\delta_{xy}$ corresponding to no damage or complete failure. These boundaries are not acceptable results, in general, for damage evolution. In brief, energy extrema does not provide a viable approach to coupling damage parameters,

d.5. The Preferred Coupling Method

The preferred approach appears to be to equate increments in d_{xy} and d_{xz} or to keep $d_{xy} = d_{xz} = d_s$. Accepting this coupling, the solution for updating δ_{xy} using Eq. (6.29)

$$\mathbb{R}_{xy} d\delta_{xy} = \frac{\frac{\tau_{xy} C_{66}}{F_{xy}^2} d\gamma_y + \frac{\tau_{xz} C_{55}}{F_{xz}^2} d\gamma_z}{\frac{\tau_{xy}^2 C_{66}}{\mathbb{R}_{xy} F_{xy}^3}\left(1 + \frac{F'_{xy}}{C_{66}}\right) + \frac{\tau_{xz}^2 C_{55}}{\mathbb{R}_{xz} F_{xz}^3}\left(1 + \frac{F'_{xz}}{C_{55}}\right)} \tag{5.34}$$

or using Eq. (5.31) gives:

$$\mathbb{R}_{xy} d\delta_{xy} = \frac{\frac{\tau_{xy} \mathbb{R}_{xy} d\gamma_y}{\varphi_{xy}} + \frac{\tau_{xz} \mathbb{R}_{xz} d\gamma_z}{\varphi_{xz}}}{\frac{\tau_{xy}^2}{F_{xy} \varphi_{xy}}\left(1 + \frac{F'_{xy}}{C_{66}}\right) + \frac{\tau_{xz}^2}{F_{xz} \varphi_{xz}}\left(1 + \frac{F'_{xz}}{C_{55}}\right)} \tag{5.35}$$

The first can be written in vector form as

$$d(d_s) = \frac{\hat{\boldsymbol{T}}_c \cdot \left(\frac{C_{66}}{F_{xy}} d\gamma_y, \frac{C_{55}}{F_{xz}} d\gamma_z\right)}{\hat{\boldsymbol{T}}_c \cdot \left(\hat{T}_{c,x} \frac{C_{66}}{\mathbb{R}_{xy} F_{xy}}\left(1 + \frac{F'_{xy}}{C_{66}}\right), \hat{T}_{c,y} \frac{C_{55}}{\mathbb{R}_{xz} F_{xz}}\left(1 + \frac{F'_{xz}}{C_{55}}\right)\right)} \tag{5.36}$$

where

$$\hat{\boldsymbol{T}}_c = \left(\frac{\tau_{xy}}{F_{xy}}, \frac{\tau_{xz}}{F_{xz}}\right) \quad \text{with} \quad \|\hat{\boldsymbol{T}}_c\| = 1$$

is a unit vector defined by the elliptical cylinder failure surface or a unit vector in direction of traction plotted by normalizing component stresses to current uniaxial strengths in that direction.

Once this result is found, the remaining parameters update by coupling equations. The updated d_{xy} and d_{xz} can be found from the relations in Eq. (5.21) using the updated δ_{xy} and δ_{xz}. Using Eq. (5.9), the cracking strain simplifies to

$$d\gamma_{c,xy} = d_s \frac{\tau_{xz} C_{55}}{F_{xz}^2} \left[\frac{\frac{\tau_{xz}}{\mathbb{R}_{xz} F_{xz}}\left(1 + \frac{F'_{xz}}{C_{55}}\right) d\gamma_y - \frac{\tau_{xy}}{\mathbb{R}_{xy} F_{xy}}\left(1 + \frac{F'_{xy}}{C_{66}}\right) d\gamma_z}{\frac{\tau_{xy}^2 C_{66}}{\mathbb{R}_{xy} F_{xy}^3}\left(1 + \frac{F'_{xy}}{C_{66}}\right) + \frac{\tau_{xz}^2 C_{55}}{\mathbb{R}_{xz} F_{xz}^3}\left(1 + \frac{F'_{xz}}{C_{55}}\right)} \right] + \frac{\tau_{xy}}{F_{xy}} d\delta_{xy} \tag{5.37}$$

See Isotropic Softening Material for special case of an isotropic material.

Ovoid Surface

This method assumes an 3D ovoid surface with axes F_n in tension and F_{xy} and F_{xz} in the two shear directions. On the compression axis, this surface is cylindrical as in the Cylindrical Surface section. When traction exceeds this surface when normal traction is positive, the first equation to solve is now:

$$\left(\frac{\sigma_{xx}^{(trial)} - C_{11}\varepsilon_n \mathbb{R}_n d\delta_n}{F_n(\delta_n + d\delta_n)}\right)^2 + \left(\frac{\tau_{xy}^{(trial)} - C_{66}\gamma_y \mathbb{R}_{xy} d\delta_{xy}}{F_{xy}(\delta_{xy} + d\delta_{xy})}\right)^2 + \left(\frac{\tau_{xz}^{(trial)} - C_{55}\gamma_z \mathbb{R}_{xz} d\delta_{xz}}{F_{xz}(\delta_{xz} + d\delta_{xz})}\right)^2 = 1 \tag{5.38}$$

Solving this equation is easier than using the gradient equation method (and the results would be the same). Expanding in a Taylor series and keeping first order terms simply ands a normal traction term to Eq. (6.29) or:

$$\frac{\sigma_{xx}^2 C_{11}(1-d_n)\left(1+\frac{F_n'}{C_{11}}\right)}{F_n^3}d\delta_n + \frac{\tau_{xy}^2 C_{66}(1-d_{xy})\left(1+\frac{F_{xy}'}{C_{66}}\right)}{F_{xy}^3}d\delta_{xy} + \frac{\tau_{xz}^2 C_{55}(1-d_{xz})\left(1+\frac{F_{xz}'}{C_{55}}\right)}{F_{xz}^3}d\delta_{xz}$$
$$= \frac{\sigma_{xx}C_{11}(1-d_n)}{F_n^2}d\varepsilon_n + \frac{\tau_{xy}C_{66}(1-d_{xy})}{F_{xy}^2}d\gamma_y + \frac{\tau_{xz}C_{55}(1-d_{xz})}{F_{xz}^2}d\gamma_z \tag{5.39}$$

or adds a term to Eq. (6.29) expressed in terms of $\mathbb{R}$ functions:

$$\frac{\sigma_{xx}^2\left(1+\frac{F_n'}{C_{11}}\right)\mathbb{R}_n d\delta_n}{(1-d_n)F_n\varphi_n} + \frac{\tau_{xy}^2\left(1+\frac{F_{xy}'}{C_{66}}\right)\mathbb{R}_{xy}d\delta_{xy}}{(1-d_{xy})F_{xy}\varphi_{xy}} + \frac{\tau_{xz}^2\left(1+\frac{F_{xz}'}{C_{55}}\right)\mathbb{R}_{xz}d\delta_{xz}}{(1-d_{xz})F_{xz}\varphi_{xz}}$$
$$= \frac{\sigma_{xx}\mathbb{R}_n d\varepsilon_n}{(1-d_n)\varphi_n} + \frac{\tau_{xy}\mathbb{R}_{xy}d\gamma_y}{(1-d_{xy})\varphi_{xy}} + \frac{\tau_{xz}\mathbb{R}_{xz}d\gamma_z}{(1-d_{xz})\varphi_{xz}}$$

For the coupling equation, we accept the linked d approach or set $d_n = d_{xy} = d_{xz}$ that is achieved by linking δ updates through

$$\mathbb{R}_n d\delta_n = \mathbb{R}_{xy}d\delta_{xy} = \mathbb{R}_{xz}d\delta_{xz}$$

The damage evolution becomes

$$\mathbb{R}_n d\delta_n = \frac{\frac{\sigma_{xx}C_{11}}{F_n^2}d\varepsilon_n + \frac{\tau_{xy}C_{66}}{F_{xy}^2}d\gamma_y + \frac{\tau_{xz}C_{55}}{F_{xz}^2}d\gamma_z}{\frac{\sigma_{xx}^2 C_{11}}{\mathbb{R}_n F_n^3}\left(1+\frac{F_n'}{C_{11}}\right) + \frac{\tau_{xy}^2 C_{66}}{\mathbb{R}_{xy}F_{xy}^3}\left(1+\frac{F_{xy}'}{C_{66}}\right) + \frac{\tau_{xz}^2 C_{55}}{\mathbb{R}_{xz}F_{xz}^3}\left(1+\frac{F_{xz}'}{C_{55}}\right)} \tag{5.40}$$

or

$$\mathbb{R}_n d\delta_n = \frac{\frac{\sigma_{xx}\mathbb{R}_n}{\varphi_n}d\varepsilon_n + \frac{\tau_{xy}\mathbb{R}_{xy}}{\varphi_{xy}}d\gamma_y + \frac{\tau_{xz}\mathbb{R}_{xz}}{\varphi_{xz}}d\gamma_z}{\frac{\sigma_{xx}^2}{F_n\varphi_n}\left(1+\frac{F_n'}{C_{11}}\right) + \frac{\tau_{xy}^2}{F_{xy}\varphi_{xy}}\left(1+\frac{F_{xy}'}{C_{66}}\right) + \frac{\tau_{xz}^2}{F_{xz}\varphi_{xz}}\left(1+\frac{F_{xz}'}{C_{55}}\right)}$$

The cracking strains increment by Eq. (5.9) in each direction. The first could be written in vector form

$$d(d) = \frac{\hat{\boldsymbol{T}}_o \cdot \left(\frac{C_{66}}{F_{xy}}d\gamma_y, \frac{C_{55}}{\tau_{xz}}d\gamma_z, \frac{C_{11}}{F_n}d\varepsilon_n\right)}{\hat{\boldsymbol{T}}_o \cdot \left(\hat{T}_{o,x}\frac{C_{66}}{\mathbb{R}_{xy}F_{xy}}\left(1+\frac{F_{xy}'}{C_{66}}\right), \hat{T}_{o,y}\frac{C_{55}}{\mathbb{R}_{xz}F_{xz}}\left(1+\frac{F_{xz}'}{C_{55}}\right), \hat{T}_{o,z}\frac{C_{11}}{\mathbb{R}_n F_n}\left(1+\frac{F_n'}{C_{11}}\right)\right)} \tag{5.41}$$

where

$$\hat{\boldsymbol{T}}_o = \left(\frac{\tau_{xy}}{F_{xy}}, \frac{\tau_{xz}}{F_{xz}}, \frac{\sigma_{xx}}{F_n}, \right) \quad \text{with} \quad \|\hat{\boldsymbol{T}}_o\| = 1$$

is a unit vector defined by the ovoid failure surface or a unit vector in direction of traction plotted by normalizing component stresses to current uniaxial strengths in that direction.

In the compression half plane, the $H(\sigma_{xx})$ in **D** means an ovoid surface reduces to an elliptical cylinder. The shear plane updates as above in the Cylindrical Surface section, but now also update the normal direction damage variable by

$$d\delta_n = \frac{\mathbb{R}_{xy}d\delta_{xy}}{\mathbb{R}_n}$$

This update happens in the background, but has no affect on cracking strains because the crack plane is in compression and the $H(\sigma_{xx})$ in **D** correctly sets normal direction cracking strain to zero.

See Isotropic Softening Material for special case of an isotropic material.

Fully Coupled Cuboid and Cylindrical Surface

If fully fully linking the d parameters works well for an Ovoid Surface, perhaps it should be added to Cuboid Surface and Cylindrical Surface as well. These surface currently have two or three decoupled d parameters. We now view them as 3D surface with return vector pointing to the origin. The solution is to set $d(d)$ (where d is the only damage parameter) to maximum increment found from the two or three decoupled equations. For cuboid surface, we get provisional $d\delta_n^*$, $d\delta_{xy}^*$, and $d\delta_{xz}^*$, and then use

$$d(d) = \max(\mathbb{R}_n d\delta_n^*, \mathbb{R}_{xy} d\delta_{xy}^*, \mathbb{R}_{xz} d\delta_{xz}^*) \quad \Longrightarrow \quad d\delta_n = \frac{d(d)}{\mathbb{R}_n}, \quad d\delta_{xy} = \frac{d(d)}{\mathbb{R}_{xy}}, \quad d\delta_{xz} = \frac{d(d)}{\mathbb{R}_{xz}}$$

For the elliptical cylinder surface:

$$d(d) = \max(\mathbb{R}_n d\delta_n^*, \mathbb{R}_s d\delta_s^*) \quad \Longrightarrow \quad d\delta_n = \frac{d(d)}{\mathbb{R}_n}, \quad d\delta_s = \frac{d(d)}{\mathbb{R}_{xy}}$$

Because some directions may be damaging when that stress is less than strength in that value, we must use the full expression for crack increment in Eq. (5.9) in each direction.

5.3.3 Failure and Post Failure

For the ovoid surface, failure occurs when the one damage variable reaches one. There is no need (and in fact no possibility) to impose a mixed mode failure criterial. This surface will have a mixed-mode failure result, but is determined by the coupling and not by some additional criiterion. For cuboid and cylindrical surfaces, there are 3 or 2 damage parameters and they may not get to 1 at the same time. To prevent too much energy being dissipated, thses surface have to be supplemented with a mixed mode failure criterion.

Cuboid Failure

For cuboid surface, the three updates are decoupled, 1D equations, meaning the total energy dissipated up to current δ can be found for each direction using Eq. (5.12). A mixed mode failure criterions can be:

$$\left(\frac{\overline{G}_n}{\overline{G}_{nc}}\right)^m + \left(\frac{\overline{G}_{xy}}{\overline{G}_{xyc}}\right)^n + \left(\frac{\overline{G}_{xz}}{\overline{G}_{xzc}}\right)^p = 1 \tag{5.42}$$

here n, m, and p are material properties, and the denominators are area under strength model in each direction (given by Eq. (5.13)). Failure may also be induced by any d reaching 1. When it fails, set $d_n = d_{xy} = d_{xz} = 1$, $\delta_n = \delta_{n,max}$, $\delta_{xy} = \delta_{xy,max}$, $\delta_{xz} = \delta_{xz,max}$, and $\sigma_{xx} = \tau_{xz} = \tau_{xy} = 0$ Cracking strains adjust by imposed increments in d's.

Cylindrical Failure

Post-Failure Frictionless Contact

In post-failure updates, the normal stress is zero if not in contact, but may go into compression if there is contact (cracking strain to zero). The stress update in the normal direction is

$$d\sigma_{xx} = C_{11}\left(d\varepsilon_n - d\varepsilon_{c,xx}\right) \tag{5.43}$$

where $d\varepsilon_{c,xx}$ is final update in crack strain and subject to constraint that total crack strain must remain positive.

First consider loading with $d\varepsilon_n > 0$ such that the crack is opening. The cracking strain updates are

$$d\varepsilon_{c,xx} = \begin{cases} d\varepsilon_n & \text{if } \varepsilon_{c,xx} > 0 \\ \max(d\varepsilon_n + \frac{\sigma_{xx}}{C_{11}}, 0) & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.44}$$

$$d\sigma_{xx} = \begin{cases} -\sigma_{xx} & \text{if } \varepsilon_{c,xx} > 0 \\ \min(-\sigma_{xx}, C_{11} d\varepsilon_n) & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.45}$$

The first case in each is for crack that started not in contact and remains not in contact. The second case in each is for crack that starts in contact. The two options possible are for the crack to overcome contact and move apart or to remain in contact.

Next consider loading with $d\varepsilon_n < 0$ such that the crack is closing. The cracking strain updates are

$$d\varepsilon_{c,xx} = \begin{cases} \max(d\varepsilon_n, -\varepsilon_{c,xx}) & \text{if } \varepsilon_{c,xx} > 0 \\ 0 & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.46}$$

$$d\sigma_{xx} = \begin{cases} -\sigma_{xx} \text{ or } C_{11}\left(d\varepsilon_n + \varepsilon_{c,xx}\right) & \text{if } \varepsilon_{c,xx} > 0 \\ C_{11} d\varepsilon_n & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.47}$$

The two options now are for the crack to move into contact or to remain in contact.

The shear updates do not need to handle contact. Subsequent updates can use elastic methods with zero stress increment in the crack plane stresses, but the cracking strains still update:

$$d\gamma_{c,xy} = d\gamma_{xy},\ d\gamma_{c,xz} = d\gamma_{xz},\ d\tau_{xy} = -\tau_{xy}, \text{ and } d\tau_{xz} = -\tau_{xz} \tag{5.48}$$

Post-Failure Frictional Constact

These previous section assumed frictionless contact. It is also possible to implement frictional contact. For a post-failure update of shear stresses, first assume that the surfaces are sticking and calculate a trial shear traction that assumes no change in cracking strains (*i.e.*, the crack surface do not slide):

$$\boldsymbol{T}_s^{(trial)} = (\tau_{xy} + C_{66} d\gamma_y, \tau_{xz} + C_{55} d\gamma_z)$$

For Coulomb friction, the magnitude of the shear traction must obey

$$\|\boldsymbol{T}_s\| \leq \mu N$$

where $N = -\sigma_{xx}$ is normal force on the crack plane. If it is less than μN, the shear stress update is accepted and shear cracking strain increments are zero. But if it is exceed, we change to a new update

$$\boldsymbol{T}_s^{(final)} = (\tau_{xy} + \phi C_{66} d\gamma_y, \tau_{xz} + \phi C_{55} d\gamma_z)$$

where ϕ is found be solving the quadratic equation

$$\|\boldsymbol{T}_s^{(final)}\|^2 = \mu^2 N^2$$

and being careful to select the physically correct root. Once ϕ is found, the shear stresses update by

$$d\tau_{xy} = \phi C_{66} d\gamma_y \qquad \text{and} \qquad d\tau_{xy} = \phi C_{55} d\gamma_z$$

and cracking strain increments corresponding to these shear stress updates are.

$$d\gamma_{c,xy} = (1-\phi) d\gamma_y \qquad \text{and} \qquad d\gamma_{c,xz} = (1-\phi) d\gamma_z$$

Physically, $\phi = 1$ is sticking, $\phi = 0$ is frictionless, and other values model Coulomb friction.

If modeling wants to account for frictional heating, the work of friction can come from force × strain increment × volume. The strain increment comes from the magnitudes of the cracking strain vector or

$$W_F = \mu N V_p \sqrt{d\gamma_{c,xy}^2 + d\gamma_{c,xz}^2}$$

In 2D, the analysis simplifies to finding $\tau_{xy} + G d\gamma_{xy}$ within the interval of $\pm\mu N$. Thus

$$\tau + \phi C_{66} d\gamma_y = \pm\mu N \quad \Longrightarrow \quad \phi = \frac{\pm\mu N - \tau}{C_{66} d\gamma_y}$$

The updates become

$$d\tau = \phi C_{66} d\gamma_y \quad \text{and} \quad d\gamma_c = (1-\phi) d\gamma_y$$

The frictional work becomes

$$W_F = \mu N V_p |d\gamma_c|$$

5.3.4 Two Dimensional Problems

Plane Strain

For plane strain analysis of generally anisotropic material (*i.e.*, crack axis frame as tension-shear and shear-shear coupling as well as shear residual strains), zero z-direction strain leads to:

$$0 = \varepsilon_{zz} = \varepsilon_{zz}^{(res)} + \sum_i S_{i3}\sigma_i \implies S_{33}\sigma_{zz} + S_{43}\tau_{yz} + S_{53}\tau_{xz} = -\varepsilon_{zz}^{(res)} - S_{13}\sigma_{xx} - S_{23}\sigma_{yy} - S_{63}\tau_{xy}$$

Combining with similar equations for zero γ_{yz} and γ_{xz} leads to

$$\begin{pmatrix} \sigma_{zz} \\ \tau_{yz} \\ \tau_{xz} \end{pmatrix} = -\begin{pmatrix} S_{33} & S_{34} & S_{35} \\ S_{34} & S_{44} & S_{45} \\ S_{35} & S_{45} & S_{55} \end{pmatrix}^{-1} \left[\begin{pmatrix} \varepsilon_{zz}^{(res)} \\ \gamma_{yz}^{(res)} \\ \gamma_{xz}^{(res)} \end{pmatrix} + \begin{pmatrix} S_{13} & S_{23} & S_{36} \\ S_{14} & S_{24} & S_{46} \\ S_{15} & S_{25} & S_{56} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} \right] \tag{5.49}$$

Substituting into compliance equation leaves equation for in-plane strains

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{16} \\ S_{12} & S_{22} & S_{26} \\ S_{16} & S_{26} & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} + \begin{pmatrix} S_{13} & S_{14} & S_{15} \\ S_{23} & S_{24} & S_{25} \\ S_{36} & S_{46} & S_{56} \end{pmatrix} \begin{pmatrix} \sigma_{zz} \\ \tau_{yz} \\ \tau_{xz} \end{pmatrix} + \begin{pmatrix} \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy}^{(res)} \\ \gamma_{xy}^{(res)} \end{pmatrix}$$

The 3×3 matrices are blocks of the $\mathbf{S}$ tensor. We define three matrices $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_3$ to write above equations as

$$\begin{pmatrix} \sigma_{zz} \\ \tau_{yz} \\ \tau_{xz} \end{pmatrix} = -\mathbf{S}_2^{-1} \begin{pmatrix} \varepsilon_{zz}^{(res)} \\ \gamma_{yz}^{(res)} \\ \gamma_{xz}^{(res)} \end{pmatrix} - \mathbf{S}_2^{-1}\mathbf{S}_3^T \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \gamma_{xy} \end{pmatrix} = \mathbf{S}_1 \begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} + \mathbf{S}_3 \begin{pmatrix} \sigma_{zz} \\ \tau_{yz} \\ \tau_{xz} \end{pmatrix} + \begin{pmatrix} \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy}^{(res)} \\ \gamma_{xy}^{(res)} \end{pmatrix}$$

The "reduced" 2D equation simplifies to a standard 2D result but has reduced compliance and residual strains

$$\varepsilon = \mathbf{S}^{(r)}\boldsymbol{\sigma} + \varepsilon^{(r)}_{res} \quad \text{where} \quad \mathbf{S}^{(r)} = \mathbf{S}_1 - \mathbf{S}_3\mathbf{S}_2^{-1}\mathbf{S}_3^T \text{ and } \varepsilon^{(r)}_{res} = \begin{pmatrix} \varepsilon^{(res)}_{xx} \\ \varepsilon^{(res)}_{yy} \\ \gamma^{(res)}_{xy} \end{pmatrix} - \mathbf{S}_3\mathbf{S}_2^{-1} \begin{pmatrix} \varepsilon^{(res)}_{zz} \\ \gamma^{(res)}_{yz} \\ \gamma^{(res)}_{xz} \end{pmatrix}$$

Then, by block matrix inversion (see "Block Matrix" in Wikipedia):

$$\boldsymbol{\sigma} = \begin{pmatrix} C_{11} & C_{12} & C_{16} \\ C_{12} & C_{22} & C_{26} \\ C_{16} & C_{26} & C_{66} \end{pmatrix} \left(\varepsilon - \begin{pmatrix} \varepsilon^{(res)}_{xx} \\ \varepsilon^{(res)}_{yy} \\ \gamma^{(res)}_{xy} \end{pmatrix} \right) - \begin{pmatrix} C_{13} & C_{14} & C_{15} \\ C_{23} & C_{24} & C_{25} \\ C_{36} & C_{46} & C_{56} \end{pmatrix} \begin{pmatrix} \varepsilon^{(res)}_{zz} \\ \gamma^{(res)}_{yz} \\ \gamma^{(res)}_{xz} \end{pmatrix} = \mathbf{C}_1 \varepsilon^{(r)}_{eff}$$

where C_{ij} are elements of the unreduced stiffness tensor, $\mathbf{C}_1$ is block of the full $\mathbf{C}$ tensor and $\varepsilon^{(r)}_{eff}$ is effective 2D strain found by subtracting reduced residual strain ($\varepsilon^{(r)}_{res}$) from the in-plane strains.

For damage mechanics, we define two strains

$$\varepsilon^{(r)}_n = \varepsilon^{(r)}_{xx} + \frac{C_{12}}{C_{11}}\varepsilon^{(r)}_{yy} + \frac{C_{16}}{C_{11}}\gamma^{(r)}_{xy} \quad \text{and} \quad \gamma^{(r)}_y = \gamma^{(r)}_{xy} + \frac{C_{16}}{C_{66}}\varepsilon^{(r)}_{xx} + \frac{C_{26}}{C_{66}}\varepsilon^{(r)}_{yy}$$

two cracking strains by

$$d\varepsilon^{(r)}_{c,xx} = d\left(d_n \varepsilon^{(r)}_n\right), \quad \text{and} \quad d\gamma_{c,xy} = d(d_{xy}\gamma^{(r)}_y)$$

and damage tensor by

$$\mathbf{D}^{(r)} = \begin{pmatrix} H(\sigma_{xx})d_n & \frac{H(\sigma_{xx})C_{12}}{C_{11}}d_n & \frac{H(\sigma_{xx})C_{16}}{C_{11}}d_n \\ 0 & 0 & 0 \\ \frac{C_{16}}{C_{66}}d_{xy} & \frac{C_{26}}{C_{66}}d_{xy} & d_{xy} \end{pmatrix}$$

The constitutive law is then

$$\boldsymbol{\sigma} = \mathbf{C}_1\left(\mathbf{I} - \mathbf{D}^{(r)}\right)\varepsilon^{(r)}_{eff}$$

The in plane stress updates beceoms

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11}(d\varepsilon^{(r)}_n - d\varepsilon^{(r)}_{c,xx}) \\ C_{22}\left(d\varepsilon^{(r)}_{yy} + \frac{C_{12}}{C_{22}}\left(d\varepsilon^{(r)}_{xx} - d\varepsilon^{(r)}_{c,xx}\right) + \frac{C_{26}}{C_{22}}\left(d\gamma^{(r)}_y - d\gamma_{c,xy}\right)\right) \\ C_{66}\left(d\gamma^{(r)}_y - d\gamma_{c,xy}\right) \end{pmatrix} \tag{5.50}$$

The out-of-plane stresses can be calculated from in-plane increments using Eq. (5.49).

Plane Stress

For plane stress, we could begin with 3D solution and then impose $d\sigma_{zz} = d\tau_{yz} = d\tau_{xz} = 0$. The resulting system of equations, however, gives effective strains (ε_n, γ_y, and γ_z) that depend on cracking strains and a non-zero value for out-of-plane cracking strain (γ_z). Instead, we extract in-plane strains from 3D compliance equation (which reduces to 3×3 due to zero stress terms), and then invert to get:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \mathbf{S}_1^{-1} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_{c,xx} \\ \varepsilon_{yy} \\ \gamma_{xy} - \gamma_{c,xy} \end{pmatrix} = \mathbf{C}_1^{(r)}(\mathbf{I} - \mathbf{D})\varepsilon \tag{5.51}$$

where $\mathbf{C}_1^{(r)}$ is the reduced, 3×3 plane-stress stiffness tenor and the strains here are *effective* strains that have subtracted the residual strains. We have to modify D for plane stress to be:

$$\mathsf{D} = \begin{bmatrix} H(\sigma_{xx})d_n & \frac{H(\sigma_{xx})C_{12}^{(r)}}{C_{11}^{(r)}}d_n & \frac{H(\sigma_{xx})C_{16}^{(r)}}{C_{11}^{(r)}}d_n \\ 0 & 0 & 0 \\ \frac{C_{16}^{(r)}}{C_{66}^{(r)}}d_{xy} & \frac{C_{26}^{(r)}}{C_{66}^{(r)}}d_{xy} & d_{xy} \end{bmatrix}$$

The stress update becomes

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11}^{(r)}\left(d\varepsilon_n - d\varepsilon_{c,xx}\right) \\ C_{22}^{(r)}\left(d\varepsilon_{yy} + \frac{C_{12}^{(r)}}{C_{22}^{(r)}}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}\right) + \frac{C_{26}^{(r)}}{C_{66}^{(r)}}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}\right)\right) \\ C_{22}^{(r)}\left(d\gamma_{xy} - d\gamma_{c,xy}\right) \end{pmatrix}$$

where

$$\varepsilon_n = \varepsilon_{xx} + \frac{C_{12}^{(r)}}{C_{11}^{(r)}}\varepsilon_{yy} + \frac{C_{16}^{(r)}}{C_{11}^{(r)}}\gamma_{xy} \qquad \gamma_y = \frac{C_{16}^{(r)}}{C_{66}^{(r)}}\varepsilon_{xx} + \frac{C_{26}^{(r)}}{C_{66}^{(r)}}\varepsilon_{yy} + \gamma_{xy}$$

and

$$d\varepsilon_{c,xx} = d(d_n\varepsilon_n) \qquad \text{and} \qquad d\gamma_{c,xy} = d(d_{xy}\gamma_y)$$

5.4 Generalized Damage Mechanics

Besides stochastic variation in strength (which is easily handled simply by using particle-specific σ_I and ε_{n0}), what if the strength depends on particle stress state? For example, what if shear strength depends on pressure and temperature. One option would be to revise the strength model to include pressure and temperature:

$$F_{xy}(\delta_{xy}, P, T) = \sigma_{II}(P, T) f_{xy}(\delta_{xy}, P, T)$$

The area under the law at constant P and T gives $G_c(P,T)$. We could assume that G_c is independent of P (perhaps reasonable, would be interesting experiments) and T (probably not reasonable), which means the maximum cracking strain at failure must decrease if $\sigma_{II}(P,T)$ increases. Figure 5.4 illustrates a sample failure surface for linear softening with strength that increases linearly with pressure (and is independent of temperature). To implement extra variables in the strength model, we need to generalize damage mechanics to allow them. The extra variable will be denoted by a vector $\boldsymbol{\alpha}$ that may include pressure, temperature, or more variables (*e.g.*, strain rate) that affect material strength.

5.4.1 Generalized 1D Damage Mechanics

This section extends the damage evolution part of the 1D Numerical Implementation section from the specialized theory. The first step is to recognize that relation between D and δ (Eq. (5.4)) now includes the extra variables:

$$D = \frac{\delta}{\delta + \frac{F(\delta,\boldsymbol{\alpha})}{E}}$$

The revised full different in damage variable becomes:

$$dD = \left(\frac{\partial D}{\partial \delta}\right)_{\boldsymbol{\alpha}} d\delta + \left(\frac{\partial D}{\partial \boldsymbol{\alpha}}\right)_{\delta} \cdot d\boldsymbol{\alpha} = \mathbb{R}\, d\delta - \mathbb{A} \cdot d\boldsymbol{\alpha}$$

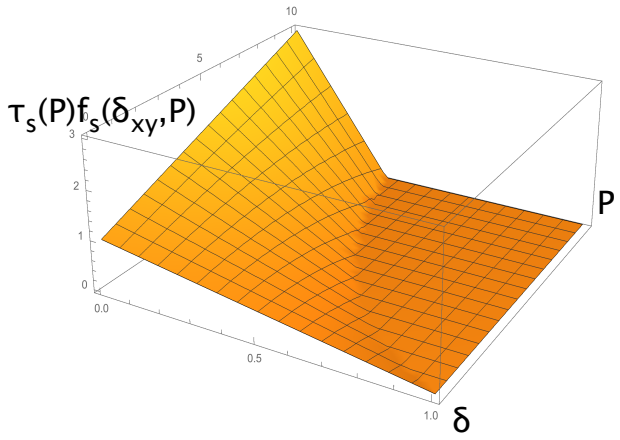

Figure 5.4: Sample total softening surface for linear softening when $\sigma_{II}(P)$ increases linearly with pressure. The area under the surface at constant P is constant or toughness does not depend on P.

and we define

$$\mathbb{A}_{,i} = -\left(\frac{\partial D}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} = \frac{\psi(\delta,\alpha_i)}{E\left(\delta + \frac{F(\delta)}{E}\right)^2} \quad \text{where} \quad \psi(\delta,\alpha_i) = \delta\left(\frac{\partial F(\delta,\boldsymbol{\alpha})}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}}$$

Other useful forms for $\mathbb{A}_{,i}$ are

$$\mathbb{A}_{,i} = \frac{E(1-D)^2\psi(\delta,\alpha_i)}{F^2(\delta)} = \frac{(1-D)D\psi(\delta,\alpha_i)}{\delta F(\delta)} = \frac{D^2\psi(\delta,\alpha_i)}{E\delta^2} = \frac{\sigma D\psi(\delta,\alpha_i)}{\varepsilon E\delta F_n(\delta)} \tag{5.52}$$

The increment in cracking strain ($d\varepsilon_c = Dd\varepsilon + \varepsilon(\mathbb{R}d\delta - \mathbb{A}\cdot d\boldsymbol{\alpha})$) that extends Eq. (5.9) to extra parameters is:

$$d\varepsilon_c = D\left[d\varepsilon - \frac{\sigma}{F(\delta)}\left(\left(1+\frac{F'(\delta)}{E}\right)d\delta + \sum_i \frac{\psi(\delta,\alpha_i)}{E\delta}d\alpha_i\right)\right] + \frac{\sigma}{F(\delta)}d\delta \tag{5.53}$$

This above equations (and others in this general theory) need α_i derivatives. All current softening laws can be written as $F(\delta,\boldsymbol{\alpha}) = \sigma_0(\boldsymbol{\alpha})f(\delta, s(\boldsymbol{\alpha})G_c(\boldsymbol{\alpha}))$ where $s = A_c/(V_p\sigma_0(\boldsymbol{\alpha}))$ and $G_c(\boldsymbol{\alpha})$ is toughness (which might depend on $\boldsymbol{\alpha}$). We can derive

$$\left(\frac{\partial F(\delta,\boldsymbol{\alpha})}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} = \left(f(\delta,sG_c) - s\frac{\partial f(\delta,sG_c)}{\partial s}\right)\left(\frac{\partial \sigma_0}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} + \sigma_0\frac{\partial f(\delta,sG_c)}{\partial G_c}\left(\frac{\partial G_c}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} \tag{5.54}$$

When allowing stochastic variation in strength and toughness, the softening law changes to

$$F(\delta,\boldsymbol{\alpha}) = r_\sigma\sigma_0(\boldsymbol{\alpha})f\left(\delta, \frac{r_G s(\boldsymbol{\alpha})G_c(\boldsymbol{\alpha})}{r_\sigma}\right) = r_\sigma\sigma_0(\boldsymbol{\alpha})f\left(\delta, s^*(\boldsymbol{\alpha})G_c(\boldsymbol{\alpha})\right)$$

where r_σ and r_G are relative strength and toughness for current particle and $s^* = r_G s/r_\sigma$ (note that s^* is the scale parameter passed to standard softening law calls). The derivative in Eq. (5.54) is scaled by r_σ and in terms of s^*.

Elastic Increments (General)

Imagine an elastic process with $\boldsymbol{\varepsilon} \to \boldsymbol{\varepsilon} + d\boldsymbol{\varepsilon}$ and $\boldsymbol{a} \to \boldsymbol{\alpha} + d\boldsymbol{a}$ such that stress remains below the current softening surface or $\boldsymbol{\sigma} + d\boldsymbol{\sigma}$ is below the softening law surface (which might be a coupled surface). Because this process must not dissipate energy, it requires $dD = 0$. Unlike with a simple strength model, however, an elastic process may now involve a change in δ. Solving for zero energy dissipation gives the "elastic" change in δ, denoted by $d\delta^{(e)}$, as:

$$d\delta^{(e)} = \frac{\mathbb{A} \cdot d\boldsymbol{a}}{\mathbb{R}} = \frac{\sum_i \psi(\delta, \alpha_i) d\alpha_i}{\varphi(\delta, \boldsymbol{\alpha})} = \frac{\delta \sum_i \left(\frac{\partial F(\delta, \boldsymbol{\alpha})}{\partial \alpha_i} \right)_{\delta, \alpha_{j \neq i}}}{\varphi(\delta, \boldsymbol{\alpha})} \tag{5.55}$$

Note that for linear softening, the denominator in Eq. (5.55) is $\sigma_0(\boldsymbol{\alpha})$. During implementation, it is better to solve a finite-increment problem using Newtons's method. The cracking strain increment in terms of $\delta^{(e)}$ can be written as $d\varepsilon_c = Dd\varepsilon + \varepsilon\mathbb{R}(d\delta - \delta^{(e)})$, which extends Eq. (5.9) to

$$d\varepsilon_c = D\left[d\varepsilon - \frac{\sigma}{F(\delta, \boldsymbol{\alpha})} \left(1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E} \right) (d\delta - d\delta^{(e)}) \right] + \frac{\sigma}{F(\delta, \boldsymbol{\alpha})} \left(d\delta - d\delta^{(e)} \right) \tag{5.56}$$

Damage Evolution Increments (General)

For damage evolution, the gradient approach changes to

$$\nabla\sigma \cdot (d\varepsilon, dD, d\boldsymbol{\alpha}) = \nabla F(\delta, \boldsymbol{\alpha}) \cdot (d\delta, d\boldsymbol{\alpha})$$
$$E(1-D)d\varepsilon - E\varepsilon\left(\mathbb{R}d\delta - \mathbb{A} \cdot d\boldsymbol{\alpha} \right) = F'(\delta, \boldsymbol{\alpha})d\delta + \sum_i \frac{\psi(\delta, \alpha_i) d\alpha_i}{\delta}$$

which evaluates to:

$$d\delta = \frac{(1-D)d\varepsilon + \varepsilon\mathbb{A} \cdot d\boldsymbol{\alpha} - \sum_i \frac{\psi(\delta, \alpha_i) d\alpha_i}{E\delta}}{\varepsilon\mathbb{R} + \frac{F'(\delta, \boldsymbol{\alpha})}{E}} \tag{5.57}$$

$$= \frac{d\varepsilon + \sum_i \left(\frac{\psi(\delta, \alpha_i)}{F(\delta, \boldsymbol{\alpha})} - \frac{\psi(\delta, \alpha_i)}{(1-D)E\delta} \right) d\alpha_i}{\frac{\varphi(\delta, \boldsymbol{\alpha})}{F(\delta, \boldsymbol{\alpha})} + \frac{F'(\delta, \boldsymbol{\alpha})}{(1-D)E}} = \frac{d\varepsilon - \sum_i \frac{\psi(\delta, \alpha_i)}{E\delta} d\alpha_i}{1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E}} = \frac{d\varepsilon - \frac{\varphi(\delta, \boldsymbol{\alpha})}{E\delta} d\delta^{(e)}}{1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E}} \tag{5.58}$$

The last two steps used $\delta = D\varepsilon$ during 1D damage evolution. This analysis assumed σ is independent of $\boldsymbol{\alpha}$. This situation holds if pressure affects only shear strength and the material has no tension-shear coupling in its constitutive law. Although constitutive law would include temperature through residual stresses, the temperature dependence of σ is accommodated in the effective stress definition (but can be added to strength model if needed). It is also possible that pressure dependences is correctly represented through the $d\boldsymbol{\varepsilon}$ terms on that trial update of pressure can be used.

Inserting the $\varphi(\delta, \boldsymbol{\alpha})$, the increment rearranges to

$$d\delta = \frac{d\varepsilon - \left(\frac{F(\delta, \boldsymbol{\alpha})}{E\delta} + 1 - 1 - \frac{F'(\delta, \boldsymbol{\alpha})}{E} \right) d\delta^{(e)}}{1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E}}$$
$$= d\delta^{(e)} + \frac{d\varepsilon - \left(\frac{F(\delta, \boldsymbol{\alpha})}{E\delta} + 1 \right) d\delta^{(e)}}{1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E}} = d\delta^{(e)} + \frac{d\varepsilon - \frac{d\delta^{(e)}}{D}}{1 + \frac{F'(\delta, \boldsymbol{\alpha})}{E}} \tag{5.59}$$

Substituting this result into Eq. (5.56), and noting $\sigma = F(\delta, \boldsymbol{\alpha})$, the 1D cracking strain increment is again $d\varepsilon_c = d\delta$. This update corresponds to a two step process to update δ:

1. Move elastically along the damage surface from $\boldsymbol{\alpha}$ to $\boldsymbol{\alpha}+d\boldsymbol{\alpha}$ with elastic update in cracking strain that occurs on the failure surface along with an elastic strain given by $d\varepsilon^{(e)} = d\delta^{(e)}/D$

2. Evolve damage at constant $\boldsymbol{\alpha}+d\boldsymbol{\alpha}$ using standard methods for single variable strength model but using the revised strain increment $d\varepsilon^{(d)} = d\varepsilon - d\varepsilon^{(e)}$. The additional change in δ due to damage can then use the special theory at $\boldsymbol{\alpha}+d\boldsymbol{\alpha}$:

$$d\delta^{(d)} = \frac{d\varepsilon^{(d)}}{1+\frac{F'(\delta,\boldsymbol{\alpha}+d\boldsymbol{\alpha})}{E}}$$

The total change in δ is then

$$d\delta = d\delta^{(e)} + d\delta^{(d)}$$

which matches the form derived above. Note that $d\delta^{(d)}$ evalates $F'(\delta,\boldsymbol{\alpha}+d\boldsymbol{\alpha})$, which corresponds only to an infinitesimal difference.

5.4.2 Generalized 3D Damage Mechanics

In 3D modeling, the updates depends on the failure surface.

Elastic Update (General)

For elastic increments, all three δ's may change using Eq. (5.55)

$$d\delta_n^{(e)} = \frac{\sum_i \psi_n(\delta_n,\alpha_i)d\alpha_i}{\varphi_n(\delta_n,\boldsymbol{\alpha})}$$

$$d\delta_{xy}^{(e)} = \frac{\sum_i \psi_{xy}(\delta_{xy},\alpha_i)d\alpha_i}{\varphi_{xy}(\delta_{xy},\boldsymbol{\alpha})} \qquad d\delta_{xz}^{(e)} = \frac{\sum_i \psi_{xz}(\delta_{xz},\alpha_i)d\alpha_i}{\varphi_{xz}(\delta_{xz},\boldsymbol{\alpha})}$$

Note that even when the d's are linked, the δ values can fluctuate due to these elastic changes.

Damage Evolution Increments (General)

When returning from trial state to any traction surface, we have to include changes in $\boldsymbol{\alpha}$ and changes in δ that happened on moving to the trial state. For tensile loading, a general update for normal traction with damage evolution adds a new term

$$d\sigma_{xx} = C_{11}\big((1-d_n)d\varepsilon_n - \varepsilon_n d(d_n)\big) = C_{11}\big((1-d_n)d\varepsilon_n - \varepsilon_n(\mathbb{R}_n d\delta_n - \mathbb{A}_n\cdot d\boldsymbol{\alpha})\big)$$

If $d\delta_n$ is the increment we seek, the return vector includes both elastic and damage changes or:

$$C_{11}\varepsilon_n\big(\mathbb{R}_n d\delta_n - \mathbb{A}_n\cdot d\boldsymbol{\alpha}\big) = C_{11}\varepsilon_n\mathbb{R}_n(d\delta_n - d\delta_n^{(e)})$$

Note that now all subscripted softening law properties implicit depend on both the appropriate δ and on $\boldsymbol{\alpha}$ (unless otherwise indicated).

5.4.3 Energy Dissipation (General)

Energy dissipation in terms of d parameters remains the same (see Eq. (5.22)), but conversion to δ's needs to include total differentials of the d parameters. The energy dissipation changes to

$$\begin{aligned} d\Omega = &\frac{H(\sigma_{xx})}{2C_{11}}\left(\frac{\sigma_{xx}}{1-d_n}\right)^2 \mathbb{R}_n(d\delta_n - d\delta_n^{(e)}) + \frac{1}{2C_{66}}\left(\frac{\tau_{xy}}{1-d_{xy}}\right)^2 \mathbb{R}_{xy}(d\delta_{xy} - d\delta_{xy}^{(e)}) \\ &+ \frac{1}{2C_{55}}\left(\frac{\tau_{xz}}{1-d_{xz}}\right)^2 \mathbb{R}_{xz}(d\delta_{xz} - d\delta_{xz}^{(e)}) = \frac{H(\sigma_{xx})}{2}\left(\frac{\sigma_{xx}}{F_n}\right)^2 \varphi_n(\delta_n)(\, d\delta_n - d\delta_n^{(e)}) \\ &+ \frac{1}{2}\left(\frac{\tau_{xy}}{F_{xy}}\right)^2 \varphi_{xy}(\delta_{xy})(d\delta_{xy} - d\delta_{xy}^{(e)}) + \frac{1}{2}\left(\frac{\tau_{xz}}{F_{xz}}\right)^2 \varphi_{xz}(d\delta_{xz} - d\delta_{xz}^{(e)}) \end{aligned} \tag{5.60}$$

Cuboid Surface (General)

Assuming this shape, the three components evolve damage independently. The update from Eq. (5.59) for normal damage becomes:

$$d\delta_n = d\delta_n^{(e)} + \frac{d\varepsilon_n - d\varepsilon_n^{(e)}}{1 + \frac{F_n'(\delta_n, \boldsymbol{\alpha})}{C_{11}}} \quad \text{where} \quad d\varepsilon_n^{(e)} = \frac{d\delta_n^{(e)}}{d_n} \tag{5.61}$$

is the strain required to move elastic on the damage surface from δ and α to $\delta_n + d\delta_n^{(e)}$ and $\alpha + d\alpha$. Using $\sigma_{xx} = F_n$ and Eq. (5.56), the cracking strain increment is $d\varepsilon_{c,n} = d\delta_n$. The shear damage equations are:

$$d\delta_{xy} = d\delta_{xy}^{(e)} + \frac{\text{sign}(\tau_{xy})d\gamma_y - d\gamma_y^{(e)}}{1 + \frac{F_{xy}'(\delta_{xy}, \boldsymbol{\alpha})}{C_{66}}} \quad \text{and} \quad d\delta_{xz} = d\delta_{xz}^{(e)} + \frac{\text{sign}(\tau_{xz})d\gamma_z - d\gamma_z^{(e)}}{1 + \frac{F_{xz}'(\delta_{xz}, \boldsymbol{\alpha})}{C_{55}}} \tag{5.62}$$

where $\text{sign}(\tau_{xy})$ and $\text{sign}(\tau_{xy})$ were inserted to work for both signs of shear stress.

Cylindrical Surface (General)

Repeating cylindrical surface from above Cylindrical Surface section, we switch $\mathbb{R}d\delta$ terms with $\mathbb{R}d\delta - \mathbb{A}\cdot d\boldsymbol{\alpha}$ in Eq. (5.29). This change adds two terms (for $ij = xy$ or xz) to right side of Eq. (6.29) or Eq. (5.31) :

$$\begin{aligned} &\frac{\tau_{ij}^2}{F_{ij}^3}\left(\frac{F_{ij}\mathbb{A}_{ij}\cdot d\boldsymbol{\alpha}}{1-d_{ij}} - \sum_i \left(\frac{\partial F_{ij}}{\partial \alpha_i}\right)_{\delta_{ij}, \alpha_{j\neq i}} d\alpha_i\right) = \frac{\tau_{ij}^2}{F_{ij}^3}\left(\frac{G_{ij}(1-d_{ij})}{F_{ij}} - \frac{1}{\delta_{ij}}\right)\sum_i \psi_{ij}(\delta_{ij}, \boldsymbol{\alpha})d\alpha_i \\ &= -\frac{\tau_{ij}^2}{F_{ij}^3}\left(\frac{1-d_{ij}}{\delta_{ij}}\right)\sum_i \psi_{ij}(\delta_{ij}, \boldsymbol{\alpha})d\alpha_i = -\frac{\tau_{ij}^2 \mathbb{R}_{ij}}{(1-d_{ij})F_{ij}\varphi_{ij}}\sum_i \frac{\psi_{ij}(\delta_{ij}, \boldsymbol{\alpha})}{G_{ij}\delta_{ij}}d\alpha_i \\ &= -\frac{\tau_{ij}^2(1-d_{ij})\varphi_{ij}}{F_{ij}^3\delta_{ij}}d\delta_{ij}^{(e)} = -\frac{\tau_{ij}^2 G_{ij}(1-d_{ij})}{F_{ij}^3}\left(\frac{F_{ij}}{G_{ij}\delta_{ij}} + 1 - 1 - \frac{F_{ij}'}{G_{ij}}\right)d\delta_{ij}^{(e)} \\ &= -\frac{\tau_{ij}G_{ij}(1-d_{ij})}{F_{ij}^2}\frac{\tau_{ij}}{F_{ij}}\left(\frac{1}{d_{ij}} - \left(1 + \frac{F_{ij}'}{G_{ij}}\right)\right)d\delta_{ij}^{(e)} \end{aligned} \tag{5.63}$$

where $G_{xy} = C_{66}$ and $G_{xz} = C_{55}$. For the coupling equation, we accept the linked d approach or set $d_{xy} = d_{xz}$ that is achieved by linking δ updates through

$$\mathbb{R}_{xy}(d\delta_{xy} - d\delta_{xy}^{(e)}) = \mathbb{R}_{xz}(d\delta_{xz} - d\delta_{xz}^{(e)})$$

The update with linked d's starts by adding the terms to Eq. (6.29) (and cancelling equal $(1-d_{ij})$ terms):

$$\begin{aligned}
&\frac{\tau_{xy}^2 C_{66}\left(1+\frac{F'_{xy}}{C_{66}}\right)}{F_{xy}^3}(d\delta_{xy} - d\delta_{xy}^{(e)}) + \frac{\tau_{xz}^2 C_{55}\left(1+\frac{F'_{xz}}{C_{55}}\right)}{F_{xz}^3}\frac{\mathbb{R}_{xy}}{\mathbb{R}_{xz}}(d\delta_{xy} - d\delta_{xy}^{(e)}) \\
&\quad = \frac{\tau_{xy} C_{66}}{F_{xy}^2}\left(d\gamma_y - \frac{\tau_{xy}}{F_{xy}}\left(\frac{1}{d_{xy}} - \left(1+\frac{F'_{xy}}{C_{66}}\right)\right)d\delta_{xy}^{(e)}\right) - \frac{\tau_{xy}^2 C_{66}\left(1+\frac{F'_{xy}}{C_{66}}\right)}{F_{xy}^3}d\delta_{xy}^{(e)} \\
&\quad + \frac{\tau_{xz} C_{55}}{F_{xz}^2}\left(d\gamma_z - \frac{\tau_{xz}}{F_{zx}}\left(\frac{1}{d_{xz}} - \left(1+\frac{F'_{xz}}{C_{55}}\right)\right)d\delta_{xz}^{(e)}\right) - \frac{\tau_{xz}^2 C_{55}\left(1+\frac{F'_{xz}}{C_{55}}\right)}{F_{xz}^3}d\delta_{xz}^{(e)}
\end{aligned} \tag{5.64}$$

which leads to

$$\mathbb{R}_{xy}(d\delta_{xy} - d\delta_{xy}^{(e)}) = \frac{\frac{\tau_{xy} C_{66}}{F_{xy}^2}\left(d\gamma_y - d\gamma_y^{(e)}\right) + \frac{\tau_{xz} C_{55}}{F_{xz}^2}\left(d\gamma_z - d\gamma_z^{(e)}\right)}{\frac{\tau_{xy}^2 C_{66}}{\mathbb{R}_{xy} F_{xy}^3}\left(1+\frac{F'_{xy}}{C_{66}}\right) + \frac{\tau_{xz}^2 C_{55}}{\mathbb{R}_{xz} F_{xz}^3}\left(1+\frac{F'_{xz}}{C_{55}}\right)} \tag{5.65}$$

where

$$d\gamma_y^{(e)} = \frac{\tau_{xy}}{F_{xy}}\frac{d\delta_{xy}^{(e)}}{d_s} \qquad \text{and} \qquad d\gamma_z^{(e)} = \frac{\tau_{xz}}{F_{xz}}\frac{d\delta_{xz}^{(e)}}{d_s}$$

are strain increment to move along the failure surface from δ_{ij} and α to $\delta_{ij} + d\delta_{ij}$ and $\alpha + d\alpha$. These increments generalize 1D results by the scaling term that equal fraction of current stress to current uniaxial strength. A vector from is

$$\mathbb{R}_{xy}(d\delta_{xy} - d\delta_{xy}^{(e)}) = \frac{\hat{\boldsymbol{T}}_c \cdot \left(\frac{C_{66}}{F_{xy}}\left(d\gamma_y - d\gamma_y^{(e)}\right), \frac{C_{55}}{F_{xz}}\left(d\gamma_z - d\gamma_z^{(e)}\right)\right)}{\hat{\boldsymbol{T}}_c \cdot \left(\hat{T}_{c,x}\frac{C_{66}}{\mathbb{R}_{xy}F_{xy}}\left(1+\frac{F'_{xy}}{C_{66}}\right), \hat{T}_{c,y}\frac{C_{55}}{\mathbb{R}_{xz}F_{xz}}\left(1+\frac{F'_{xz}}{C_{55}}\right)\right)} \tag{5.66}$$

with

$$d\gamma_y^{(e)} = \hat{T}_{c,x}\frac{d\delta_{xy}^{(e)}}{d_s} \qquad \text{and} \qquad d\gamma_z^{(e)} = \hat{T}_{c,y}\frac{d\delta_{xz}^{(e)}}{d_s} \tag{5.67}$$

See Isotropic Softening Material for special case of an isotropic material.

Ovoid Surface (General)

Repeating ovoid surface from the above Ovoid Surface section, we switch $\mathbb{R}d\delta$ terms with $\mathbb{R}d\delta - \boldsymbol{\mathbb{A}}\cdot d\boldsymbol{\alpha}$ in Eq. (5.38). This change adds three terms (for $ij = n$, xy, or xz in Eq. (5.63)) to right side of Eq. (5.39). When the d's are linked, the end result follows the analysis in the previous Cylindrical Surface (General) section with another term for normal direction. The normal update becomes:

$$\mathbb{R}_n(d\delta_n - d\delta_n^{(e)}) = \frac{\hat{\boldsymbol{T}}_o \cdot \left(\frac{C_{66}}{F_{xy}}\left(d\gamma_y - d\gamma_y^{(e)}\right), \frac{C_{55}}{\tau_{xz}}\left(d\gamma_z - d\gamma_z^{(e)}\right), \frac{C_{11}}{F_n}\left(d\varepsilon_n - d\varepsilon_n^{(e)}\right)\right)}{\hat{\boldsymbol{T}}_o \cdot \left(\hat{T}_{o,x}\frac{C_{66}}{\mathbb{R}_{xy}F_{xy}}\left(1+\frac{F'_{xy}}{C_{66}}\right), \hat{T}_{o,y}\frac{C_{55}}{\mathbb{R}_{xz}F_{xz}}\left(1+\frac{F'_{xz}}{C_{55}}\right), \hat{T}_{o,z}\frac{C_{11}}{\mathbb{R}_n F_n}\left(1+\frac{F'_n}{C_{11}}\right)\right)} \tag{5.68}$$

with

$$d\gamma_y^{(e)} = \hat{T}_{o,x}\frac{d\delta_{xy}^{(e)}}{d}, \qquad d\gamma_z^{(e)} = \hat{T}_{0,y}\frac{d\delta_{xz}^{(e)}}{d}, \qquad \text{and} \qquad d\varepsilon_n^{(e)} = \hat{T}_{0,z}\frac{d\delta_n^{(e)}}{d}, \tag{5.69}$$

being strain increments to move along the failure surface from δ_{ij} and α to $\delta_{ij} + d\delta_{ij}$ and $\alpha + d\alpha$.

The compression plane uses the Cylindrical Surface (General) methods but also increments the normal direction damage parameter by

$$d\delta_n = d\delta_n^{(e)} + \frac{\mathbb{R}_{xy}(d\delta_{xy} - d\delta_{xy}^{(e)})}{\mathbb{R}_n} \tag{5.70}$$

See Isotropic Softening Material for special case of an isotropic material.

Fully Coupled Cuboid and Cylindrical Surface (General)

This options uses the methods in Fully Coupled Cuboid and Cylindrical Surface but subtracts $d\delta^{(e)}$ from each $d\delta$ term and uses Eq. (5.53) for cracking strain increments.

5.5 Isotropic Softening Material

5.5.1 Damage Initiation

One damage initiation model for isotropic materials is to use principle stress. If the maximum principle stress exceeds tensile strength (from $F_n(0)$), damage initiates with normal in the maximum principle stress direction. If the maximum shear stress (give by $(\sigma_1 - \sigma_3)/2$ where σ_1 and σ_3 are maximum and minimum principle stresses, respectively). Caution: maybe shear failure has to look out for normal stress on the shear surface?

Another option might be a directional failure. This approach might replace cohesive zones for modeling delamination of adhesive failure between two isotropic adherends.

5.5.2 Post Damage Initiation Constitutive Law

The **D** tensor is given by Eq. (5.16). This tensor is used for both elastic updates and updates with damage evolution.

Elastic Update

An elastic update is as explained in Elastic Update above, but using **C** and **D** for an isotropic material.

Damage Evolution Update

The damage evolution is derived as special case in Damage Evolution Update above. For an isotropic material, $C_{55} = C_{66} = G$, $F_{xy} = F_{xz} = F_s$, and the effective strains simplify to:

$$\varepsilon_n = \varepsilon_{xx} + \frac{\nu}{1-\nu}\left(\varepsilon_{yy} + \varepsilon_{zz}\right) \qquad \gamma_z = \gamma_{xz} \qquad \gamma_y = \gamma_{xy}$$

The net effect of damage parameters is to convert the isotropic material to a damaged, orthotropic material (with crack normal along the x axis) using $E_{xx} = (1 - d_n^*)E$ (tension), $E_{xx} = E$ (compression),

$\nu_{xz} = \nu_{xy} = (1-d_n^*)\nu$ (tension) $\nu_{xz} = \nu_{xy} = \nu$ (compression), $G_{xz} = (1-d_{xz})G$, $G_{xy} = (1-d_{xy})G$, $C_{11,eff} = (1-d_n)C_{11}$ (tension) and $C_{11,eff} = C_{11}$ (compression), where d_n and d_n^* are related by

$$d_n = \frac{d_n^*(1-\nu)}{1-\nu-2(1-d_n^*)\nu^2} \qquad \text{and} \qquad d_n^* = \frac{d_n(1+\nu)(1-2\nu)}{1-\nu-2d_n\nu^2} \tag{5.71}$$

Energy Dissipation

From above section on Energy Dissipation, energy dissipation for an isotropic material simplifies to

$$d\Omega = \frac{1}{2}H(\sigma_{xx})C_{11}\varepsilon_n^2 dd_n + \frac{1}{2}G\gamma_{xz}^2 dd_{xz} + \frac{1}{2}G\gamma_{xy}^2 dd_{xy}$$

Using Eq. (5.7), energy dissipation can be written in terms of critical cracking strain increments:

$$\begin{aligned} d\Omega &= \frac{H(\sigma_{xx})}{2C_{11}}\left(\frac{\sigma_{xx}}{1-d_n}\right)^2 \mathbb{R}_n\, d\delta_n + \frac{1}{2G}\left(\frac{\tau_{xy}}{1-d_{xy}}\right)^2 \mathbb{R}_{xy}\, d\delta_{xy} + \frac{1}{2G}\left(\frac{\tau_{xz}}{1-d_{xz}}\right)^2 \mathbb{R}_{xz}\, d\delta_{xz} \\ &= \frac{H(\sigma_{xx})}{2}\left(\frac{\sigma_{xx}}{F_n}\right)^2 \varphi_n\, d\delta_n + \frac{1}{2}\left(\frac{\tau_{xy}}{F_s(\delta_{xy})}\right)^2 \varphi_s(\delta_{xy})\, d\delta_{xy} + \frac{1}{2}\left(\frac{\tau_{xz}}{F_s(\delta_{xz})}\right)^2 \varphi_s(\delta_{xy})\, d\delta_{xz} \end{aligned} \tag{5.72}$$

To handle $\boldsymbol{\alpha}$ variables, replace $d\delta_i$ with $d\delta_i - d\delta_i^{(e)}$ (see Eq. (5.60)). These simplify further when for surface that couple damage paramaters.

Strength Models or Damage Surfaces

We use the Strength Models or Damage Surfaces from above, but specialize to an isotropic materials. Finding damage increments and their energy dissipation requires some traction failure surface and its associated strength model. This section considers three rational surfaces.

Cuboid Surface (Iso)

This decoupled approach in Cuboid Surface (or in Cuboid Surface (General) with $\boldsymbol{\alpha}$ variables) above is unchanged (expect to use isotropic properties).

Cylindrical Surface (Iso)

Using the recommended method to link d parameters, will have a single damage variable $d_s = d_{xy} = d_{xz}$ and single cracking strain $\delta_s = \delta_{xy} = \delta_{xz}$ and a single strength model (F_s and $\mathbb{R}_s$) and properties $C_{55} = C_{66} = G$. The elliptical cylinder will evolve as a circular cylinder. Using the vector for in Eq. (5.66) and defining shear traction vector as $\boldsymbol{T}_s = (\tau_{xy}^0, \tau_{xz}^0)$ (such that $\|\boldsymbol{T}_s\| = F_s$ and $\hat{\boldsymbol{T}}_c = \boldsymbol{T}_s/\|\boldsymbol{T}_s\| = \hat{\boldsymbol{T}}_s$ is unit vector in current traction direction, leads to

$$\mathbb{R}_s\left(d\delta_s - d\delta_s^{(e)}\right) = \frac{\hat{\boldsymbol{T}}_s \cdot \left[\left(d\gamma_y, d\gamma_z\right) - \hat{\boldsymbol{T}}_s \frac{d\delta_s^{(e)}}{d_s}\right]}{\hat{\boldsymbol{T}}_s \cdot \hat{\boldsymbol{T}}_s \frac{1}{\mathbb{R}_s}\left(1 + \frac{F_s'}{G}\right)} \implies d\delta_s = d\delta_s^{(e)} + \frac{\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma} - \frac{d\delta_s^{(e)}}{d_s}}{1 + \frac{F_s'}{G}}$$

where $d\boldsymbol{\gamma} = (d\gamma_{xy}, d\gamma_{xz})$. This equation works for any sign of shear stress by formation of the unit vector (*i.e.*, damage only evolves when $\boldsymbol{\gamma}$ is in same direction as shear traction).

Making using of Eq. (5.56) and using $F_s = \|\boldsymbol{T}_s\|$, the cracking strain increments can be written as:

$$d\gamma_{c,xy} = d_s\left(d\gamma_{xy} - \hat{T}_{s,x}\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}\right) + \hat{T}_{s,x}d\delta_s = d_s\left(\hat{T}^2_{s,y}d\gamma_{xy} - \hat{T}_{s,x}\hat{T}_{s,y}d\gamma_{xz}\right) + \hat{T}_{s,x}d\delta_s$$
$$d\gamma_{c,xz} = d_s\left(\hat{T}^2_{s,x}d\gamma_{xz} - \hat{T}_{s,x}\hat{T}_{s,y}d\gamma_{xy}\right) + \hat{T}_{s,y}d\delta_s$$

Notice that all $d\delta_s^{(e)}$ terms canceled out. These components can be written in vector form:

$$d\boldsymbol{\gamma}_c = \hat{\boldsymbol{T}}_s d\delta_s + d_s\big(d\boldsymbol{\gamma} - \hat{\boldsymbol{T}}_s(\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma})\big) = \hat{\boldsymbol{T}}_s d\delta_s + d_s\hat{\boldsymbol{T}}_t(\hat{\boldsymbol{T}}_t \cdot d\boldsymbol{\gamma}) \tag{5.73}$$

where $\hat{\boldsymbol{T}}_t$ is unit vector tangential to the shear traction vector. These reduce to 1D result for uniaxial shear.

Once shears are coupled, the energy dissipation simplifies to:

$$\begin{aligned} d\Omega &= \frac{1}{2C_{11}}\left(\frac{\sigma_{xx}}{1-d_n}\right)^2 \mathbb{R}_n\left(d\delta_n - d\delta_e^{(e)}\right) + \frac{1}{2G}\left(\frac{\|\boldsymbol{T}_s\|}{1-d_s}\right)^2 \mathbb{R}_s\left(d\delta_s - d\delta_s^{(e)}\right) \\ &= \frac{1}{2}\varphi_n(\delta_n)\left(d\delta_n - d\delta_e^{(e)}\right) + \frac{1}{2}\varphi_s(\delta_s)\left(d\delta_s - d\delta_s^{(e)}\right) \end{aligned}$$

Unlike for cuboid surface, the integral of $d\Omega$ is not a function of δ_n and δ_s. It will depend on how $\boldsymbol{\alpha}$ changed during the simulation. The code will need to track dissipated energy rather the calculate it on each time step.

Ovoid Surface (Iso)

Using the recommended method to link d parameters from Ovoid Surface (and from Ovoid Surface (General)) above, will have a single damage variable $d_n = d_{xy} = d_{xz} = d$ and single shear cracking strain $\delta_s = \delta_{xy} = \delta_{xz}$ (as well as ($C_{55} = C_{66} - G$, $F_{xy} = F_{xz} = G$, $\mathbb{R}_{xy} = \mathbb{R}_{xz} = \mathbb{R}_s$). The incremental solution in Eq. (5.68) than simplifies to:

$$\begin{aligned} \mathbb{R}_n(d\delta_n - d\delta_n^{(e)}) &= \frac{\hat{\boldsymbol{T}}_o \cdot \left[\left(\frac{G}{F_s}d\gamma_{xy}, \frac{G}{\tau_{xz}}d\gamma_{xz}, \frac{C_{11}}{F_n}d\varepsilon_n\right) - \left(\hat{T}_{o,x}\frac{G}{F_s}\frac{d\delta_s^{(e)}}{d_s}, \hat{T}_{o,y}\frac{G}{F_s}\frac{d\delta_s^{(e)}}{d_s}, \hat{T}_{o,z}\frac{C_{11}}{F_n}\frac{d\delta_n^{(e)}}{d_n}\right)\right]}{\hat{\boldsymbol{T}}_o \cdot \left(\hat{T}_{o,x}\frac{G}{\mathbb{R}_s F_s}\left(1+\frac{F_s'}{G}\right), \hat{T}_{o,y}\frac{G}{\mathbb{R}_s F_s}\left(1+\frac{F_s'}{G}\right), \hat{T}_{o,z}\frac{C_{11}}{\mathbb{R}_n F_n}\left(1+\frac{F_n'}{C_{11}}\right)\right)} \\ &= \frac{\frac{G}{F_s}\left(\hat{T}_{o,x}, \hat{T}_{o,y}\right)\cdot d\boldsymbol{\gamma} + \frac{\hat{T}_{o,z}C_{11}}{F_n}d\varepsilon_n - \frac{G}{F_s}\left(\hat{T}^2_{o,x} + \hat{T}^2_{o,y}\right)\frac{d\delta_s^{(e)}}{d} - \frac{\hat{T}^2_{o,z}C_{11}}{F_n}\frac{d\delta_n^{(e)}}{d}}{\frac{(\hat{T}^2_{o,x}+\hat{T}^2_{o,y})G}{\mathbb{R}_s F_s}\left(1+\frac{F_s'}{G}\right) + \frac{\hat{T}^2_{o,z}C_{11}}{\mathbb{R}_n F_n}\left(1+\frac{F_n'}{C_{11}}\right)} \end{aligned} \tag{5.74}$$

where $d\boldsymbol{\gamma} = (d\gamma_{xy}, d\gamma_{xz})$ and $\boldsymbol{T}_s = (\tau^0_{xy}, \tau^0_{xz})$. The cracking strain increments (with $d_n = d_{xy} = d_{xz} = d$) and using Eq. (5.56) are:

$$\begin{aligned} d\gamma_{c,xy} &= \hat{T}_{o,x}(d\delta_s - d\delta_s^{(e)}) + d\left(d\gamma_{xy} - \hat{T}_{o,x}\left(1+\frac{F_s'}{G}\right)(d\delta_s - d\delta_s^{(e)})\right) \\ d\gamma_{c,xz} &= \hat{T}_{o,y}(d\delta_s - d\delta_s^{(e)}) + d\left(d\gamma_{xz} - \hat{T}_{o,y}\left(1+\frac{F_s'}{G}\right)(d\delta_s - d\delta_s^{(e)})\right) \\ d\varepsilon_{c,xx} &= \hat{T}_{o,z}(d\delta_n - d\delta_n^{(e)}) + d\left(d\varepsilon_n - \hat{T}_{o,z}\left(1+\frac{F_n'}{C_{11}}\right)(d\delta_n - d\delta_n^{(e)})\right) \end{aligned} \tag{5.75}$$

which all reduce to 1D result for uniaxial loading.

5.5.3 Pressure and Deviatoric Stress

Sometimes it is beneficial to partition stress into pressure and deviatoric stress. For isotropic materials this separation leads to two decoupled equations that can simplify implementation. Because a crack converts an isotropic to an anisotropic material, that separation is not as useful. If done, the pressure (P) and deviatoric stress (s) are related to volumetric strain ($e = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$) deviatoric strain ($e_d$) by:

$$P = -K(e - d_n\varepsilon_n)$$

$$s_{xx} = 2G\left(e_{xx} - \frac{2d_n\varepsilon_n}{3}\right) \qquad s_{yy} = 2G\left(e_{yy} + \frac{d_n\varepsilon_n}{3}\right) \qquad s_{yy} = 2G\left(e_{yy} + \frac{d_n\varepsilon_n}{3}\right)$$

$$s_{yz} = 2Ge_{yz} \qquad s_{xz} = 2G(1-d_{xz})e_{xz} \qquad s_{xy} = 2G(1-d_{xy})e_{xy}$$

The crack "normal" strain can be expressed in terms of volumetric and deviatoric strain using

$$\varepsilon_n = \frac{1-2\nu}{1-\nu}e_{xx} + \frac{1+\nu}{1-\nu}e = \frac{1}{3K+4G}\left(Ke + \frac{2G}{3}e_{xx}\right)$$

5.5.4 Two Dimensional Problems

Plane Strain

For plane strain, we need to insert residual strains and focus on in-plane properties. Inserting all three effective strains (with $d\varepsilon_{zz}^{(eff)} = -d\varepsilon_{res}$) the key terms are:

$$d\varepsilon_n = d\varepsilon_{xx} - d\varepsilon_{res} + \frac{\nu}{1-\nu}d\varepsilon_{yy} - \frac{2\nu}{1-\nu}d\varepsilon_{res}, \tag{5.76}$$

or

$$d\varepsilon_n = d\varepsilon_{xx} + \frac{\nu}{1-\nu}d\varepsilon_{yy} - \frac{1+\nu}{1-\nu}d\varepsilon_{res}, \qquad \text{and} \qquad d\gamma_t = d\gamma_{xy} \tag{5.77}$$

The normal strain can be rewritten as:

$$d\varepsilon_n^{(r)} = d\varepsilon_{xx} - (1+\nu)d\varepsilon_{res} + \frac{\nu}{1-\nu}(d\varepsilon_{yy} - (1+\nu)d\varepsilon_{res}) = d\varepsilon_{xx}^{(r)} + \frac{\nu}{1-\nu}d\varepsilon_{yy}^{(r)} \tag{5.78}$$

where effective increments are called "reduced" because they subtract the reduced residual strain given by $d\varepsilon_{res}^{(r)} = (1+\nu)d\varepsilon_{res}$. The cracking strain increments are

$$d\varepsilon_{c,xx}^{(r)} = d\left(d_n\varepsilon_n^{(r)}\right), \quad d\gamma_{c,xy} = d(d_{xy}\gamma_{xy}), \quad \text{and} \quad d\gamma_{c,xz} = 0 \tag{5.79}$$

The stress updates become

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11}(d\varepsilon_n^{(r)} - d\varepsilon_{c,xx}^{(r)}) \\ C_{11}\left(d\varepsilon_{yy}^{(r)} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(r)} - d\varepsilon_{c,xx}^{(r)}\right)\right) \\ C_{11}\left(-d\varepsilon_{res} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}^{(r)} + d\varepsilon_{yy} - 2d\varepsilon_{res}\right)\right) \\ G(d\gamma_{xy} - d\gamma_{c,xy}) \end{pmatrix} \tag{5.80}$$

Here shear strains do not need to be reduces and σ_{zz} is a separate calculation and uses total strain increments and a residual strain term.

Plane Stress

Taking the special case for isotropic material in section Plane Stress, the key terms are

$$\mathbf{C}_1^{(r)} = \begin{bmatrix} \frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\ \frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & G \end{bmatrix} \quad \text{and} \quad \mathbf{D} = \begin{bmatrix} H(\sigma_{xx})d_n & H(\sigma_{xx})\nu d_n & 0 \\ 0 & 0 & 0 \\ 0 & 0 & d_{xy} \end{bmatrix} \tag{5.81}$$

The stress update becomes

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \frac{E}{1-\nu^2}\left(d\varepsilon_n - d\varepsilon_{c,xx}\right) \\ \frac{E}{1-\nu^2}\left(d\varepsilon_{yy} + \nu\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}\right)\right) \\ G\left(d\gamma_{xy} - d\gamma_{c,xy}\right) \end{pmatrix} \tag{5.82}$$

$$\varepsilon_n = \varepsilon_{xx} + \nu\varepsilon_{yy} \tag{5.83}$$

and

$$d\varepsilon_{c,xx} = d(d_n\varepsilon_n) \qquad \text{and} \qquad d\gamma_{c,xy} = d(d_{yz}\gamma_{xy}) \tag{5.84}$$

5.6 Numerical Algorithm

Each particle is marked as "undamaged" (before initiation occurs), "damaged" (while damage is evolving), or "failed" (post failure state). In most simulations, all particles start as undamaged, but they could alternatively be initialized as damaged or failed. The following steps depend on particle state.

1. From input ∇u, find $d\boldsymbol{\varepsilon}_0$ in the initial configuration (using large rotation methods in chapter 3). In the process, find R^0_{n-1} and R^0_{tot} as rotation matrices between initial configuration and $(n-1)^{th}$ and n^{th} configurations and $d\mathsf{R} = \mathsf{R}^0_{tot}(\mathsf{R}^0_{n-1})^T$ as the incremental rotation.

2. If the particle is undamaged, rotate current stress to initial configuration and then find trial stress update in those initial axes using

$$\boldsymbol{\sigma}^{(trial)} = (\mathsf{R}^0_{n-1})^T\boldsymbol{\sigma}^{(p)}_{n-1}\mathsf{R}^0_{n-1} + \mathbf{C}d\boldsymbol{\varepsilon}_0 \tag{5.85}$$

   If failure criterion has not been reached, finish update by standard methods for a never-damaged material (depending on parent material model being used).

3. If the failure surface has been reached, mark the particle as "damaged," calculate (and store) rotation matrix, $\mathsf{R}^{(p)}_c$, as rotation from crack axis system where crack normal is along the x axis, to initial axes and calculate (and store) $A_c/(V_p\rho)$. Note that A_c is intersection between the particle and a plane through the particle center with the determined crack normal and ρ is included for subsequent calculations based on specific stress. Proceed to update methods for a "damaged" particle.

4. For "damaged" and "failed" particles, revise rotation matrices to $\mathsf{R}_{tot} = \mathsf{R}^0_{tot}\mathsf{R}^{(p)}_c$ and $\mathsf{R}_{n-1} = \mathsf{R}^0_{n-1}\mathsf{R}^{(p)}_c$ or to matrices that rotate from crack axis system to $(n-1)^{th}$ and n^{th} configurations. Next, rotate $d\boldsymbol{\varepsilon}_0$ (which was found above in initial axes) and previous particle stress to the crack axis system:

$$d\boldsymbol{\varepsilon} = \mathsf{R}^{(p)T}_c d\boldsymbol{\varepsilon}_0\mathsf{R}^{(p)}_c \quad \text{and} \quad \boldsymbol{\sigma} = \mathsf{R}^T_{n-1}\boldsymbol{\sigma}^{(p)}_{n-1}\mathsf{R}_{n-1} \tag{5.86}$$

5. Find strain increments. Assuming crack axis x axis is normal to a symmetry plane, we have

$$d\varepsilon_n = d\varepsilon^*_{xx} + \frac{C_{12}}{C_{11}}\varepsilon^*_{yy} + \frac{C_{13}}{C_{11}}\varepsilon^*_{zz}, \quad d\gamma_{xy} = d\varepsilon_{xy} + d\varepsilon_{yx}, \quad \text{and} \quad d\gamma_{xz} = d\varepsilon_{xz} + d\varepsilon_{zx}$$

For an isotropic material, $C_{1j}/C_{11} = \nu/(1-\nu)$. The damage calculation depends on traction surface being used and the options for cuboid, cylindrical, and ovoid are in the next three sections. Note that for 2D, cuboid and cylindrical are the same. All methods start by finding trial tractions that assume an elastic deformation or

$$d\sigma^{(trial)}_{xx} = C_{11}(1-d_n)d\varepsilon_n, \quad d\tau^{(trial)}_{xy} = C_{66}(1-d_{xy})d\gamma_{xy}, \quad d\tau^{(trial)}_{xz} = C_{55}(1-d_{xz})d\gamma_{xz}$$

and

$$T^{(trial)}_n = \sigma_{xx} + d\sigma^{(trial)}_{xx}, \quad T^{(trial)}_{xy} = \tau_{xy} + d\tau^{(trial)}_{xy}, \quad T^{(trial)}_{xz} = \tau_{xz} + d\tau^{(trial)}_{xz}$$

5.6.1 Cuboid Surface (Implementation)

This surface decouples tension and the two shear axes. The methods for tension are given and then they are repeated for the two shear directions except shear direction might damage with negative stresses and strain increments.

- *Special Theory*: set elastic critical cracking strain increment to $d\delta^{(e)}_n = 0$.
- *General Theory*: Find the elastic critical cracking strain increment $d\delta^{(e)}_n$, which is defined by integration of Eq. (5.55) from $\boldsymbol{\alpha}$ to $\boldsymbol{\alpha} + d\boldsymbol{\alpha}$. A more practical numerical methods is to treat it as a single-variable, finite increment solution by solving for $d\delta^{(e)}$ such that d remains constant:

$$\frac{\delta}{\delta + \frac{F(\delta,\boldsymbol{\alpha})}{E}} = \frac{\delta + d\delta^{(e)}}{\delta + d\delta^{(e)} + \frac{F(\delta+d\delta^{(e)},\boldsymbol{\alpha}+d\boldsymbol{\alpha})}{E}}$$

This equation can be solved for $d\delta^{(e)}$:

$$d\delta^{(e)} = \frac{\delta}{F(\delta,\boldsymbol{\alpha})}\left(F(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) - F(\delta,\boldsymbol{\alpha})\right) \tag{5.87}$$

For small increments, this equation matches Eq. 5.55; starting with that equation:

$$\varphi d\delta^{(e)} = F d\delta^{(e)} - \delta F' d\delta^{(e)} = \delta \sum_i \left(\frac{\partial F}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} d\alpha_i$$

$$d\delta^{(e)} = \frac{\delta}{F}\left(\left(\frac{\partial F}{\partial \delta}\right)_{\boldsymbol{\alpha}} d\delta^{(e)} + \sum_i \left(\frac{\partial F}{\partial \alpha_i}\right)_{\delta,\alpha_{j\neq i}} d\alpha_i\right)$$

The term in parentheses is incremental form of $F(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) - F(\delta,\boldsymbol{\alpha})$, thus showing equivalence of the two approaches. Also note that a key term can be written:

$$\frac{d\delta^{(e)}}{d} = \frac{F(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) - F(\delta,\boldsymbol{\alpha})}{E(1-d)} \tag{5.88}$$

For finite increments we can solve the discrete/implicit equation by Newton's method by solving

$$\begin{aligned} g(x) &= xF(\delta,\boldsymbol{\alpha}) - \delta\left(F(\delta + x, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) - F(\delta,\boldsymbol{\alpha})\right) = 0 \\ g'(x) &= F(\delta,\boldsymbol{\alpha}) - \delta\frac{\partial F(\delta + x, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{\partial \delta} \end{aligned}$$

If $F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) > F(\delta, \boldsymbol{\alpha})$ (*i.e.*, increase in $\boldsymbol{\alpha}$ causes strength at δ to increase) then $g(0) < 0$. The solution is for positive x bracketed by $g(\delta_{max} - \delta) = \delta_{max} > 0$ or $0 < x < \delta_{max} - \delta$ and δ_{max} is evaluated for $\boldsymbol{\alpha} + d\boldsymbol{\alpha}$. But, if an increase in $\boldsymbol{\alpha}$ causes strength to decrease at δ, then $g(0) > 0$ and the solution is for negative x. Because

$$g(-\delta) = -\delta F(0, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) < 0$$

The solution is bracked by $-\delta < x < 0$. This problem can be stably solved using Newton's method with bracketing. Note that for linear softening, $g'(x)$ is constant and the equation can be solved analytically using

$$\begin{aligned} x &= -\frac{g(0)}{g'(0)} = \frac{\delta\left(F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) - F(\delta, \boldsymbol{\alpha})\right)}{F(\delta, \boldsymbol{\alpha}) - \delta \frac{\partial F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{\partial \delta}} \\ F(\delta, \boldsymbol{\alpha}) &= \sigma^*(\boldsymbol{\alpha})\left(1 - \frac{\delta}{2G_c(\boldsymbol{\alpha}) s^*(\boldsymbol{\alpha})}\right) \\ \frac{\partial F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{\partial \delta} &= -\frac{\sigma^*(\boldsymbol{\alpha} + d\boldsymbol{\alpha})}{2G_c(\boldsymbol{\alpha} + d\boldsymbol{\alpha}) s^*(\boldsymbol{\alpha} + d\boldsymbol{\alpha})} \end{aligned}$$

Substituting and simplifying in Mathematica leads to:

$$x = \delta\left(\frac{\delta_{max}(\boldsymbol{\alpha})\delta_{max}(\boldsymbol{\alpha} + d\boldsymbol{\alpha})\sigma_i^*(\boldsymbol{\alpha} + d\boldsymbol{\alpha})}{(\delta_{max}(\boldsymbol{\alpha}) - \delta)\,\delta_{max}(\boldsymbol{\alpha} + d\boldsymbol{\alpha})\sigma_i^*(\boldsymbol{\alpha}) + \delta\,\delta_{max}(\boldsymbol{\alpha})\sigma_i^*(\boldsymbol{\alpha} + d\boldsymbol{\alpha})} - 1\right)$$

where $s^*(\boldsymbol{\alpha}) = r_G A_c / (V_p r_\sigma \sigma_i(\boldsymbol{\alpha}))$, $\sigma_i^*(\boldsymbol{\alpha}) = r_\sigma \sigma_i(\boldsymbol{\alpha})$ is initiation stress at $\boldsymbol{\alpha}$, and $\delta_{max}(\boldsymbol{\alpha}) = 2G_c(\boldsymbol{\alpha}) s^*(\boldsymbol{\alpha})$. This result only needs strength model to be linear in δ; it can be nonlinear in $\boldsymbol{\alpha}$ and both G_c and σ can vary with $\boldsymbol{\alpha}$.

A better approach is to lump left side of the equation as the current value of the tracked damage variable. For this case, an alternate finite increment solution is found by solving for $d\delta^{(e)}$ such new d equals the tracked current d:

$$d = \frac{\delta + d\delta^{(e)}}{\delta + d\delta^{(e)} + \frac{F(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{E}}$$

This equation can be solved for $d\delta^{(e)}$:

$$d\delta^{(e)} = -\delta + \frac{dF(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{E(1-d)} \tag{5.89}$$

For finite increments we can solve the discrete/implicit equation by Newton's method by solving for x in $g(x) = 0$ where

$$\begin{aligned} g(x) &= E(1-d)(x + \delta) - dF(\delta + x, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) \\ g'(x) &= E(1-d) - d\frac{\partial F(\delta + x, \boldsymbol{\alpha} + d\boldsymbol{\alpha})}{\partial \delta} \end{aligned}$$

If $F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha}) > F(\delta, \boldsymbol{\alpha})$ (*i.e.*, increase in $\boldsymbol{\alpha}$ causes strength at δ to increase) then using

$$\frac{g(0)}{(1-d)F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha})} = \frac{E\delta}{F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha})} - \frac{d}{1-d} = E\delta\left(\frac{1}{F(\delta, \boldsymbol{\alpha} + d\boldsymbol{\alpha})} - \frac{1}{F(\delta, \boldsymbol{\alpha})}\right)$$

implies that $g(0) < 0$. We also note that $g(\delta_{max}(\boldsymbol{\alpha}+d\boldsymbol{\alpha})-\delta) = E(1-d)\delta_{max}(\boldsymbol{\alpha}+d\boldsymbol{\alpha}) > 0$. This the solution is for positive x bracketed by $0 < x < \delta_{max}(\boldsymbol{\alpha}+d\boldsymbol{\alpha})-\delta$. But, if an increase in $\boldsymbol{\alpha}$ causes strength to decrease at δ, then $g(0) > 0$ and the solution is for negative x. Because $g(-\delta) = -dF(0, \boldsymbol{\alpha}+d\boldsymbol{\alpha}) < 0$, the solution is bracketed by $-\delta < x < 0$.

For linear softening (*i.e.*, $g'(x)$ independent of x) and substituting $F(\delta, \boldsymbol{\alpha})$ and $\partial F(\delta, \boldsymbol{\alpha}+d\boldsymbol{\alpha})/\partial\delta$ from above, a closed-form solution is

$$x = -\frac{g(0)}{g'(0)} = \frac{d\delta_{max}(\boldsymbol{\alpha}+d\boldsymbol{\alpha})\sigma_i^*(\boldsymbol{\alpha}+d\boldsymbol{\alpha})}{E(1-d)\delta_{max}(\boldsymbol{\alpha}+d\boldsymbol{\alpha}) + d\sigma_i^*(\boldsymbol{\alpha}+d\boldsymbol{\alpha})} - \delta$$

where $\delta_{max}(\boldsymbol{\alpha}) = 2G_c(\boldsymbol{\alpha})s^*(\boldsymbol{\alpha})$.

For non-linear softening, the above problems can be stably solved using Newton's method with bracketing. The input required for this calculation is to know strength and toughness at $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}+d\boldsymbol{\alpha}$. These can be combined into softening law scaling term in the two states where relative toughness is included in the scaling terms. The initiation law and softening laws can calculate these terms. When done, set $\sigma_I \to \sigma_I(\boldsymbol{\alpha}+d\boldsymbol{\alpha})$ and $f_I(\delta_n) \to f_I(\delta_n + d\delta^{(e)}, \boldsymbol{\alpha}+d\boldsymbol{\alpha})$.

- *Pressure Dependence*: The previous step to find elastic increment in δ assumes that $d\boldsymbol{\alpha}$ is known. This step is therefore complicated by pressure dependent properties because the increment in pressure depends the cracking strain increment ($-d\varepsilon_{c,xx}$), but that increment is not known until after calculation of $d\delta^{(e)}$. Considering all possible analysis states, the pressure increment for an isotropic material is

$$\begin{aligned}
dP &= -C_{11}\left(1+\frac{2\nu}{1-\nu}\right)\left(d\varepsilon_{xx}^{(eff)} - d\varepsilon_{c,xx} + d\varepsilon_{yy}^{(eff)} + d\varepsilon_{zz}^{(eff)}\right) && \text{3D and Axisymetric}\\
dP &= -C_{11}\left(1+\frac{\nu}{1-\nu}\right)\left(d\varepsilon_{xx}^{(r,eff)} - d\varepsilon_{c,xx} + d\varepsilon_{yy}^{(r,eff)}\right)\\
&\quad - C_{11}\left(\frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(eff)} - d\varepsilon_{c,xx} + d\varepsilon_{yy}^{(eff)}\right) - \varepsilon_{zz}^{(res)}\right) && \text{Plane Strain}\\
dP &= -C_{11}^{(r)}(1+\nu)\left(d\varepsilon_{xx}^{(eff)} - d\varepsilon_{c,xx} + d\varepsilon_{yy}^{(eff)}\right) && \text{Plane Stress}
\end{aligned}$$

where $d\varepsilon_{ii}^{(eff)} = d\varepsilon_{ii} - d\varepsilon_{ii}^{(res)}$, $d\varepsilon_{ii}^{(r,eff)} = d\varepsilon_{ii} - d\varepsilon_{ii}^{(r,res)}$, r means to use reduced stiffness (in plane stress) or residual expansion coefficient (in plane strain) analysis. In cuboid implementation with pressure dependence only in shear properties, $d\varepsilon_{c,xx}$ can be calculated before needing to find $d\delta^{(e)}$ in shear. But if normal direction depends on pressure or for coupled methods (cylindrical and ovoid methods), $d\varepsilon_{c,xx}$ is not know before it is needed to find increment in pressure. A recursive method that appears effective is:

  1. Start with $d\varepsilon_{c,xx}^{(0)}$ equal to increment that would occur for an elastic step and set $i = 1$.
  2. Evaluate damage evolution using pressure increment found from $d\varepsilon_{c,xx}^{(i-1)}$, which will result in new evaluation of $d\varepsilon_{c,xx}^{(i)}$.
  3. If $|d\varepsilon_{c,xx}^{(i)} - d\varepsilon_{c,xx}^{(i-1)}|/\delta_{max}^{(n)} <$ (tol) then accept the result for damage evolution. If not, set $i = i+1$ and go to step 2. To prevent endless loop, accept answer if reach some specified maximum number of passes. Note the (tol) is tolerance and the evaluation is a dimensionless quantity in range of 0 to 1.

If $T_n^{(trial)} < F_I(\delta_n)$ (*General Theory*: use updated $F_I(\delta_n + d\delta^{(e)}, \boldsymbol{\alpha}+d\boldsymbol{\alpha})$), then the update is elastic (note that right side is always positive, which means no normal-direction damage when in compression

or when $T_n^{(trial)} < 0$). Set $d\varepsilon_{c,xx} = d_n d\varepsilon_n$ to update cracking strain, make no change to d_n, increment δ_n by $d\delta_n^{(e)}$, and proceed to final update for normal stresses. In normal direction, this change cannot let total $\varepsilon_{c,xx}$ becoming negative. If it does, change $d\varepsilon_{c,xx}$ to $-\varepsilon_{c,xx}$ to end up with zero cracking strain after the update. All elastic updates have zero energy dissipation.

If the trial update exceeds the current normal strength, then partition the elastic and damage strains during the step. We partition total strain into $d\varepsilon_n = d\varepsilon_n^{(1)} + d\varepsilon_n^{(2)}$ where $d\varepsilon_n^{(1)}$ is strain to reach the failure envelope and $d\varepsilon_n^{(2)}$ is strain from failure envelop at the trial stress:

$$d\varepsilon_n^{(1)} = \frac{F_I - \sigma_{xx}}{C_{11}(1-d_n)} \quad \text{and} \quad d\varepsilon_n^{(2)} = d\varepsilon_n - d\varepsilon_n^{(1)} = \frac{T_n^{(trial)} - F_I}{C_{11}(1-d_n)}$$

- *General Theory*: We imagine three steps — one to reach $F_I(\delta, \boldsymbol{\alpha})$ (or $d\varepsilon_n^{(1)}$), one to move along the damage surface at constant d_n (or $d\varepsilon_n^{(e)}$) to reach $F_I(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$, and last to cause damage (or $d\varepsilon_n^{(2)}$). By definition of $d\varepsilon_n^{(e)}$ in Eq. (5.61) and using Eq. (5.88):

$$d\varepsilon_n^{(1*)} = d\varepsilon_n^{(1)} + d\varepsilon_n^{(e)} = \frac{F_I - \sigma_{xx}}{C_{11}(1-d_n)} + \frac{d\delta_n^{(e)}}{d_n} = \frac{F_I^* - \sigma_{xx}}{C_{11}(1-d_n)}$$

  where $F_I^* = F_I(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$. The general theory then proceeds by special theory by setting $d\varepsilon_n^{(1)} = d\varepsilon_n^{(1*)}$ and updating F_I to F_I^* and δ is already updated to $\delta + d\delta_n^{(e)}$.

The portion of strain above the failure envelop is used to find damage by solving (*General Theory*: which is done at $\boldsymbol{\alpha} + d\boldsymbol{\alpha}$).

$$d\varepsilon_n^{(2)} = d\delta_n + \varepsilon_{n0}\big(f_I(\delta_n + d\delta_n) - f_I(\delta_n)\big) \tag{5.90}$$

For small increments, this equation reduces to:

$$d\delta_n = \frac{1}{1 + \varepsilon_{n0} f_I'(\delta_n)} d\varepsilon_n^{(2)} \tag{5.91}$$

For larger increments (which may occur if the softening is rapid or large negative stiffness), the equation is better solved numerically to find δ_n. For Newton's methods, we need to solve

$$g(d\delta_n) = d\delta_n - d\varepsilon_n^{(2)} + \varepsilon_{n0}\big(f_I(\delta_n + d\delta_n) - f_I(\delta_n)\big) = 0 \tag{5.92}$$

with

$$g'(d\delta_n) = 1 + \varepsilon_{n0} f_I'(\delta_n + d\delta_n) \tag{5.93}$$

For bracketing, we begin with

$$g(0) = -d\varepsilon_n^{(2)} < 0 \tag{5.94}$$

$$g(d\varepsilon_n^{(2)}) = \varepsilon_{n0}\big(f_I(\delta_n + d\varepsilon_n^{(2)}) - f_I(\delta_n)\big) < 0 \tag{5.95}$$

$$g(d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)) = \varepsilon_{n0} f_I(\delta_n + d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)) \geq 0 \tag{5.96}$$

where the equals of the last result is if failure occurs (the end point is then the solution or $d\delta_n = d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)$). Our bracketing becomes $d\varepsilon_n^{(2)} < d\delta_n < d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)$. We normalize $g(x)$ (where x is $d\delta_n$) to be of order unity by changing to:

$$g(x) = \frac{x - d\varepsilon_n^{(2)}}{b} + \frac{f_I(\delta_n + x)}{f_I(\delta)} - 1 = 0 \tag{5.97}$$

$$g'(x) = \frac{1}{b} + \frac{f_I'(\delta_n + x)}{f_I(\delta)} \tag{5.98}$$

where $b = \varepsilon_{n0} f_I(\delta_n)$ is the width of the bracket window. Over the window, the function will vary from

$$\frac{f_I(\delta_n + d\varepsilon_n^{(2)})}{f_I(\delta_n)} - 1 < g(x) < \frac{f_I(\delta_n + d\varepsilon_n^{(2)} + b)}{f_I(\delta_n)} \tag{5.99}$$

Derivatives of softening laws are rather well behaved meaning simple Newton's method is usually OK, but some issues can arise especially near failure. The numerical options that seemed to work are:

1. Use Newton's method with bracketing and the initial guess close to the lower limit of $d\varepsilon_n^{(2)}$

2. A step outside the bracket is most likely round off error. The best approach is to change such a guess to just inside the current bracket. Normal bracketing uses midpoint when outside the brackets, but changing to close to the edge is better for softening laws.

3. Standard Newton's method with bracketed uses midpoint if Newton's step is larger than half the current bracket. This option can be ignored for softening laws.

4. The special case of linear softening with $f_I(\delta_n) = 1 - \delta_n/\delta_{max}$ can be solved explicitly:

$$d\varepsilon_n^{(2)} = d\delta_n - \varepsilon_{n0}\frac{d\delta_n}{\delta_{max}} \qquad \text{or} \qquad d\delta_n = \frac{d\varepsilon_n^{(2)}}{1 - \frac{\varepsilon_{n0}}{\delta_{max}}} \tag{5.100}$$

   along with attention to surpassing the maximum crack strain. The increment in damage variable (in case that is more stable) is

$$d(d_n) = \mathbb{R}_n(\delta_n)d\delta_n = \frac{\varepsilon_{n0}}{\left(\delta_n + \varepsilon_{n0}\left(1 - \frac{\delta_n}{\delta_{max}}\right)\right)^2}\frac{d\varepsilon_n^{(2)}}{1 - \frac{\varepsilon_{n0}}{\delta_{max}}}$$

When done, if failure, set $\delta_n = \delta_{max}$ and $d_n = 1$. If not failed, set $\delta_n \to \delta_n + d\delta_n + d\delta_n^{(e)}$. The total cracking strain increment for the two steps is

$$d\varepsilon_{c,xx} = d_n d\varepsilon_n^{(1)} + d\delta_n = d_n(d\varepsilon_n - d\varepsilon_n^{(2)}) + d\delta_n$$

The first term is cracking strain increment during elastic portion of the step while second is cracking strain increment during damage evolution. Calculate updated d_n and the store it along with updated δ_n on the particle. Finally, calculate dissipated energy.

- *General Theory*: The same equation applies in general theory. Or explicitly, the general cracking stain increment adds elastic step to $F_I(\delta, \boldsymbol{\alpha})$ to total δ change to get

$$d\varepsilon_{c,xx} = d_n(d\varepsilon_n^{(1)}) + d\delta_n + d\delta_n^{(e)} = d_n(d\varepsilon_n^{(1)} + d\varepsilon_n^{(e)}) + d\delta_n = d_n(d\varepsilon_n - d\varepsilon_n^{(2)}) + d\delta_n$$

  The energy dissipation using total change in δ minus $d\delta_n^{(e)}$, which here is equal to $d\delta_n$.

Finally, repeat for shear directions (x-y in 2D and also x-z in 3D). The implementation accounts for sign of the shear stress by using sign(τ_{ij}) on both the damage evolution and on the cracking strain increment.

5.6.2 Cyindrical Surface (Implementation)

This surface couples shear and therefore only occurs in 3D modeling that has two shears on the crack plane. This implementation is also limited to isotropic materials. Coupling shears in anisotropic materials needs to develop an appropriate strength model (and it need not be elliptical). The normal update is the same as for cuboid surface in the previous step, but the shear updates are coupled and their damage parameters and strength models are equal (for isotropic). The trial shear traction is $\boldsymbol{T}_s^{(trial)} = (T_{xy}^{(trial)}, T_{xz}^{(trial)})$. Find $d\delta_s^{(e)}$ by same methods used for cuboid surface for general theory or set $d\delta_s^{(e)} = 0$ for special theory. If trial state is within the elliptical failure envelop, the update is elastic. Set $d\gamma_{c,xy} = d_s d\gamma_{xy}$ and $d\gamma_{c,xz} = d_s d\gamma_{xz}$ to update each cracking strain, increment δ_s by $d\delta_s^{(e)}$, make no change to d_s, and proceed to final update for stresses.

If the trial update exceeds the current elliptical envelop (*General theory*: envelope at $\delta + d\delta^{(e)}$ and $\boldsymbol{\alpha} + d\boldsymbol{\alpha}$), partition into two increments as in cuboid methods, but scaling traction magnitude and strain increment vectors. First move to ellipse along the current traction vector by increment $d\boldsymbol{T}_s = \phi \hat{\boldsymbol{T}}_s \|\boldsymbol{T}_s\|$ until reaching the failure surface via:

$$(1+\phi)^2 \|\boldsymbol{T}_s\|^2 \left(\hat{T}_{s,x}^2 + \hat{T}_{s.y}^2\right) = F_s(\delta_s, \boldsymbol{\alpha})^2 \quad \Longrightarrow \quad \phi = \frac{F_s(\delta_s, \boldsymbol{\alpha}) - \|\boldsymbol{T}_s\|}{\|\boldsymbol{T}_s\|}$$

the strain increment to reach the failure surface becomes

$$d\boldsymbol{\gamma}^{(1)} = \frac{\phi \hat{\boldsymbol{T}}_s \|\boldsymbol{T}_s\|}{G(1-d_s)} = \hat{\boldsymbol{T}}_s \frac{F_s(\delta_s, \boldsymbol{\alpha}) - \|\boldsymbol{T}_s\|}{G(1-d_s)}$$

- *General Theory*: We imagine three steps — one to reach $F_s(\delta, \boldsymbol{\alpha})$ (or $d\boldsymbol{\gamma}^{(1)}$), one to move along the damage surface at constant d_s (or $d\boldsymbol{\gamma}^{(e)}$) to reach $F_s(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$, and last to cause damage (or $d\boldsymbol{\gamma}^{(2)}$). The total elastic increment to move to $F_s(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$ is sum of $d\boldsymbol{\gamma}^{(1)}$ and $d\boldsymbol{\gamma}^{(e)}$ using Eq. (5.67) and Eq. (5.88):

  $$d\boldsymbol{\gamma}^{(1*)} = d\boldsymbol{\gamma}^{(1)} + d\boldsymbol{\gamma}^{(e)} = \hat{\boldsymbol{T}}_s \frac{F_s^* - \|\boldsymbol{T}_s\|}{G(1-d_s)}$$

  where $F_s^* = F_s(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$. The general theory proceeds by updating F_s to F_s^* and δ_s is already updated to $\delta_s + d\delta_s^{(e)}$. The special theory proceeds by same methods but sets $d\boldsymbol{\gamma}^{(e)} = 0$

Next find strain to cause damage or $d\boldsymbol{\gamma}^{(2)} = d\boldsymbol{\gamma} - d\boldsymbol{\gamma}^{(1)} - d\boldsymbol{\gamma}^{(e)} = 0$. Given this biaxial strain, find $d\delta_s$ using Cuboid methods with $d\gamma_{eff} = \hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}^{(2)}$ (note that we do not need to recalculate $\hat{\boldsymbol{T}}_s$ on the failure surface because the increment to get this point is parallel to $\boldsymbol{T}_s$). If failure, set $\delta_s = \delta_{max}$ and $d_s = 1$. If not failed, set $\delta_s \to \delta_s + d\delta_s^{(e)} + d\delta_s$. The total cracking strain increment sums elastic change to $F_s(\delta, \boldsymbol{\alpha})$ to damage increment accounting for $d\delta_s^{(e)}$ in general theory (see Eq. (5.73)) to get.

$$\begin{aligned}
d\boldsymbol{\gamma}_c &= d_s\left(d\boldsymbol{\gamma}^{(1)}\right) + d_s\left(d\boldsymbol{\gamma}^{(2)} - \hat{\boldsymbol{T}}_s(\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}^{(2)})\right) + \hat{\boldsymbol{T}}_s\left(d\delta_s + d\delta_s^{(e)}\right) \\
&= d_s\left(d\boldsymbol{\gamma}^{(1)} + d\boldsymbol{\gamma}^{(e)}\right) + d_s\left(d\boldsymbol{\gamma}^{(2)} - \hat{\boldsymbol{T}}_s(\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}^{(2)})\right) + \hat{\boldsymbol{T}}_s d\delta_s \\
&= d_s\left(d\boldsymbol{\gamma} - d\boldsymbol{\gamma}^{(2)}\right) + d_s\left(d\boldsymbol{\gamma}^{(2)} - \hat{\boldsymbol{T}}_s(\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}^{(2)})\right) + \hat{\boldsymbol{T}}_s d\delta_s \\
&= d_s\left(d\boldsymbol{\gamma} - \hat{\boldsymbol{T}}_s(\hat{\boldsymbol{T}}_s \cdot d\boldsymbol{\gamma}^{(2)})\right) + \hat{\boldsymbol{T}}_s d\delta_s
\end{aligned}$$

Finally, calculate updated d_s and the store it along with updated δ_s on the particle and then calculate dissipated energy. The energy dissipation uses total change in δ_s minus $d\delta_s^{(e)}$, which here is equal to $d\delta_s$.

5.6.3 Ovoid Surface (Implementation)

This implementation is also limited to isotropic materials with three damage parameters ($d_n = d_s = d$. δ_n, and δ_s) and two softening laws (F_n and F_s). The trial traction is

$$\boldsymbol{T}^{(trial)} = (T_{xy}^{(trial)}, T_{xz}^{(trial)}, T_n^{(trial)})$$

Find $d\delta_n^{(e)}$ and $d\delta_s^{(e)}$ by same methods used for cuboid surface for general theory or set $d\delta_n^{(e)} = d\delta_s^{(e)} = 0$ for special theory. If trial tractions are within the ovoid failure envelop, the update is elastic. Set $d\varepsilon_{c,xx} = d_n d\varepsilon_n$ and $d\gamma_{c,ij} = d_s d\gamma_{ij}$ to update cracking strain, make no change to d, add $d\delta_n^{(e)}$ to δ_n, add $d\delta_s^{(e)}$ to δ_s, and proceed to final update for normal stresses.

If the trial update exceeds the current elliptical envelop, partition into two increments by moving parallel to the traction vector until reaching the failure surface. We change the current traction by $d\boldsymbol{T} = \phi \boldsymbol{T} = \phi \hat{\boldsymbol{T}} \|\boldsymbol{T}\|$ and find ϕ to match current failure envelop using

$$\begin{aligned} 1 &= \left(\frac{\hat{\boldsymbol{T}}_n(1+\phi)\|\boldsymbol{T}\|}{F_n}\right)^2 + \left(\frac{\hat{\boldsymbol{T}}_{xy}(1+\phi)\|\boldsymbol{T}\|}{F_s}\right)^2 + \left(\frac{\hat{\boldsymbol{T}}_{xz}(1+\phi)\|\boldsymbol{T}\|}{F_s}\right)^2 \\ &= (1+\phi)^2\|\boldsymbol{T}\|^2\left(\frac{\hat{\boldsymbol{T}}_n^2}{F_n^2} + \frac{\hat{\boldsymbol{T}}_{xy}^2 + \hat{\boldsymbol{T}}_{xz}^2}{F_s^2}\right) \\ \phi\|\boldsymbol{T}\| &= \frac{F_n F_s}{\sqrt{F_s^2\hat{\boldsymbol{T}}_n^2 + F_n^2\left(\hat{\boldsymbol{T}}_{xy}^2 + \hat{\boldsymbol{T}}_{xz}^2\right)}} - \|\boldsymbol{T}\| \end{aligned}$$

The strain to reach the yield surface (and remaining strain to cause damage) become

$$d\boldsymbol{\varepsilon}^{(1)} = \frac{\phi\|\boldsymbol{T}\|}{1-d}\left(\frac{\hat{T}_{xy}}{G}, \frac{\hat{T}_{xz}}{G}, \frac{\hat{T}_n}{C_{11}}\right) \quad \text{and} \quad d\boldsymbol{\varepsilon}^{(2)} = d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^{(1)}$$

- *General Theory*: We imagine three steps — one to reach $(\delta, \boldsymbol{\alpha})$ (or $d\boldsymbol{\varepsilon}^{(1)}$), one to move along the damage surface at constant d (or $d\boldsymbol{\varepsilon}^{(e)}$ form Eq. (5.69)) to reach $(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$, and last to cause damage (or $d\boldsymbol{\varepsilon}^{(2)}$). The total elastic increment to move to $(\delta + d\delta^{(e)}, \boldsymbol{\alpha} + d\boldsymbol{\alpha})$ on the failure surface is

$$\begin{aligned} d\boldsymbol{\varepsilon}^{(1*)} = d\boldsymbol{\varepsilon}^{(1)} + d\boldsymbol{\varepsilon}^{(e)} = \frac{\phi\|\boldsymbol{T}\|}{1-d}\left(\frac{\hat{T}_{xy}}{G}, \frac{\hat{T}_{xz}}{G}, \frac{\hat{T}_n}{C_{11}}\right) + \Bigg(\frac{\hat{\boldsymbol{T}}_{xy}(1+\phi)\|\boldsymbol{T}\|}{F_s}\frac{d\delta_s^{(e)}}{d}, \\ \frac{\hat{\boldsymbol{T}}_{xz}(1+\phi)\|\boldsymbol{T}\|}{F_s}\frac{d\delta_s^{(e)}}{d}, \frac{\hat{\boldsymbol{T}}_n(1+\phi)\|\boldsymbol{T}\|}{F_n}\frac{d\delta_n^{(e)}}{d}\Bigg) \end{aligned}$$

  Using Eq. (5.88), this simplifies to:

$$d\boldsymbol{\varepsilon}^{(1*)} = \frac{\|\boldsymbol{T}\|}{1-d}\left(\frac{\hat{T}_{xy}}{G}\left(\frac{(1+\phi)F_s^*}{F_s} - 1\right), \frac{\hat{T}_{xz}}{G}\left(\frac{(1+\phi)F_s^*}{F_s} - 1\right), \frac{\hat{T}_n}{C_{11}}\left(\frac{(1+\phi)F_n^*}{F_n} - 1\right)\right)$$

  It is easy to show that this increment falls on the update failure surface. The general theory then proceeds by updating F_s and F_n to F_s^* and F_n^* and δ_s and δ_n are already updated to $\delta_s + d\delta_s^{(e)}$ and $\delta_n + d\delta_n^{(e)}$. The special theory proceeds by same methods but sets $d\boldsymbol{\varepsilon}^{(e)} = 0$. But note, that is $d\delta_n^{(e)} \neq 0$ the traction in the update state may not be along the initial traction directions. We thus have to find traction on the update failure surface as

$$\boldsymbol{T}^* = (1+\phi)\|\boldsymbol{T}\|\left(\frac{\hat{T}_{xy}F_s^*}{F_s}, \frac{\hat{T}_{xz}F_s^*}{F_s}, \frac{\hat{T}_n F_n^*}{F_n}\right)$$

Next find strain to cause damage or $d\boldsymbol{\varepsilon}^{(2)} = d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^{(1)} - d\varepsilon^{(e)} = 0$. Find new tractions (they are needed in cracking strain updates and in energy dissipation) and find $\boldsymbol{T}_o$ components (should automatically be a unit vector). Using the 3D strain increment, find $\mathbb{R}_n(d\delta_n - d\delta_n^{(e)})$ using Eq. (5.74) (without its $d\delta_i^{(e)}$ terms) If failure, set $\delta_n = \delta_{n,max}$, $\delta_s = \delta_{s,max}$, and $d_n = d_s = 1$. If not failed, set $\delta_n \to \delta_n + d\delta_n^{(e)} + d\delta_n$ and update $\delta_s \to \delta_s + d\delta_s^{(e)} + \mathbb{R}_n(d\delta_n - d\delta_n^{(e)})/\mathbb{R}_s$, and set each to have the same d.

The cracking strain increments add elastic steps to change during evolution. For shear (from Eq. (5.75)), use

$$\begin{aligned} d\gamma_{c,xy} &= d(d\gamma_{xy}^{(1)} + d\gamma_{xy}^{(e)}) + \hat{T}_{o,x} d\delta_s^* + d\left(d\gamma_{xy}^{(2)} - \hat{T}_{o,x}\left(1 + \frac{F_s'}{G}\right) d\delta_s^* \right) \\ &= \hat{T}_{o,x} d\delta_s^* + d\left(d\gamma_{xy} - \hat{T}_{o,x}\left(1 + \frac{F_s'}{G}\right) d\delta_s^* \right) \end{aligned}$$

where $d\delta_s^*$ is increment found from the damage step alone (*i.e.*, equal to $d\delta_s - d\delta_s^{(e)}$). Note that we add $d\gamma_{xy}^{(e)}$ to the elastic step because we are treating the last step by special theory on the updated surface state with updated tractions and unit vectors. Similar results apply for the other two cracking strains.

If in compression, use the cylindrical shear method, but update $d\delta_n$ using Eq. (5.70).

5.6.4 Needs Editing

1. In calculations, the increment in dissipated energy due to any damage variable change is:

$$d\Omega_i = d\overline{G}_i = \overline{G}_i(\delta_i + d\delta_i) - \overline{G}_i(\delta_i) \tag{5.101}$$

Alternatively, the energy increment can be found from

$$d\Omega_n = C_{0,11}\left(\varepsilon_n + d\varepsilon_n^{(1)}\right)\left(d\delta_n - d_n d\varepsilon_n^{(2)}\right) \tag{5.102}$$

$$d\Omega_{ij} = G_{ij}\left(\gamma_{ij} + d\gamma_{ij}^{(1)}\right)\left(d\delta_{ij} - d_{ij} d\gamma_{ij}^{(2)}\right) \qquad \text{for } ij = (xy, xz) \tag{5.103}$$

These were checked in code and found identical provided $d\delta_i$ was not very small. When it is small, they differed by round off errors in subtracting two similar numbers.

2. Finally, the stress updates in the non-cracking directions become

$$\begin{pmatrix} d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \end{pmatrix} = \begin{pmatrix} C_{0,11}\left(d\varepsilon_{yy} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx} + \nu d\varepsilon_{zz}\right)\right) \\ C_{0,11}\left(d\varepsilon_{zz} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx} + \nu d\varepsilon_{yy}\right)\right) \\ G d\gamma_{yz} \end{pmatrix} \tag{5.104}$$

Note that pressure change is

$$dP = -\frac{C_{11}}{3}\frac{1+\nu}{1-\nu}(de - d\varepsilon_{c,xx}) = -K(de - d\varepsilon_{c,xx}) \tag{5.105}$$

5.7 Examples of Softening Laws

It is easy to add softening laws to the code and several are implemented. It is likely a fool's errand to determine some "true" softening law or to think that results will be best if softening law is chosen "realistically." Results tend not to depend much on the softening law. For stability reasons, linear softening appears best. Power-law softening is potentiall very unstable (and not implemented). Linear softening also improves numerical efficiency because some numerical steps can be done analytically.

5.7.1 Linear Softening

Linear softening law is

$$F(\delta,\delta_{max}) = \sigma_0\left(1-\frac{\delta}{\delta_{max}}\right)$$

where σ_0 is initiation stress and δ_{max} is failure cracking strain. Equating area under the law to toughness gives:

$$G_c = \frac{V_p}{A_c}\int_0^{\delta_{max}} \sigma_0\left(1-\frac{\delta}{\delta_{max}}\right)d\delta = \frac{\delta_{max}}{2s}$$

where $s = A_c/(V_p\sigma_0)$ is a scaling factor and $\delta_{max} = 2sG_c$. Here V_p is particle volume and A_c is area of crack plane within the particle. We write softening law in terms of s along with other terms potentially needed during numerical modeling:

$$\begin{aligned}
F(\delta,s) &= \sigma_0\left(1-\frac{\delta}{\delta_{max}}\right)\\
\frac{\partial F(\delta,s)}{\partial\delta} &= -\frac{\sigma_0}{\delta_{max}}\\
\Omega(\delta,s) &= \int_0^{\delta} F(u,s)\,du - \frac{\delta F(\delta,s)}{2} = \frac{\sigma_0\delta}{2}\\
\frac{\Omega(\delta,s)}{\Omega(\delta_{max},s)} &= \frac{\delta}{2sG_c}\\
\varphi(\delta,s) = F(\delta,s) - \delta\frac{\partial F(\delta,s)}{\partial\delta} &= \sigma_0\left(1-\frac{\delta}{2sG_c}\right)+\delta\frac{\sigma_0}{2sG_c} = \sigma_0\\
\mathbb{R}(\delta,s,\varepsilon_i) &= \frac{\varepsilon_i}{\left(\delta+\varepsilon_i\left(1-\frac{\delta}{2sG_c}\right)\right)^2}
\end{aligned}$$

The incremental $d\delta$ during damage evolution equation can be solved analytically:

$$\begin{aligned}
d\delta &= d\varepsilon - \frac{1}{E}\left(F(\delta+d\delta,s)-F(\delta,s)\right)\\
d\delta &= \frac{d\varepsilon}{1-\frac{\sigma_0}{2sG_cE}}
\end{aligned}$$

If ever needed, the relation between d and δ can be inverted to give

$$\delta = \frac{2\sigma_0 sG_c d}{2sG_cE(1-d)+\sigma_0 d} \quad \text{and} \quad d = \frac{2sG_cE\delta}{2sG_c\sigma_0+(2sG_cE-\sigma_0)\delta}$$

For stability analysis, we use

$$\frac{1}{\eta} = \frac{1}{\delta_{max}}\frac{\Omega(\delta_{max},s)}{\sigma_0} = \frac{1}{2}$$

If σ_0 depends on one extra variable (such as pressure), a useful derivative is

$$\left(\frac{\partial F(\delta,\alpha)}{\partial\alpha_i}\right)_\delta = \sigma_0'(\alpha)\left(1-\frac{\delta}{sG_c}\right)+\frac{G_c'(\alpha)}{G_c}\left(\frac{\sigma_0\delta}{2sG_c}\right)$$

leading to:

$$d\delta^{(e)} = \delta\left(\frac{\sigma_0(\alpha+d\alpha)}{\sigma_0(\alpha)}-1\right)\left(1-\frac{\delta}{sG_c}\right)+\delta\left(\frac{G_c(\alpha+d\alpha)}{G_c(\alpha)}-1\right)\left(\frac{\delta}{2sG_c}\right)$$

5.7.2 Exponential Softening

The basic exponential softening law is

$$F(\delta,k)=\sigma_0 e^{-k\delta}$$

where σ_0 is (note this law never fails). Equating area under the law to toughness gives:

$$G_c=\frac{V_p}{A_c}\int_0^{\delta_{max}}\sigma_0 e^{-k\delta}\,d\delta=\frac{1}{ks}$$

where $s=A_c/(V_p\sigma_0)$ is a scaling factor and $k=1/(sG_c)$. Here V_p is particle volume and A_c is area of crack plane within the particle. We write softening law in terms of s along with other terms potentially needed during numerical modeling:

$$\begin{aligned}
F(\delta,s)&=\sigma_0 e^{-\delta/(sG_c)}\\
\frac{\partial F(\delta,s)}{\partial\delta}&=-\frac{\sigma_0 e^{-\delta/(sG_c)}}{sG_c}\\
\Omega(\delta,s)=\int_0^{\delta}F(u,s)\,du-\frac{\delta F(\delta,s)}{2}&=\sigma_0\left(sG_c-e^{\delta/(sG_c)}\left(sG_c+\frac{\delta}{2}\right)\right)\\
\frac{\Omega(\delta,s)}{\Omega(\infty,s)}&=1-e^{\delta/(sG_c)}\left(1+\frac{\delta}{2sG_c}\right)\\
\varphi(\delta,s)=F(\delta,s)-\delta\frac{\partial F(\delta,s)}{\partial\delta}&=\sigma_0 e^{-\delta/(sG_c)}\left(1+\frac{\delta}{sG_c}\right)\\
\mathbb{R}(\delta,s,\varepsilon_i)&=\frac{\varepsilon_i e^{-\delta/(sG_c)}\left(1+\frac{\delta}{sG_c}\right)}{\left(\delta+\varepsilon_i e^{-\delta/(sG_c)}\right)^2}
\end{aligned}$$

The incremental $d\delta$ during damage evolution equation can be solved using inverse functions, but otherwise needs numerical method. Similarly, the relation between d and δ can only be inverted with inverse function. The required function is `ProductLog[]`. If ever needed, the relation between d and δ can be inverted to give

$$\delta=sG_c\texttt{ProductLog}\left[\frac{\sigma_0 d}{sG_c(1-d)E}\right]\quad\text{and}\quad d=\frac{E\delta}{E\delta+\sigma_0 e^{-\delta/(sG_c)}}$$

Note that the maximum slope of exponential softening is $-\frac{\sigma_0}{sG_c}$, which is twice the maximum (and constant) slope for linear softening. For stability analysis, we use

$$\frac{1}{\eta}=\frac{1}{sG_c}\frac{\Omega(\delta_{max},s)}{\sigma_0}=1$$

If σ_0 depends on one extra variable (such as pressure), a useful derivative is

$$\left(\frac{\partial F(\delta,\alpha)}{\partial\alpha_i}\right)_{\delta}=\left(\sigma_0'(\alpha)\left(1-\frac{\delta}{sG_c}\right)+\frac{G_c'(\alpha)}{G_c(\alpha)}\frac{\sigma_0\delta}{sG_c}\right)e^{-\delta/(sG_c)}$$

leading to:

$$d\delta^{(e)}=\delta\left(\frac{\sigma_0(\alpha+d\alpha)}{\sigma_0(\alpha)}-1\right)\frac{1-\frac{\delta}{sG_c}}{1+\frac{\delta}{sG_c}}+\delta\left(\frac{G_c(\alpha+d\alpha)}{G_c(\alpha)}-1\right)\frac{\frac{\delta}{sG_c}}{1+\frac{\delta}{sG_c}}$$

5.7.3 Smooth Step Function

The implement smooth step functions uses a cubic function

$$F(\delta,\delta_{max}) = \sigma_0\left(1-3x^2+2x^3\right) \qquad \text{where} \qquad x = \frac{\delta}{\delta_{max}}$$

where σ_0 is initiation stress and δ_{max} is failure cracking strain. Equating area under the law to toughness gives:

$$G_c = \frac{V_p}{A_c}\int_0^{\delta_{max}} \sigma_0\left(1+2x^3-3x^2\right)\delta_{max}\,dx = \frac{\delta_{max}}{2s}$$

where $s = A_c/(V_p\sigma_0)$ is a scaling factor and $\delta_{max} = 2sG_c$. Here V_p is particle volume and A_c is area of crack plane within the particle. We write softening law in terms of s along with other terms potentially needed during numerical modeling:

$$F(\delta,s) = \sigma_0\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(\frac{2\delta}{\delta_{max}}-3\right)\right)$$

$$\frac{\partial F(\delta,s)}{\partial\delta} = -\frac{6\sigma_0}{\delta_{max}}\frac{\delta}{\delta_{max}}\left(1-\frac{\delta}{\delta_{max}}\right)$$

$$\Omega(\delta,s) = \int_0^{\delta} F(u,s)\,du - \frac{\delta F(\delta,s)}{2} = \frac{\sigma_0\delta}{2}\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(1-\frac{\delta}{\delta_{max}}\right)\right)$$

$$\frac{\Omega(\delta,s)}{\Omega(\delta_{max},s)} = \frac{\delta}{\delta_{max}}\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(1-\frac{\delta}{\delta_{max}}\right)\right)$$

$$\varphi(\delta,s) = \sigma_0\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(3-\frac{4\delta}{\delta_{max}}\right)\right)$$

$$\mathbb{R}(\delta,s,\varepsilon_i) = \frac{\varepsilon_i\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(3-\frac{4\delta}{\delta_{max}}\right)\right)}{\left[\delta+\varepsilon_i\left(1+\left(\frac{\delta}{\delta_{max}}\right)^2\left(\frac{2\delta}{\delta_{max}}-3\right)\right)\right]^2}$$

The incremental $d\delta$ during damage evolution equation :

$$d\delta = d\varepsilon - \frac{1}{E}\left(F(\delta+d\delta,s)-F(\delta,s)\right)$$

is a cubic equation. It can be solved analytically (and that solution in implemented in the code). Similarly, the relation between d and δ is a cubic equation:

$$\frac{2\sigma_0 d}{E}x^3 - \frac{3\sigma_0 d}{E}x^3 - (1-d)\delta_{max}x + \frac{\sigma_0 d}{E} = 0 \qquad \text{where} \qquad x = \frac{\delta}{\delta_{max}}$$

Because this is only used for setting initial damage state, the solution in code is found numerically instead of using the cubic equation. Note that the maximum slope of smooth step softening is $-\frac{3\sigma_0}{4sG_c}$, which is 50% higher than the maximum (and constant) slope for linear softening. For stability analysis, we use

$$\frac{1}{\eta} = \frac{3}{2\delta_{max}}\frac{\Omega(\delta_{max},s)}{\sigma_0} = \frac{3}{4}$$

If σ_0 depends on one extra variable (such as pressure), a useful derivative is

$$\left(\frac{\partial F(\delta,\alpha)}{\partial\alpha_i}\right)_\delta = \sigma_0'(\alpha)\left(1-\left(\frac{\delta}{2sG_c}\right)^2\left(9-\frac{4\delta}{sG_c}\right)\right) + \frac{G_c'(\alpha)}{G_c}\left(3\sigma_0\left(\frac{\delta}{2sG_c}\right)^2\left(2-\frac{\delta}{sG_c}\right)\right)$$

leading to:

$$d\delta^{(e)} = \delta\left(\frac{\sigma_0(\alpha+d\alpha)}{\sigma_0(\alpha)}-1\right)\frac{1-\left(\frac{\delta}{2sG_c}\right)^2\left(9-\frac{4\delta}{sG_c}\right)}{1+\left(\frac{\delta}{2sG_c}\right)^2\left(3-\frac{2\delta}{sG_c}\right)}+\delta\left(\frac{G_c(\alpha+d\alpha)}{G_c(\alpha)}-1\right)\frac{3\left(\frac{\delta}{2sG_c}\right)^2\left(2-\frac{\delta}{sG_c}\right)}{1+\left(\frac{\delta}{2sG_c}\right)^2\left(3-\frac{2\delta}{sG_c}\right)}$$

5.7.4 Cubic Softening with Initial Stiffness

This cubic law starts at σ_0, but then increases to a peak value. The start is tied to initiation stress while peak is stress that can be reached in the material. It is generalization of the smotth step law that changes initial slope to k instead of zero:

$$F(\delta,\delta_{max}) = \sigma_0\big(1+(2+k)x\big)\big(1-x\big)^2 \qquad \text{where} \qquad x=\frac{\delta}{\delta_{max}}$$

This function reverts to smooth step if $k=0$. Thus code only needs one of these laws with k as a parameter. The peak stress is given by

$$\max\big(F(\delta,\delta_{max})\big) = \frac{4(3+k)^3}{27(2+k)^2}\sigma_0$$

where σ_0 is initiation stress and δ_{max} is failure cracking strain. Equating area under the law to toughness gives:

$$G_c = \frac{V_p}{A_c}\int_0^{\delta_{max}}\sigma_0\big(1+(2+k)x\big)\big(1-x\big)^2\delta_{max}\,dx = \frac{(6+k)\delta_{max}}{12s}$$

where $s=A_c/(V_p\sigma_0)$ is a scaling factor and $\delta_{max}=12sG_c/(6+k)$. Here V_p is particle volume and A_c is area of crack plane within the particle. We write softening law in terms of s along with other terms potentially needed during numerical modeling:

$$F(\delta,s) = \sigma_0\left(1+\frac{(2+k)\delta}{\delta_{max}}\right)\left(1-\frac{\delta}{\delta_{max}}\right)^2$$

$$\frac{\partial F(\delta,s)}{\partial\delta} = -\frac{\sigma_0}{\delta_{max}}\left(\frac{3(2+k)\delta}{\delta_{max}}-k\right)\left(1-\frac{\delta}{\delta_{max}}\right)$$

$$\Omega(\delta,s) = \int_0^{\delta}F(u,s)\,du - \frac{\delta F(\delta,s)}{2} = \frac{\sigma_0\delta}{2}\left(1+\frac{3+k}{3}\left(\frac{\delta}{\delta_{max}}\right)^2-\frac{2+k}{2}\left(\frac{\delta}{\delta_{max}}\right)^3\right)$$

$$\frac{\Omega(\delta,s)}{\Omega(\delta_{max},s)} = \frac{6\delta}{(6+k)\delta_{max}}\left(1+\frac{3+k}{3}\left(\frac{\delta}{\delta_{max}}\right)^2-\frac{2+k}{2}\left(\frac{\delta}{\delta_{max}}\right)^3\right)$$

$$\varphi(\delta,s) = \sigma_0\left(1-\frac{\delta}{\delta_{max}}\right)\left(1+\frac{\delta}{\delta_{max}}+2(2+k)\left(\frac{\delta}{\delta_{max}}\right)^2\right)$$

$$\mathbb{R}(\delta,s,\varepsilon_i) = \frac{\varepsilon_i\left(1-\frac{\delta}{\delta_{max}}\right)\left(1+\frac{\delta}{\delta_{max}}+2(2+k)\left(\frac{\delta}{\delta_{max}}\right)^2\right)}{\left[\delta+\varepsilon_i\left(1+\frac{(2+k)\delta}{\delta_{max}}\right)\left(1-\frac{\delta}{\delta_{max}}\right)^2\right]^2}$$

For stability analysis, we use

$$\frac{1}{\eta} = \frac{(3+k)^2}{3(2+k)\delta_{max}}\frac{\Omega(\delta_{max},s)}{\sigma_0} = \frac{(6+k)(3+k)^2}{36(2+k)}$$

Chapter 6

Cohesive Zone Modeling

6.1 Introduction

`NairnMPM` (and `OSParticulas`) fully supports cohesive zone modeling. Each cohesive zone model is defined using a material model that is a subclass of `TractionLaw` material. Cohesive zones are used in modeling by adding them to crack particles on explicit cracks. They can be created at the start of a simulation or dynamically inserted whenever a crack propagates.

6.2 Unidirectional Cohesive Zone Modeling

This section describes cohesive zone modeling for unidirectional loading. The main intent is to define all terms and clarify the proposed semantics used later to extend the modeling to mixed-mode loading. All real simulations must be capable of handling mixed-mode loading.

Figure 6.1 shows a possible traction response during monotonic, 1D loading (pure mode I or pure mode II) of a cohesive zone as $F(u)$. This response has a linear portion with stiffness k (SI units N/m^3), ending at COD= $u^{(e)}$, followed by non-linear portion (the plot is drawn using part of the cubic variation, introduced by Needleman, but almost any function could be used). The traction drops to zero at critical COD= $u^{(c)}$.

Traction responses like Fig. 6.1 in the literature have been called the "traction law" for the cohesive zone, but that is a poor terminology. Rather $F(u)$ is an envelop of possible tractions as a function of u; it is equal to tractions in cohesive zone *only* when the zone is subjected to monotonic increases in displacement. This interpretation holds for both plastic and elastic/damage cohesive zones. To handle elastic/damage zones with unloading, a better terminology is to define a zone's strength model denoted as $S(\delta)$ where δ is equal to max(u) during the deformation and is a state variable characterizing the extent of damage. The strength model corresponding to any "traction law" is

$$S(\delta) = \begin{cases} F(u^{(e)}) & \delta < u^{(e)} \\ F(\delta) & u^{(e)} \le \delta \le u^{(c)} \\ 0 & \text{otherwise} \end{cases}$$

If we initialize $\delta = u^{(e)}$ for the state with no damage, we can dispense with the initial region or the region for $\delta < u^{(e)}$ and simply write $S(\delta) = F(\delta)$ (understanding that $\delta \ge u^{(e)}$).

It might seem superfluous to have "traction law" $F(\delta)$ and strength model $S(\delta)$ as two separate concepts, but it is not merely semantics. Some of the literature has been confused by the terminology and sometimes made errors by misinterpreting the area under the traction law as "potential energy" (or

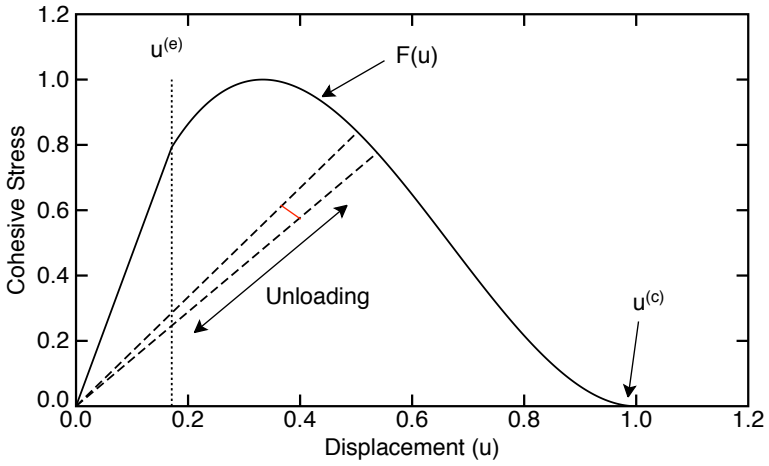

Figure 6.1: A sample trraction response of a cohesive zone in unidirectional loading. The dashed lines show trractions during unloading at constant state of damage. The area between two dashed lines is the energy released on an increase in damage. The area between the two dashed lines capped by the red line is energy released if damage evolves with current traction is less than current strength.

alternatively that a potential energy exists and tractions can be found from its derivatives). A proper analysis must supplement the "traction law" with how the zone responds when unloaded. Early CZM work (*e.g.*, Dugdale and others) imagined a plastic zone. Those models typically did not address unloading and specifically limit analysis to monotonic loading. When CZMs are used in numerical modeling, it is not possible to guarantee monotonically increasing loads throughout the entire cohesive zone. As a result, numerical methods must handle unloading. The most common numerical application of CZMs is to imagine them as modeling an elastic material with damage. The zone tractions are thus always a linear elastic response but the slope for the linear elasticity is a function of the current damage state δ. Such linear unloading and reloading tractions are shown in Fig. 6.1 by the dashed loading and unloading lines for any u below the current δ. The slope is determined by the current strength meaning the cohesive zone tractions are defined not by $F(u)$, but by

$$T(u) = \frac{S(\delta)}{\delta} u = k_{eff} u \qquad \text{where} \qquad k_{eff} = \frac{S(\delta)}{\delta} \tag{6.1}$$

At constant state of damage, the material is linear elastic (with effective stiff k_{eff}) and can be characterized by its current strain energy, U, found by integrating the linear elastic traction or

$$U(u,\delta) = \int_0^u T(u)\, du = \frac{1}{2} \frac{S(\delta)}{\delta} u^2 \tag{6.2}$$

Although δ is a sufficient damage parameter (and one most commonly used in the literature), it is worth defining two alternate damage parameters. Modeling can use anyone of the three, or move between them if beneficial (*i.e.*, a given damage state can be defined by any one of the damage parameters). We start by dividing the total COD in the cohesive zone, u, into COD within the elastic material in the cohesive zone, u_e, and COD within the damaged material consisting of opening of microcracks or voids, u_d. In other words, $u = u_e + u_d$. Next we consider that tractions are caused only by elastic COD and the stiffness is identical to initial stiffness of the undamaged zone or

$$T = k u_e = k(u - u_d)$$

For two more damage parameters, we can propose

$$D = \frac{u_d}{u} \quad \text{and} \quad \zeta = \max(u_d)$$

The first, D, is a dimensionless damage parameter commonly used in continuum damage mechanics (CDM) that evolves from 0 to 1 at failure. Substituting into the traction equation gives

$$T = k(u-u_d) = k(1-D)u = k_{\mathit{eff}}u \qquad \text{where} \qquad \mathrm{k}_{\mathit{eff}} = \mathrm{k}(1-\mathrm{D}) \tag{6.3}$$

By this equation, D is commonly described in the literature as a measure of stiffness reduction due to damage. I claim that defining D as ratio of u_d to u is the more compelling definition of this damage parameter (*i.e.*, the displacement ratio concept is more useful in deriving 3D CDM models than a stiffness reduction concept, although in 1D, the distinction is not important). Comparing Eq. (6.3) to Eq. (6.1) gives relation between D and δ and a new form for strain energy:

$$D = 1 - \frac{S(\delta)}{k\delta} \qquad \text{and} \qquad U(u,D) = \frac{1}{2}k(1-D)u^2 = (1-D)U(u,0) \tag{6.4}$$

where $U(u,0)$ is strain energy of an undamaged cohesive zone.

To relate ζ to other damage parameters, recognize that when $u = \delta$, the traction is $S(\delta)$ and the damage parameters are related by

$$\delta = u_e + \zeta = \frac{S(\delta)}{k} + \zeta \quad \text{or} \quad \zeta = \delta - \frac{S(\delta)}{k} = D\delta \quad \text{or} \quad D = \frac{\zeta}{\delta} = \frac{\delta - \frac{S(\delta)}{k}}{\delta}$$

In comparison, δ evolves from $u^{(e)}$ to $u^{(c)}$ at final failure while ζ evolves from 0 to $u^{(c)}$. The later paramater is common in CDM. To calculate δ from ζ, we postulate a strength model in terms of ζ or $s(\zeta)$ such that

$$\delta = u_e + \zeta = \zeta + \frac{s(\zeta)}{k} \quad \Longrightarrow \quad s(\zeta) = S\left(\zeta + \frac{s(\zeta)}{k}\right) \quad \text{and} \quad s'(\zeta) = S'(\delta)\left(1 + \frac{s'(\zeta)}{k}\right) \tag{6.5}$$

and

$$D = \frac{\zeta}{\zeta + \frac{s(\zeta)}{k}}$$

In brief, using δ is based on total displacement while ζ is based on damage displacement requiring use of different softening laws, but the end results are identical or either method could be used. Whether the CDM approach is better than the CZM approach, or vice versa, I cannot say. These notes will continue using the CZM approach because that allows better comparison to prior cohesive zone methods.

Before continuing, we define restrictions on $S(\delta)$. As drawn in Fig. 6.1, $S(\delta)$ need not be a monotonically decreasing function. But because D is a state function of damage that can only increase (it evolves monotonically from 0 to 1), differentiating Eq. (6.4), therefore shows that all acceptable strength models must satisfy

$$\varphi(\delta) = S(\delta) - \delta S'(\delta) \geq 0$$

It will be shown later that $\varphi(\delta)$ (SI units $\mathrm{N/m^2}$) is related to energy dissipation. In other words, requiring $\varphi(\delta) \geq 0$ guarantees that dissipated energy is always positive or that the damage evolution obeys second law of thermodynamics.

6.2.1 Damage Evolution

The next step in cohesive zone modeling is to postulate a traction-failure surface — when tractions are below the failure surface, the deformation is elastic; when they exceed the surface, damage evolves to return to an updated surface. Like δ, D, and ζ, thermodynamics requires the traction-failure surface to be a state variable that depends only on the current state of damage. In unidirectional loading, the traction failure surface is simply the strength model, $S(\delta)$, that depends only on δ. Note that robust material-property modeling might need the failure surface to depend on other state variables, besides damage state variables, such as temperature, pressure, or strain rate. Other state variables can (and should be) added, but are not yet implemented in `NairnMPM`)

In displacement driven, numerical modeling, each step will correspond to an imposed change in COD — du. For a cohesive zone at some current damage state (defined by current value of δ), the trial traction caused by du is:

$$T^{(trial)} = \frac{S(\delta)}{\delta}(u+du)$$

If this traction is below the failure surface (*i.e.*, $T^{(trial)} \le S(\delta)$), the deformation is elastic — the trial traction is accepted and no changes are mode to damage state variables.

But, if the trial traction extends beyond the failure surface (*i.e.*, $T^{(trial)} > S(\delta)$), the current step causes damage. Three methods can be used to get the same answer for damage evolution:

- *Use δ Definition*: Observing that $u = \delta$ during damage evolution and that by definition $\delta = \max(u)$, damage evolution obviously corresponds to $d\delta = du$.

- *General Method*: When the traction exceeds the strength model, the traction update can be expressed as

$$T^{(0)} + \nabla T \cdot (du, d\delta) = S(\delta) + \frac{\partial S(\delta)}{\partial \delta} d\delta$$

  where $T^{(0)}$ and $S(\delta)$ are traction and strength at the beginning of the displacement increment. For small increments, these will be equal and therefore cancel (*i.e*, the problem evolves until reaching the strength model and then subsequent steps evolve damage while tractions remain equal to the evolving strength). The damage evolution equation becomes:

$$\nabla T \cdot (du, d\delta) = S'(\delta) d\delta \implies \frac{\partial \big(S(\delta) - T\big)}{\partial \delta} d\delta = \frac{\partial T}{\partial u} du \tag{6.6}$$

  Substituting linear elastic traction ($T(u) = S(\delta)u/\delta$) leads to

$$d\delta = \frac{\frac{S(\delta)}{\delta} du}{S'(\delta) + \frac{u\varphi(\delta)}{\delta^2}}$$

  Realizing that $u = \delta$ during uniaxial loading and substituting for $\varphi(\delta) = S(\delta) - \delta S'(\delta)$, this result reduces to $d\delta = du$.

- *Return to Failure Surface*: this solution finds the damage by equating traction at an evolved damage state (which affects its stiffness through Eq. (6.1)) to the strength at that new state of damage. In other words, the new traction "returns" to the traction failure surface by:

$$\frac{S(\delta + d\delta)}{\delta + d\delta}(u + du) = S(\delta + d\delta) \qquad \implies \qquad d\delta = u - \delta + du \tag{6.7}$$

During unidirectional, incremental numerical modeling, δ remains synchronized with u such that at the beginning of a damage evolution step, the state would be $u = \delta$ leading to update in damage state again given by $d\delta = du$.

A detail that arises during implementation is that increments du are discrete increments rather than infinitesimal ones. As a consequence u may start out below δ and then jump to above it. Such steps are handled by partitioning du into $du^{(1)}$ and $du^{(2)}$ defined by:

$$du^{(1)} = \delta - u \qquad \text{and} \qquad du^{(2)} = du - du^{(1)} = u + du - \delta$$

Here $du^{(1)}$ is the elastic increment required to reach the failure surface where $u = \delta$ and $du^{(2)}$ is the increment causing damage or the damage evolution becomes $d\delta = du^{(2)}$.

6.2.2 Energy Dissipation

The energy dissipation increment (SI units J/m^2 or N/m) caused by an increment in δ is equal to the area between the two dashed lines in Fig. 6.1 or, more mathematically, by derivative of potential energy:

$$d\Omega = -d\Pi = d(W - U)$$

The total work input, W, during monotonic loading is area under the traction response function:

$$W = \int_0^u F(u)du$$

and U is strain energy defined in Eq. (6.2). The energy dissipation becomes:

$$\frac{d\Omega}{du} = F(u) - \frac{u}{\delta}S(\delta) + \frac{u^2}{2}\frac{\varphi(\delta)}{\delta^2}\frac{d\delta}{du}$$

For monotonic loading and $u < u^{(e)}$, $F(u) = ku$, $\delta = u^{(e)}$, and $\varphi(u^{(e)}) = 0$ leading correctly to no energy dissipation during elastic loading. For $u > u^{(e)}$, $u = \delta$ and $F(u) = S(\delta)$ leading to

$$\frac{d\Omega}{du} = \frac{1}{2}\varphi(\delta)$$

Alternatively, the energy release rate can come by differentiating strain energy at constant u:

$$d\Omega = -\left(\frac{\partial U(u,\delta)}{\partial \delta}\right)_u d\delta = \frac{1}{2}u^2\frac{\varphi(\delta)}{\delta^2}d\delta = \frac{1}{2}\varphi(\delta)d\delta \tag{6.8}$$

where last step recognizes that $u = \delta$ during 1D damage evolution. These results show that $\varphi(\delta)$ is energy dissipation rate for any strength model.

Alternatively, the energy area can be found from the intersection points in Fig. 6.1 using D and CODs (*i.e.*, using Eq. (6.3)):

$$d\Omega = \frac{k}{2}\big((1-D)u(u+du) - (1-D-dD)(u+du)u\big) = \frac{1}{2}ku^2\,dD \tag{6.9}$$

where second order differential terms are ignored. This same result can be derived by strain energy:

$$d\Omega = -\left(\frac{\partial U(u,D)}{\partial D}\right)_u dD = \frac{1}{2}ku^2 dD$$

These two forms using $d\delta$ or dD are interrelated by

$$dD = \frac{dD}{d\delta}d\delta = \frac{\varphi(\delta)\,d\delta}{k\delta^2} = \mathbb{R}(\delta)d\delta \quad \text{where} \quad \mathbb{R}(\delta) = \frac{\varphi(\delta)}{k\delta^2} \tag{6.10}$$

and setting $u = \delta$. The relation between dD and $d\delta$ will arise frequently making $\mathbb{R}(\delta)$ a useful cohesive zone function, which is derived from the strength model. Other potentially-useful forms for $\mathbb{R}(\delta)$ (SI units $1/m$) are:

$$\mathbb{R}(\delta) = \frac{(1-D)\varphi(\delta)}{\delta S(\delta)} = \frac{k(1-D)^2\varphi(\delta)}{S(\delta)^2} = \frac{T^2\varphi(\delta)}{ku^2S(\delta)^2} = \frac{(1-D)T\varphi(\delta)}{uS(\delta)^2}$$

which follow by various uses of

$$u = \frac{T}{k(1-D)} = \frac{T\delta}{S(\delta)} \tag{6.11}$$

Because none of these relations assume $u = \delta$, they apply during mixed-mode loading as well.

6.2.3 Potential Energy *vs.* Input Work

Some cohesive zone models find a "potential energy" by integrating the so-called "traction law" or

$$W = \phi = \int_0^u F(u)\,du \tag{6.12}$$

Because energy release rate is derivative of potential energy, Högberg associates this integral with the cumulative energy released. All papers using that approach are making an error. During monotonic loading, this integral is cumulative work done on the cohesive zone, while potential energy, Π, for an elastic/damaging material is strain energy minus work or

$$\Pi = U - W = \frac{1}{2}\frac{S(\delta)}{\delta}u^2 - \int_0^u F(u)\,du$$

The cumulative (Ω) and incremental ($d\Omega$) energy released should be found from this potential energy (see Energy Dissipation) or:

$$\Omega = -\Pi = W - U \qquad \text{and} \qquad d\Omega = -d\Pi = dW - dU$$

Note that $U \to 0$ at failure which means $\Omega(u^{(c)}) = W(u^{(c)}) = G_c$ or the total energy released during deformation. But for any $u < u^{(c)}$, $W(u)$ is not equal to Ω. During damage evolution with $u = \delta$, cumulative energy released is

$$\Omega = \int_0^\delta F(u)\,du - \frac{1}{2}S(\delta)\delta$$

which is area under the traction law up to δ minus area under the linear unloading curve from δ to 0 — it is not area under the traction law except when $\delta = u^{(c)}$.

What are the consequences of using the wrong potential energy to find tractions? If we consider monotonic, unidirectional loading and attempt to get tractions by differentiation the "erroneous" potential

$$T(u) = \frac{\partial\phi}{\partial u} = F(u)$$

If we avoid this error and get tractions from the elastic strain energy, we get:

$$T = \frac{\partial U(u,\delta)}{\partial u} = \frac{S(\delta)}{\delta} u = S(\delta) = F(u)$$

where the second steps used the special case of monotonic loading ($u = \delta$) and connection between strength model and the traction law. These two approaches give the same results. The difference, however, is that differentiating ϕ is *only* correct during monotonic 1D loading. Differentiating $U(u,\delta)$ to get tractions is a general result that applies for any loading history.

6.2.4 Tangent Stiffness

The tangent stiffness for 1D deformation is

$$\frac{dT}{du} = k(1-D) - ku\frac{dD}{du} = \frac{S(\delta)}{\delta} - ku\mathbb{R}\frac{d\delta}{du} = \frac{S(\delta)}{\delta} - k\delta\mathbb{R} = \frac{S(\delta)}{\delta} - \frac{\varphi(\delta)}{\delta} = S'(\delta) \tag{6.13}$$

but would use dD during elastic deformation. The conversion to δ used $\delta = u$ and $d\delta = du$ during 1D damage evolution and would not apply during mixed-mode loading.

6.2.5 Connection to Continuum Damage Mechanics

Switching to ζ damage state instead of δ would need a different damage evolution analysis. To connect the two methods, 1D damage increments by $d\delta = du$ and D is given by ζ/δ. These increment for ζ is thus found by:

$$d\zeta = d(\delta D) = \left(1 - \frac{S'(\delta)}{k}\right) d\delta \tag{6.14}$$

Using Eq. (6.5) leads to

$$d\zeta = \frac{du}{1 + \frac{s'(\zeta)}{k}}$$

This results agrees with CDM methods (see Eq. (5.8)).

If the CDM approach was adopted instead, a challenge in comparing to prior CZM models would be that in general, one cannot calculate $s(\zeta)$ from $S(\delta)$ (because the conversion requires inverse functions). One exception is the Linear Sawtooth Strength Model; this strength model corresponds to CDM-style strength model of

$$s(\zeta) = ku^{(e)}\left(1 - \frac{\zeta}{u^{(c)}}\right)$$

or monotonic linear softening from $s(0) = ku^{(e)}$ to 0 when $\zeta = u^{(c)}$. Note the areas under both $S(\delta)$ and $s(\zeta)$ are both $ku^{(e)}u^{(c)}/2$ or the unidirectional toughness of the cohesive zone. The CDM version of the strength model is simpler in that it starts from 0 instead of from $u^{(e)}$. Both approaches end when ζ or δ reach $u^{(c)}$.

Recognizing the $d\zeta > 0$ for any damage evolution, implies that the strength model must be selected such that $-s'(\zeta) < k$. This relation was used in CDM to derive maximum cell size allowed for given softening properties to get stable calculations. The same analysis like explains snap-back instability in CZM implementation. Using Eq. (6.5), CZM stability requires

$$-\frac{S'(\delta)}{1 - \frac{S'(\delta)}{k}} < k \quad \Longrightarrow \quad k > 0$$

This result does not provide help in determining stability.

6.3 Mixed-Mode Cohesive Zone Modeling

To model mixed-mode problems, the single strength model is replaced with $S_n(\delta_n)$ and $S_t(\delta_t)$ for strength models in normal and tangential directions or mode I and mode II deformation. The two laws are characterized with separate damage parameters — $\boldsymbol{\delta} = (\delta_n, \delta_t)$. While still damage state variables, the damage evolution analysis below shows that δ_n and δ_t in mixed-mode loading differ from 1D by no longer being equal to maximum values of u_n and u_t (*i.e.*, normal and tangential CODs). The normal and shear tractions independently follow Eq (6.1) leading to strain energy

$$U(\boldsymbol{u}, \boldsymbol{\delta}) = \int \boldsymbol{T} \cdot d\boldsymbol{u} = \frac{1}{2}\frac{S_n(\delta_n)}{\delta_n}u_n^2 + \frac{1}{2}\frac{S_t(\delta_t)}{\delta_t}u_n^2 \tag{6.15}$$

The scalar D parameter in 1D analysis changes to a second-rank tensor defined by:

$$(u_{t,c}, u_{n,c}) = \mathbf{D}(u_t, u_n)$$

Perhaps $\mathbf{D}$ could be fully populated, but here it will be restricted to diagonal with elements D_t and D_n. The strain energy can then be written as

$$U(\boldsymbol{u}, \mathsf{D}) = \mathsf{K}(\mathsf{I} - \mathbf{D})\boldsymbol{u} \cdot \boldsymbol{u}$$

where K is diagonal tensor with initial tangential and normal stiffness (k_t and k_n) on the diagonal. The energy dissipation increment becomes:

$$d\Omega = -\left(\frac{\partial U(\boldsymbol{u}, \mathsf{D})}{\partial \mathsf{D}}\right)_{\boldsymbol{u}} d\mathsf{D} = \frac{1}{2}k_n u_n^2 dD_n + \frac{1}{2}k_t u_t^2 dD_t$$

The released energy partitions into sum of mode I and mode II energy release rates (which might justify the choice of diagonal $\mathbf{D}$ and K tensors). Using Eq. (6.10) and (6.11), the energy release in terms of δ_n and δ_t becomes

$$d\Omega = \frac{1}{2}\left(\frac{u_n}{\delta_n}\right)^2 \varphi_n(\delta_n) d\delta_n + \frac{1}{2}\left(\frac{u_t}{\delta_t}\right)^2 \varphi_t(\delta_t) d\delta_t \tag{6.16}$$

The next step is to postulate a traction-failure surface. Extending 1D modeling to mixed mode involves defining a failure that, in general, depends on $S_n(\delta_n)$, $S_t(\delta_t)$, and the current mode mixity. A rational starting point (which is only a cross section of the surface) is shown in Fig. 6.2. This example surface is a half ellipse in the tensile half plane where normal traction is positive and the normal COD means an opened cohesive zone. The ellipse intersects the x axis at $S_t(\delta_t)$ and the y axis at $S_n(\delta_n)$, which are the current unidirectional strengths. The negative normal half plane corresponds to when the cohesive zone is in contact. Under compression, only shear traction can cause damage.

The surface in Fig. 6.2 plots vector components for damage evolution as a function of normal and tangential strength models. The underlying model is to find the magnitude of the traction (vector $\boldsymbol{T}$ in Fig. 6.2) needed to cause damage as a function of δ_n, δ_t, and the current mode-mixity. In other words, while 1D traction failure surface is a simply a 2D plot of $S(\delta)$ as a function of δ, the required mixed-mode failure surface is a 4D plot for strength as a function of δ_n, δ_t, and θ where θ is the current mode-mixity defined by

$$\tan\theta = \frac{u_n}{u_t} \quad \Longrightarrow \quad u_n = \|\boldsymbol{u}\| \sin\theta \text{ and } u_t = \|\boldsymbol{u}\| \cos\theta$$

In other words, $\theta = \pi/2$ for pure mode I and $\theta = 0$ or π for pure mode II. The range of $0 < \theta < \pi$ includes the normal-opening direction half plane where u_t may be positive or negative. For any phase

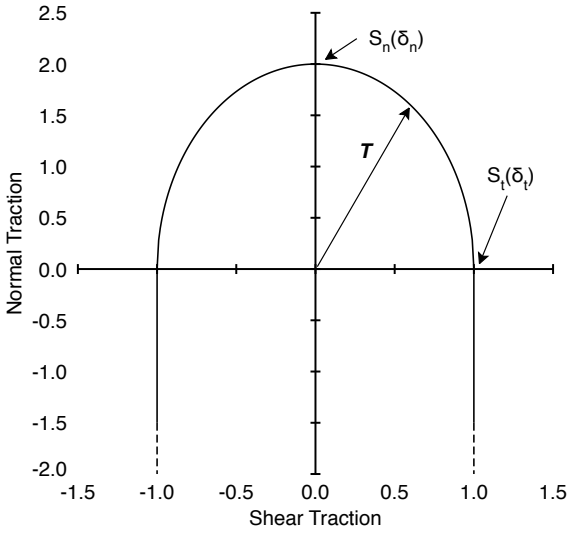

Figure 6.2: Traction Surface

angle, the traction magnitude as function of COD magnitude is

$$\|\boldsymbol{T}\| = \|\boldsymbol{u}\|\sqrt{k_n^2(1-D_n)^2\sin^2\theta + k_t^2(1-D_t)^2\cos^2\theta} = \|\boldsymbol{u}\|\sqrt{\frac{S_n(\delta_n)^2}{\delta_n^2}\sin^2\theta + \frac{S_t(\delta_t)^2}{\delta_t^2}\cos^2\theta} \quad (6.17)$$

This loading causes damage when the elliptical surface is reached and that happens when

$$\begin{aligned} 1 &= \left(\frac{T_n}{S_n(\delta_n)}\right)^2 + \left(\frac{T_t}{S_t(\delta_t)}\right)^2 = \|\boldsymbol{u}_d\|^2\left(\frac{\sin^2\theta}{\delta_n^2} + \frac{\cos^2\theta}{\delta_t^2}\right) \\ \|\boldsymbol{u}_d\| = \delta_d &= \frac{1}{\sqrt{\frac{\sin^2\theta}{\delta_n^2} + \frac{\cos^2\theta}{\delta_t^2}}} \quad \text{or} \quad \delta_d^2 = \frac{\delta_n^2\delta_t^2}{\delta_t^2\sin^2\theta + \delta_n^2\cos^2\theta} \end{aligned} \quad (6.18)$$

This defines an *effective* damage parameter δ_d that is equal to the displacement magnitude when the traction is on the traction failure surface. It extends to pure mode result of $\delta = u$ to mixed mode loading. The strength model can now be represented by a 4D surface given by traction when $\|\boldsymbol{u}\| = \delta_d$:

$$S(\delta_n, \delta_t, \theta) = k_{mm}\delta_d = \sqrt{\frac{\frac{S_n(\delta_n)^2}{\delta_n^2}\sin^2\theta + \frac{S_t(\delta_t)^2}{\delta_t^2}\cos^2\theta}{\frac{\sin^2\theta}{\delta_n^2} + \frac{\cos^2\theta}{\delta_t^2}}} \quad (6.19)$$

where k_{mm} is effective mixed-mode stiffness or slope of $\|\boldsymbol{T}\|$ *vs.* $\|\boldsymbol{u}\|$:

$$k_{mm} = \sqrt{\frac{S_n(\delta_n)^2}{\delta_n^2}\sin^2\theta + \frac{S_t(\delta_t)^2}{\delta_t^2}\cos^2\theta}$$

Here $S(\delta_n, \delta_t, \theta)$, without a subscript on S, is full strength model that depends on three variables. The strength models $S_n(\delta_n)$ and $S_t(\delta_t)$ remain as current strengths if the object was unloaded and then reloading in pure mode I or mode II loading, respectively. Note that coupling happens in the strength

model but not in the zone tractions; in other words, it is important to distinguish strength model from "traction law."

The modeling is initialized with $\delta_n = u_n^{(e)}$, $\delta_t = u_t^{(e)}$ and $D_n = D_t = 0$. For displacement increment du_n, du_t, and $d\theta$, the trial traction vector is found from

$$\boldsymbol{T}^{(trial)} = \left(\frac{S_t(\delta_t)}{\delta_t}(u_t + du_t), \frac{S_n(\delta_n)}{\delta_n}(u_n + du_n)\right)$$

$$\|\boldsymbol{T}^{(trial)}\| = \|\boldsymbol{u} + d\boldsymbol{u}\|\sqrt{\frac{S_n(\delta_n)^2}{\delta_n^2}\sin^2(\theta + d\theta) + \frac{S_t(\delta_t)^2}{\delta_t^2}\cos^2(\theta + d\theta)}$$

If $\boldsymbol{T}^{(trial)}$ is within the failure surface, the deformation is elastic — the trial tractions are accepted and no changes are made to D_n, D_t, δ_n, or δ_t. The next sections give options for handling damage evolution when the traction failure surface is surpassed.

6.3.1 General Method

In mixed-mode, damage evolution consists of the traction magnitude moving along the failure surface under conditions that $\|\boldsymbol{u}\| = \delta_d$ given by Eq. (6.18). Extending the general method for 1D loading (see Eq. (6.6)) to mixed mode loading, the evolution equation becomes:

$$\nabla\|\boldsymbol{T}\| \cdot (d\|\boldsymbol{u}\|, d\theta, d\delta_n, d\delta_t) = \nabla S(\theta, \delta_n, \delta_t) \cdot (d\theta, d\delta_n, d\delta_t) \tag{6.20}$$

Using Eq. (6.17), the left hand side is

$$\begin{aligned}
\nabla\|\boldsymbol{T}\| \cdot (d\|\boldsymbol{u}\|, d\theta, d\delta_n, d\delta_t) &= k_{mm} d\|\boldsymbol{u}\| + \|\boldsymbol{u}\|\left(\frac{S_n(\delta_n)^2}{k_{mm}\delta_n^2} - \frac{S_t(\delta_t)^2}{k_{mm}\delta_t^2}\right)\sin\theta\cos\theta d\theta \\
&- \frac{\|\boldsymbol{u}\| S_n(\delta_n)\varphi_n(\delta_n)\sin^2\theta}{k_{mm}\delta_n^3} d\delta_n - \frac{\|\boldsymbol{u}\| S_t(\delta_t)\varphi_t(\delta_t)\cos^2\theta}{k_{mm}\delta_t^3} d\delta_t \\
&= \frac{\delta_d S_n(\delta_n)^2}{k_{mm}\delta_n^2}\left(\frac{\sin^2\theta}{\delta_d} d\|\boldsymbol{u}\| + \sin\theta\cos\theta d\theta - \frac{\varphi_n(\delta_n)\sin^2\theta}{\delta_n S_n(\delta_n)} d\delta_n\right) \\
&+ \frac{\delta_d S_t(\delta_t)^2}{k_{mm}\delta_t^2}\left(\frac{\cos^2\theta}{\delta_d} d\|\boldsymbol{u}\| - \sin\theta\cos\theta d\theta - \frac{\varphi_t(\delta_t)\cos^2\theta}{\delta_t S_t(\delta_t)} d\delta_t\right)
\end{aligned} \tag{6.21}$$

The second form is for traction on the failure surface (by setting for $\|\boldsymbol{u}\| = \delta_d$). Using the mixed-mode strength model in Eq. (6.19) gives:

$$\begin{aligned}
\nabla S(\theta, \delta_n, \delta_t) \cdot (d\theta, d\delta_n, d\delta_t) &= \frac{\delta_d^3\left(S_n(\delta_n)^2 - S_t(\delta_t)^2\right)\sin\theta\cos\theta d\theta}{k_{mm}\delta_n^2\delta_t^2} \\
&+ \left(\frac{\delta_d^3\left(S_t(\delta_t)^2 - S_n(\delta_n)^2\right)\sin^2\theta\cos^2\theta}{k_{mm}\delta_n^3\delta_t^2} + \frac{\delta_d S_n(\delta_n) S_n'(\delta_n)\sin^2\theta}{k_{mm}\delta_n^2}\right) d\delta_n \\
&+ \left(\frac{\delta_d^3\left(S_n(\delta_n)^2 - S_t(\delta_t)^2\right)\sin^2\theta\cos^2\theta}{k_{mm}\delta_t^3\delta_n^2} + \frac{\delta_d S_t(\delta_t) S_t'(\delta_t)\cos^2\theta}{k_{mm}\delta_t^2}\right) d\delta_t \\
&= \frac{\delta_d S_n(\delta_n)^2}{k_{mm}\delta_n^2}\left(\frac{\delta_d^2\sin\theta\cos\theta d\theta}{\delta_t^2} - \frac{\delta_d^2\sin^2\theta\cos^2\theta d\delta_n}{\delta_n\delta_t^2} + \frac{\delta_d^2\sin^2\theta\cos^2\theta d\delta_t}{\delta_t^3} + \frac{S_n'(\delta_n)\sin^2\theta d\delta_n}{S_n(\delta_n)}\right) \\
&+ \frac{\delta_d S_t(\delta_t)^2}{k_{mm}\delta_t^2}\left(-\frac{\delta_d^2\sin\theta\cos\theta d\theta}{\delta_n^2} + \frac{\delta_d^2\sin^2\theta\cos^2\theta d\delta_n}{\delta_n^3} - \frac{\delta_d^2\sin^2\theta\cos^2\theta d\delta_t}{\delta_t\delta_n^2} + \frac{S_t'(\delta_t)\cos^2\theta d\delta_t}{S_t(\delta_t)}\right)
\end{aligned}$$

Finally, equating the above two results gives damage evolution equation:

$$0 = \frac{S_n(\delta_n)^2}{\delta_n^2}\left(\frac{\sin^2\theta}{\delta_d}d\|\boldsymbol{u}\| + \left(1-\frac{\delta_d^2}{\delta_t^2}\right)\sin\theta\cos\theta d\theta - \frac{\sin^2\theta}{\delta_n}\left(1-\frac{\delta_d^2\cos^2\theta}{\delta_t^2}\right)d\delta_n - \frac{\delta_d^2\sin^2\theta\cos^2\theta}{\delta_t^3}d\delta_t\right) + \frac{S_t(\delta_t)^2}{\delta_t^2}\left(\frac{\cos^2\theta}{\delta_d}d\|\boldsymbol{u}\| - \left(1-\frac{\delta_d^2}{\delta_n^2}\right)\sin\theta\cos\theta d\theta - \frac{\cos^2\theta}{\delta_t}\left(1-\frac{\delta_d^2\sin^2\theta}{\delta_n^2}\right)d\delta_t - \frac{\delta_d^2\sin^2\theta\cos^2\theta}{\delta_n^3}d\delta_n\right) \tag{6.22}$$

The results for pure mode I and mode II reduce correctly to $d\delta_n = du_n$ and $d\delta_t = du_t$. Some potentially useful relations are

$$1-\frac{\delta_d^2}{\delta_t^2} = \frac{(\delta_t^2-\delta_n^2)\sin^2\theta}{\delta_t^2\sin^2\theta+\delta_n^2\cos^2\theta} \quad \text{and} \quad 1-\frac{\delta_d^2}{\delta_n^2} = \frac{(\delta_n^2-\delta_t^2)\cos^2\theta}{\delta_t^2\sin^2\theta+\delta_n^2\cos^2\theta}$$
$$1-\frac{\delta_d^2\cos^2\theta}{\delta_t^2} = \frac{\delta_t^2\sin^2\theta}{\delta_t^2\sin^2\theta+\delta_n^2\cos^2\theta} = \frac{\delta_d^2\sin^2\theta}{\delta_n^2} \quad 1-\frac{\delta_d^2\sin^2\theta}{\delta_n^2} = \frac{\delta_n^2\cos^2\theta}{\delta_t^2\sin^2\theta+\delta_n^2\cos^2\theta} = \frac{\delta_d^2\cos^2\theta}{\delta_t^2} \tag{6.23}$$

In computer modeling, the increments du_n and du_t will be more practically available. Athough $d\|\boldsymbol{u}\|$ and $d\theta$ could be calculated from them, it is easy to convert to using du_n and du_t. Furthermore, the conversion reveals a significant simplification. Recognizing that $u_n = \|\boldsymbol{u}\|\sin\theta$ and $u_t = \|\boldsymbol{u}\|\cos\theta$, their differentials are

$$du_n = \sin\theta d\|\boldsymbol{u}\| + \|\boldsymbol{u}\|\cos\theta d\theta \quad \text{and} \quad du_t = \cos\theta d\|\boldsymbol{u}\| - \|\boldsymbol{u}\|\sin\theta d\theta$$

These component differentials can be inverted to derive

$$d\|\boldsymbol{u}\| = \sin\theta du_n + \cos\theta du_t \quad \text{and} \quad d\theta = \frac{\cos\theta du_n - \sin\theta du_t}{\|\boldsymbol{u}\|} \tag{6.24}$$

The first two terms of each block in Eq. (6.22) can be recast as

$$\frac{\sin^2\theta}{\delta_d}d\|\boldsymbol{u}\| + \left(1-\frac{\delta_d^2}{\delta_t^2}\right)\sin\theta\cos\theta d\theta = \delta_d\sin^2\theta\left(\frac{\sin\theta}{\delta_n^2}du_n + \frac{\cos\theta}{\delta_t^2}du_t\right)$$
$$\frac{\cos^2\theta}{\delta_d}d\|\boldsymbol{u}\| - \left(1-\frac{\delta_d^2}{\delta_n^2}\right)\sin\theta\cos\theta d\theta = \delta_d\cos^2\theta\left(\frac{\sin\theta}{\delta_n^2}du_n + \frac{\cos\theta}{\delta_t^2}du_t\right)$$

The evolution equation can then be rewritten

$$0 = \frac{S_n(\delta_n)^2\sin^2\theta}{\delta_n^2}\left(\frac{\delta_d\sin\theta}{\delta_n^2}du_n + \frac{\delta_d\cos\theta}{\delta_t^2}du_t - \frac{\delta_d^2\sin^2\theta}{\delta_n^3}d\delta_n - \frac{\delta_d^2\cos^2\theta}{\delta_t^3}d\delta_t\right) + \frac{S_t(\delta_t)^2\cos^2\theta}{\delta_t^2}\left(\frac{\delta_d\sin\theta}{\delta_n^2}du_n + \frac{\delta_d\cos\theta}{\delta_t^2}du_t - \frac{\delta_d^2\sin^2\theta}{\delta_n^3}d\delta_n - \frac{\delta_d^2\cos^2\theta}{\delta_t^3}d\delta_t\right) \tag{6.25}$$

which simplifies even further to

$$\frac{\delta_d\sin^2\theta}{\delta_n^3}d\delta_n + \frac{\delta_d\cos^2\theta}{\delta_t^3}d\delta_t = \frac{\sin\theta}{\delta_n^2}du_n + \frac{\cos\theta}{\delta_t^2}du_t \tag{6.26}$$

Using displacements instead of θ leads to

$$\frac{u_n^2}{\delta_n^3}d\delta_n + \frac{u_t^2}{\delta_t^3}d\delta_t = \frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t \tag{6.27}$$

6.3.2 Define δ_d From $\|\boldsymbol{u}\|$

During mixed-mode loading, $\delta_d = \|\boldsymbol{u}\|$. One can proceed as in 1D modeling where an increment results in $d\delta_d = d\|\boldsymbol{u}\|$. One is tempted (and several people have) to model mixed mode failure with δ_d as a single damage parameter and effectively approach the problem using 1D methods. That approach is not sufficient to model general loading. Instead, we have to retain δ_d as a function of two damage variables (δ_n and δ_t) as well as θ, all of which may change during general loading. Finding *full* differential of δ_d leads to:

$$\frac{\delta_d^3 \sin^2\theta}{\delta_n^3} d\delta_n + \frac{\delta_d^3 \cos^2\theta}{\delta_t^3} d\delta_t = d\|\boldsymbol{u}\| + \delta_d^3 \left(\frac{1}{\delta_n^2} - \frac{1}{\delta_t^2}\right) \sin\theta\cos\theta d\theta$$

Converting the right hand side from using $d\|\boldsymbol{u}\|$ and $d\theta$ to du_n and du_t using Eq. (6.24) gives

$$\begin{aligned}\sin\theta \left(1 + \delta_d^2 \left(\frac{1}{\delta_n^2} - \frac{1}{\delta_t^2}\right)\cos^2\theta\right) du_n + \cos\theta \left(1 - \delta_d^2 \left(\frac{1}{\delta_n^2} - \frac{1}{\delta_t^2}\right)\sin^2\theta\right) du_t \\ = \frac{\delta_d^3 \sin^2\theta}{\delta_n^3} d\delta_n + \frac{\delta_d^3 \cos^2\theta}{\delta_t^3} d\delta_t\end{aligned}$$

Using Eq. (6.23), this approach thus correctly reduces the general method in Eq. (6.26) or Eq. (6.27).

This *effective* damage parameter and effective displacement has been tried in the literature, but they are all wrong. The only time an effective displacement can be used is when failure occurs at some function of u_n and u_t alone (*i.e.*, that is independent of δ_n and δ_t). By Eq. (6.18), an effective displacement approach when using an elliptical traction failure surface is only acceptable with $\delta_t = \chi\delta_n$ where χ is a constant. When this relation holds, failure occurs when

$$1 = \left(\frac{T_n}{S_n(\delta_n)}\right)^2 + \left(\frac{T_t}{S_t(\delta_t)}\right)^2 \quad \Longrightarrow \quad (u_n)^2 + \left(\frac{u_t}{\chi}\right)^2 = \delta_n^2$$

The left side defines a suitable effective displacement of displacement components alone, but any uniform modification can be used as well. For example, if $\chi = u_n^{(c)}/u_t^{(c)}$, we could define an effective displacement as:

$$u_{eff} = \sqrt{\left(\frac{u_n}{u_n^{(c)}}\right)^2 + \left(\frac{u_t}{u_t^{(c)}}\right)^2}$$

This form has been used (*e.g.*, Högberg), was was not recognized that it is only acceptable when it can be shown that $\delta_n/u_n^{(c)} = \delta_t/u_t^{(c)}$. The use of a single D, likes the strength models by $D(\delta_n) = D(\delta_t)$ or:

$$\frac{S_n(\delta_n)}{k_n\delta_n} = \frac{S_t(\delta_t)}{k_t\delta_t} \quad \text{and} \quad \delta_t = \chi\delta_n \quad \Longrightarrow \quad S_t(\delta_t) = \frac{k_t\chi}{k_n} S_n\left(\frac{\delta_t}{\chi}\right)$$

In other words, the tangential strength must match the normal strength by scaling strength and damage parameter axis. If $\chi = 1$ (*i.e.*, $u_{eff} = \|\boldsymbol{u}\|$), the tangential strength can scale only the strength axis.

6.3.3 Return to Failure Surface

If $\boldsymbol{T}^{(trial)}$ extends beyond the current fracture surface, the task is to solve for $d\delta_n$ and $d\delta_t$ (which will correspond to increments dD_n and dD_t). The final tractions (once $d\delta_n$ and $d\delta_t$ are found) can be written as

$$\boldsymbol{T}^{(final)} = \left(\frac{S_t(\delta_t + d\delta_t)}{\delta_t + d\delta_t}(u_t + du_t), \frac{S_n(\delta_n + d\delta_n)}{\delta_n + \delta_n}(u_n + du_n)\right)$$

Extending the 1D methods of returning to the failure surface, this final state must fall on the updated ellipse with update major an minor radii of $S_t(\delta_t + d\delta_t)$ and $S_n(\delta_n + d\delta_n)$:

$$1 = \left(\frac{S_t(\delta_t + d\delta_t)(u_t + du_t)}{(\delta_t + d\delta_t)S_t(\delta_t + d\delta_t)}\right)^2 + \left(\frac{S_n(\delta_n + d\delta_n)(u_n + du_n)}{(\delta_n + d\delta_n)S_n(\delta_n + d\delta_n)}\right)^2$$
$$1 = \left(\frac{u_t + du_t}{\delta_t + d\delta_t}\right)^2 + \left(\frac{u_n + du_n}{\delta_n + d\delta_n}\right)^2 \tag{6.28}$$

Conveniently, the normal and tangental strength models cancel out.

We assume trial state is in the positive quadrant ($T_n^{(trial)} > 0$ and $T_t^{(trial)} > 0$) (and if $T_t^{(trial)} < 0$, move it to quadrant by changing signs on u_t and du_t). Noting $\delta_t + d\delta_t > 0$ and $u_t + du_t$, the solution for $d\delta_t$ is

$$d\delta_t = \frac{u_t + du_t}{\sqrt{1 - \left(\frac{u_n + du_n}{\delta_n + d\delta_n}\right)^2}} - \delta_t$$

Expanding this solution in Taylor series (with help and verification using Mathematica) and keeping up to first order terms gives

$$\frac{u_n^2}{\delta_n^3}d\delta_n + \frac{u_t^2}{\delta_t^3}d\delta_t = \frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t + 1 - \left(\frac{u_t}{\delta_t}\right)^2 + \left(\frac{u_n}{\delta_n}\right)^2 = \frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t \tag{6.29}$$

The second step noted that the constant terms evaluate to zero by assuming the prior tractions were on the failure surface (which applies for small increments in deformation). This result is again identical to general methods in Eq. (6.27).

6.3.4 The Need for a Second Equation

Reassuringly, all methods give the same evolution equation, but it is a single equation in two unknowns. To update both δ_n and δ_t, we need a second equation, which basically means a method to couple the two variables.

Equal Damage Parameter Evolution

A desirable property in prior mixed-model models is that all tractions drop to zero simultaneously, which means $d\delta_n \to u_n^{(c)}$ and $d\delta_t \to u_n^{(c)}$ and the same amount of deformation and independently of mixed-mode ratio (it should even happen in pure mode I or mode II loading). Expressing the coupling in terms of D damage parameters

$$dD_n = \mathbb{R}_n(\delta_n)d\delta_n \text{ and } dD_t = \mathbb{R}_t(\delta_t)d\delta_t \implies dD_n = dD_t = dD \text{ or } \mathbb{R}_n(\delta_n)d\delta_n = \mathbb{R}_t(\delta_t)d\delta_t$$

In other words, coupling means to keep D_n and D_t equal. This choice might in fact might be the only way to couple the two directions. The normal and tangential strength models, however, can have any form. The coupled by $\mathbb{R}_n$ and $\mathbb{R}_t$ functions and the δ_n and δ_t will differ (in general).

Return Vector Methods

A common methods in plasticity modeling is that trial states falling outside a plastic potential function must return to that function (often by a vector normal to the plastic potential surface). We can try this

scheme for cohesive zones as well. First, derive the "return vector" in terms of damage parameters by writing the initial, trial, and final tractions using D_n and D_t or:

$$\begin{aligned}\boldsymbol{T}^0 &= \left(k_t(1-D_t)u_t, k_n(1-D_n)u_n\right)\\ \boldsymbol{T}^{(trial)} &= \left(T_t^0 + k_t(1-D_t)du_t, T_n^0 + k_n(1-D_n)du_n\right)\\ \boldsymbol{T}^{(final)} &= \left(T_t^0 + k_t(1-D_t)du_t - k_t u_t dD_t, T_n^0 + k_n(1-D_n)du_n - k_n u_n dD_n\right)\end{aligned}$$

The return vector is defined by

$$\boldsymbol{r} = \boldsymbol{T}^{(trial)} - \boldsymbol{T}^{(final)} = \left(k_t u_t dD_t, k_n u_n dD_n\right) = \left(k_t u_t \mathbb{R}_n(\delta_n)d\delta_n, k_n u_n \mathbb{R}_n(\delta_t)d\delta_t\right)$$

We consider possible return methods in the following items:

- *Parallel to the Traction Vector* By this model, the return vector is parallel to the initial traction vector. A second equation is derived from

$$\begin{aligned}0 = \|\boldsymbol{r}\times\boldsymbol{T}^0\| &= k_n u_n dD_n k_t(1-D_t)u_t - k_t u_t dD_t k_n(1-D_n)u_n\\ \frac{dD_t}{1-D_t} &= \frac{dD_n}{1-D_n}\end{aligned}$$

  At initiation of damage evolution when $D_t = D_n = 0$, the first damage increment will be $dD_t = dD_n$. The next increment will have the same $D_t = D_n$, which means $dD_t = dD_n$ again. In brief, this return vector is equivalent to assuming there is only one damage variable or that $D_n = D_t$. When $dD_n = dD_t$, the $\boldsymbol{\delta}$ parameters are connected by $\mathbb{R}_n(\delta_n)\delta_n = \mathbb{R}_t(\delta_t)\delta_t$. Conversely, a claim that the cohesive law has a single D damage variable is equivalent to asserting the return vector is parallel to the traction vector.

  Note that this analysis divided through by $u_n u_t$, which formally means that in only applies when both are nonzero. Because the final answer, however, is independent of u_t and u_n, we can assume the result applies in the limit of unidirectional loading as well. It does give the correct update, with the only new result that unidirectional evolution of damage induces evolution of damage parameters in the unloaded direction as well.

- *Parallel to the Trial Traction Vector* By this model, the return vector is parallel to the trial traction vector. A second equation is derived from

$$\begin{aligned}0 = \|\boldsymbol{r}\times\boldsymbol{T}^{(trial)}\| &= k_n u_n dD_n k_t(1-D_t)(u_t+du_t) - k_t u_t dD_t k_n(1-D_n)(u_n+du_n)\\ \frac{dD_t}{(1-D_t)\left(1+\frac{du_t}{u_t}\right)} &= \frac{dD_n}{(1-D_n)\left(1+\frac{du_n}{u_n}\right)}\end{aligned}$$

  Eliminating the second-order terms, this result reduces to the parallel return vector (as expected for small increments). This option is thus identical to that option.

- *Normal to the Evolved Failure Surface*: By this model, the return vector is parallel to a vector normal to the evolved damage surface. The (unnormalized) normal vector for the elliptical failure surface is

$$\boldsymbol{n} = \left(\frac{(u_t+du_t)}{(\delta_t+d\delta_t)F_t(\delta_t+d\delta_t)}, \frac{(u_n+du_n)}{(\delta_n+d\delta_n)F_n(\delta_n+d\delta_n)}\right)$$

  The second equation is

$$0 = \|\boldsymbol{r}\times\boldsymbol{n}\| = \frac{k_n u_n dD_n(u_t+du_t)}{(\delta_t+d\delta_t)F_t(\delta_t+d\delta_t)} - \frac{k_t u_t dD_t(u_n+du_n)}{(\delta_n+d\delta_n)F_n(\delta_n+d\delta_n)}$$

Expanding in Taylor series and keeping only first order terms gives

$$\begin{aligned}
k_n\delta_n S_n(\delta_n)\mathbb{R}_n(\delta_n)d\delta_n &= k_t\delta_t F_t(\delta_n)\mathbb{R}_t(\delta_t)d\delta_t \\
\frac{F_n^2(\delta_n)\mathbb{R}_n(\delta_n)}{1-D_n}d\delta_n &= \frac{F_t^2(\delta_n)\mathbb{R}_t(\delta_t)}{1-D_t}d\delta_t \\
k_n(1-D_n)\varphi_n(\delta_n)d\delta_n &= k_t(1-D_t)\varphi_t(\delta_t)d\delta_t \\
\frac{S_n(\delta_n)\varphi_n(\delta_n)}{\delta_n}d\delta_n &= \frac{S_t(\delta_t)\varphi_t(\delta_t)}{\delta_t}d\delta_t
\end{aligned}$$

This approach gives coupling such that tractions will not simultaneously drop to zero at failure. A normal return might be appropriate for plasticity theory, but it not physically justified for an elastic/damage cohesive zone.

Energy Minimization or Maximization

Perhaps damage is coupled such that each process minimizes or maximized energy. Minimization energy dissipation corresponds to find the path that is closest to elastic. Maximizing energy is a concept in fracture modeling, such as predicting crack growth direction in mixed-mode loading by finding the direction that maximized the amount of energy released (and is same as maximum hoop stress direction). Whether or not minimization or maximization is correct, the approach may not be feasible. Below are some attempts at explaining why.

Begin with a linearized increment in dissipated energy in Eq. (6.16):

$$d\Omega = \frac{1}{2}\left[\left(\frac{u_n}{\delta_n}\right)^2\varphi_n(\delta_n)d\delta_n + \left(\frac{u_t}{\delta_t}\right)^2\varphi_t(\delta_t)d\delta_t\right] \tag{6.30}$$

To minimize energy, solve Eq. (6.27) for $(u_t^2/\delta_t^2)d\delta_t$:

$$\frac{u_t^2}{\delta_t^2}d\delta_t = \delta_t\left(\frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t - \frac{u_n^2}{\delta_n^3}d\delta_n\right)$$

and substitute into Eq. (6.30) to get

$$2d\Omega = \frac{u_n^2}{\delta_n^3}\big(\delta_n\varphi_n(\delta_n) - \delta_t\varphi_t(\delta_t)\big)d\delta_n + \delta_t\varphi_t(\delta_t)\left(\frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t\right) \tag{6.31}$$

This linearized energy will always have its minimum on the boundary of the region of acceptable $d\delta_n$ values. For example, with linearized increments, Eq. (6.29) maps the constraints in the positive x-y quadrant as shown graphically (and schematically) in Fig. 6.3. The intercepts on the x and y axes are at:

$$\left(0, \frac{\delta_t^3 u_n}{u_t^2\delta_n^2}du_n + \frac{\delta_t}{u_t}du_t\right) \quad \text{and} \quad \left(\frac{\delta_n}{u_n}du_n + \frac{\delta_n^3 u_t}{u_n^2\delta_t^2}du_t, 0\right)$$

and the final solution is constrained to values on the line connecting these two points. The above return vector methods result in $d\delta_t$ being proportional to $d\delta_n$. These functions plot as lines from the origin (see Fig. 6.3) and their solutions are when those lines intersect the line based on the ellipse. In contrast, the dissipated energy varies linearly with $d\delta_n$. Thus, if the first term in Eq. (6.31) is negative, the minimum energy will be the intercept with the x axis ("Energy Min 1"); if it positive, the minimum energy will be at the intercept with the y axis ("Energy Min 1"); and if it is zero, the energy is the same for all

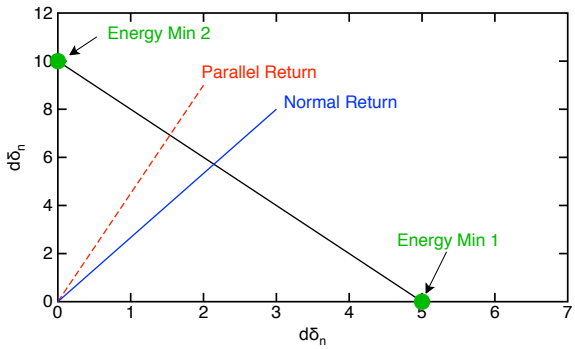

Figure 6.3: Graphical Surface

values of $d\delta_n$ (*i.e.*, the solution is not unique). The energy maximum will be at the opposite boundary. None of these options are acceptable. For example, if that first term is positive, the evolution always has $d\delta_n = 0$, but what if that is applied to unidirectional normal opening? The energy extrema would predict that normal opening deformation only induces damage only in the tangential direction.

Perhaps the problem is linearizing energy, which is a quadratic function of displacements. A discrete calculation of dissipated energy for mixed-mode loading gives:

$$\Delta\Omega = \frac{1}{2}\left(\frac{S_n(\delta_n)}{\delta_n} - \frac{S_n(\delta_n + d\delta_n)}{\delta_n + d\delta_n}\right)u_n(u_n + du_n) + \frac{1}{2}\left(\frac{S_t(\delta_t)}{\delta_t} - \frac{S_t(\delta_t + d\delta_t)}{\delta_t + d\delta_t}\right)u_t(u_t + du_t) \tag{6.32}$$

Expanding one direction to second order (because energy is a quadratic function) results in

$$\begin{aligned} d\Omega &= \frac{1}{2}\left(\frac{\varphi_n(\delta_n)}{\delta_n^2}d\delta_n - \left(\frac{\varphi_n(\delta_n)}{\delta_n^3} + \frac{S_n''(\delta_n)}{2\delta_n}\right)d\delta_n^2\right)u_n(u_n + du_n) \\ &= \frac{1}{2}\left(\mathbb{R}_n d\delta_n - \frac{1}{2}\mathbb{R}_n' d\delta_n^2\right)u_n(u_n + du_n) \end{aligned}$$

where $\mathbb{R}_n$ is implicitly a function of δ_n. The energy released by both direction sis

$$d\Omega = \frac{1}{2}\left(\mathbb{R}_n d\delta_n - \frac{1}{2}\mathbb{R}_n' d\delta_n^2\right)u_n(u_n + du_n) + \frac{1}{2}\left(\mathbb{R}_t d\delta_t - \frac{1}{2}\mathbb{R}_t' d\delta_t^2\right)u_t(u_t + du_t)$$

Combine thi analysis with second-order expansions in $\boldsymbol{u}$ and $\boldsymbol{\delta}$ increments did not resolve the issue. For example, it found extrema outside the acceptable range, which means the boundaries remain as extrema points within constraints of the solution.

6.3.5 Selection of the Best Method

The best (and maybe only) option for coupling appears to link D parameters such that $dD_n = dD_t = dD$ and $\mathbb{R}_n(\delta_n)d\delta_n = \mathbb{R}_t(\delta_t)d\delta_t$. Using Eq. (6.29), the damage increment then becomes:

$$dD = \mathbb{R}_n d\delta_n = \frac{\frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t}{\frac{1}{\mathbb{R}_n}\frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t}\frac{u_t^2}{\delta_t^3}} \implies d\delta_n = \frac{dD}{\mathbb{R}_n} \quad \text{and} \quad d\delta_t = \frac{dD}{\mathbb{R}_t} \tag{6.33}$$

By Eq. (6.13), the tractions update by:

$$dT_n = \frac{S_n}{\delta_n} du_n - k_n u_n \mathbb{R}_n d\delta_n = \frac{S_n}{\delta_n} du_n - \frac{k_n u_n \left(\frac{u_n}{\delta_n^2} du_n + \frac{u_t}{\delta_t^2} du_t \right)}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}}$$

$$dT_t = \frac{S_t}{\delta_t} du_t - k_t u_t \mathbb{R}_t d\delta_t = \frac{S_t}{\delta_t} du_t - \frac{k_t u_t \left(\frac{u_n}{\delta_n^2} du_n + \frac{u_t}{\delta_t^2} du_t \right)}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}}$$

In matrix form, the tangent stiffness matrix is:

$$\begin{pmatrix} dT_n \\ dT_t \end{pmatrix} = \begin{pmatrix} \frac{S_n}{\delta_n} - \frac{\frac{k_n u_n^2}{\delta_n^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} & - \frac{\frac{k_n u_n u_t}{\delta_t^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} \\ - \frac{\frac{k_t u_t u_n}{\delta_n^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} & \frac{S_t}{\delta_t} - \frac{\frac{k_t u_t^2}{\delta_t^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} \end{pmatrix} \begin{pmatrix} du_n \\ du_t \end{pmatrix}$$

Using $\mathbb{R}\delta^2 = \varphi/k$ and

$$\frac{S}{\varphi} - 1 = \frac{S}{S - \delta S'} - 1 = \frac{S - S + \delta S'}{S - \delta S'} = \frac{\delta S'}{\varphi}$$

the tangent stiffness matrix becomes:

$$\begin{pmatrix} dT_n \\ dT_t \end{pmatrix} = \frac{1}{\frac{k_n u_n^2}{\varphi_n \delta_n} + \frac{k_t u_t^2}{\varphi_t \delta_t}} \begin{pmatrix} \frac{S_n' k_n u_n^2}{\varphi_n \delta_n} + \frac{S_n k_t u_t^2}{\delta_n \varphi_t \delta_t} & - \frac{k_n u_n u_t}{\delta_t^2} \\ - \frac{k_t u_t u_n}{\delta_n^2} & \frac{S_t' k_t u_t^2}{\varphi_t \delta_t} + \frac{S_t k_n u_n^2}{\delta_t \varphi_n \delta_n} \end{pmatrix} \begin{pmatrix} du_n \\ du_t \end{pmatrix} \tag{6.34}$$

An alternate derivation uses the single D parameter and damage tensor $D\mathsf{I}$, the tractions can be written as

$$\boldsymbol{T} = (1-D)\mathsf{K}\boldsymbol{u} \quad \Longrightarrow \quad d\boldsymbol{T} = (1-D)\mathsf{K}d\boldsymbol{u} - \mathsf{K}\boldsymbol{u}dD$$

Looking an normal component:

$$\begin{aligned} dT_n &= k_n \left(1 - D - \frac{\frac{u_n^2}{\delta_n^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} \right) du_n - \frac{\frac{k_n u_n u_t}{\delta_t^2}}{\frac{1}{\mathbb{R}_n} \frac{u_n^2}{\delta_n^3} + \frac{1}{\mathbb{R}_t} \frac{u_t^2}{\delta_t^3}} du_t \\ &= \frac{1}{\frac{k_n u_n^2}{\varphi_n \delta_n} + \frac{k_t u_t^2}{\varphi_t \delta_t}} \left[\left(\left(\frac{S_n}{\varphi_n} - 1 \right) \frac{k_n u_n^2}{\delta_n^2} + \frac{S_n k_t u_t^2}{\delta_n \varphi_t \delta_t} \right) du_n - \frac{k_n u_n u_t}{\delta_t^2} du_t \right] \end{aligned}$$

This result matches the previous result (and can expressed using various functions). For elastic loading, the tangent stiffness is trivially $d\boldsymbol{T} = (1-D)\mathsf{K}d\boldsymbol{u}$.

Some observations are:

1. The damage parameters D will remain in synch and thus reach failure ($D = 1$) at the same time. This coupling avoids the problem of extra failure criterion causing loads to suddenly drop to zero.

2. Any other coupling would not have synched failure property. In fact any coupling could lead to case where a cohesive zone in tangential direction causes failure even when loaded in pure normal direction. The only alternative to coupling proposed here is a decoupled approach. That approach does not have erroneous failures, but would have the sudden traction drop problem still.

3. This coupling avoids the need to even have a mixed-mode failure law. But how does a zone fail during mixed mode loading or is it possible to model materials that might experimental exhibit different mixed-mode failure criteria? See section 6.3.8.

6.3.6 Special Case if No Elastic Regime

If the strength model has no elastic region (such as Needleman cubic law), the modeling will start with $\delta_n = \delta_t = 0$ and the above equations no longer work. To handle such laws, the initiation of damage must use a special case. If one or both strength models start at zero, the modeling needs a special case to get started. If both directions have zero initial strength, the first increment will exceed the strength and the first equation reduces to:

$$\left(\frac{du_n}{d\delta_n}\right)^2 + \left(\frac{du_t}{d\delta_t}\right)^2 = \left(\frac{\mathbb{R}_n(0)du_n}{dD}\right)^2 + \left(\frac{\mathbb{R}_t(0)du_t}{dD}\right)^2 = 1 \tag{6.35}$$

which can be solved for initial damage increment

$$dD = \sqrt{(\mathbb{R}_n(0)du_n)^2 + (\mathbb{R}_t(0)du_t)^2}$$

Once initiated, the analysis can revert to previous equations.

If only the normal direction sas zero strength, steps will proceed until either tangential damage occurs or the first non-zero du_n occurs. If damage initiates in tential direction while $u_n = du_n =$, the first damage increment is:

$$dD = \frac{\mathbb{R}_t(\delta_t)\delta_t du_t}{u_t} = \mathbb{R}_t(\delta_t)\delta_t d(\ln u_t)$$

But if $du_n > 0$ defore initiating tangential damage, the equation to solve is

$$\left(\frac{du_n}{d\delta_n}\right)^2 + \left(\frac{u_t + du_t}{\delta_t + d\delta_t}\right)^2 = \left(\frac{\mathbb{R}_n(0)du_n}{dD}\right)^2 + \left(\frac{\mathbb{R}_t(\delta_t)(u_t + du_t)}{\mathbb{R}_t(\delta_t)\delta_t + dD}\right)^2 = 1 \tag{6.36}$$

Solving for dD gives

$$(\mathbb{R}_t(\delta_t)\delta_t + dD)^2(\mathbb{R}_n(0)du_n)^2 + dD^2(\mathbb{R}_t(\delta_t)(u_t + du_t))^2 = dD^2(\mathbb{R}_t(\delta_t)\delta_t + dD)^2 \tag{6.37}$$

which is a quartic equation for dD.

6.3.7 Compression Half-Plane Damage Evolution

In the compression half plane, the failure can only happen by shear deformation. Because the surface does not include normal traction, the damage evolution can use 1D methods or:

$$d\delta_t = du_t$$

It is not obvious how this damage should couple to normal direction damage. Two options are to assume no normal direction damage evolves when in compression or to assume the normal direction variable couples in compression the same it does in tension or

$$dD_n = dD_t = dD$$

This approach appears the most consistent with physical picture of a damaged zone.

The increments when in compression will also include du_n, which will need to be converted to a negative traction load. Three options for handling the compression region are:

1. Extend in the compression direction elastically using initial stiffness k_n (or chose another elastic stiffness)

2. Extend in the compression direction elastically using the current effective stiffness $k_{eff} = k_0(1-D)$.

3. Set the traction to prevent interpenetration or to bring u_n back to zero.

Options 1 or 3 are probably best.

6.3.8 Mixed-Mode Failure Criterion

Constant Mode Mixity

Coupling to get equal $D_n = D_t = D$ means the cohesive zone fails when $D = 1$ and not by an imposed-mixed mode failure criterion. The question remains — how does a cohesive zone fail at a constant state of mode mixity loading? Under monotonic, constant mode loading (if that is even possible), using Eq. (6.16), and realizing the $\|\boldsymbol{u}\| = \delta_d$ during damage evolution, the energy partitions into mode I and mode II by

$$d\Omega = dG_I + dG_2 \quad \text{where} \quad dG_I = \frac{1}{2}\left(\frac{\delta_d \sin\theta}{\delta_n}\right)^2 \varphi_n(\delta_n)d\delta_n \quad dG_{II} = \frac{1}{2}\left(\frac{\delta_d \cos\theta}{\delta_t}\right)^2 \varphi_t(\delta_t)d\delta_t$$

Each mode is linked to the other by the δ_d term. To complete each integral, we need δ_t and function of δ_n (and vice versa). By the linking functions, we know that

$$\int_{u_n^{(e)}}^{\delta_n} \mathbb{R}_n(\delta_n)d\delta_n = \int_{u_t^{(e)}}^{\delta_t} \mathbb{R}_t(\delta_t)d\delta_t \quad \Longrightarrow \quad D_n(\delta_n) = D_t(\delta_t)$$

We can solve using inverse functions

$$\delta_t = D_t^{-1}\big(D_n(\delta_n)\big)$$

The mode I energy released up to failure becomes

$$G_I = \frac{1}{2}\int_{u_n^{(e)}}^{u_n^{(c)}} \frac{\varphi_n(\delta_n)\sin^2\theta}{\sin^2\theta + \left(\frac{\delta_n}{D_t^{-1}\left(D_n(\delta_n)\right)}\right)^2 \cos^2\theta} d\delta_n$$

The corresponding expression for mode II is

$$G_{II} = \frac{1}{2}\int_{u_t^{(e)}}^{u_t^{(c)}} \frac{\varphi_t(\delta_t)\cos^2\theta}{\left(\frac{\delta_t}{D_n^{-1}\left(D_t(\delta_t)\right)}\right)^2 \sin^2\theta + \cos^2\theta} d\delta_t$$

In general, the inverse functions for arbitrary softening laws cannot be analytically integrated. One exception is the often used saw tooth law (the inverse function is given in section 6.6.1), which leads to

$$\delta_t(\delta_n) = \frac{u_t^{(e)}u_t^{(c)}}{u_t^{(c)} - \left(1 - \frac{u_n^{(e)}}{\delta_n}\frac{u_n^{(c)}-\delta_n}{u_n^{(c)}-u_n^{(e)}}\right)(u_t^{(c)} - u_t^{(e)})}$$

Performing the (still-challenging) integrations in Mathematics, the mode I and mode II energies released at failure in pure mode loading are

$$G_I = \begin{cases} 0 & \theta = 0 \\ G_{Ic}\dfrac{\arctan(r_e\cot\theta)-\arctan(r_c\cot\theta)}{r_e-r_c}\tan\theta & 0<\theta<\frac{\pi}{2} \\ G_{Ic} & \theta=\frac{\pi}{2} \end{cases}$$

$$G_{II} = \begin{cases} G_{IIc} & \theta = 0 \\ G_{IIc}\dfrac{r_e r_c\left(\arctan\left(\frac{\tan\theta}{r_c}\right)-\arctan\left(\frac{\tan\theta}{r_e}\right)\right)}{r_e-r_c}\cot\theta & 0<\theta<\frac{\pi}{2} \\ 0 & \theta=\frac{\pi}{2} \end{cases}$$

where

$$r_e = \frac{u_n^{(e)}}{u_t^{(e)}} \qquad r_c = \frac{u_n^{(c)}}{u_t^{(c)}} \qquad G_{IIc} = \frac{k_t}{k_n r_e r_c}G_{Ic}$$

Note that these results assume that $r_e \neq r_c$. If they are equal, the inversion simplifies to $\delta_t = \delta_n/r_e$ (or r_c; they are the same). The much simpler integrals evaluate to

$$G_I = \frac{G_{Ic}}{1+r_c^2\cot^2\theta} \qquad G_{II} = \frac{r_c^2 G_{IIc}}{r_c^2+\tan^2\theta} \qquad G_{IIc} = \frac{k_t}{k_n r_c^2}G_{Ic}$$

In terms of $\overline{u}_{np} = \frac{u_n^{(e)}}{u_n^{(c)}}$ and $\overline{u}_{tp} = \frac{u_t^{(e)}}{u_t^{(c)}}$, these are recast as:

$$G_I = \begin{cases} 0 & \theta = 0 \\ G_{Ic}\dfrac{\arctan\left(\frac{r_c\overline{u}_{np}}{\overline{u}_{tp}}\cot\theta\right)-\arctan(r_c\cot\theta)}{r_c\left(\frac{\overline{u}_{np}}{\overline{u}_{tp}}-1\right)}\tan\theta & 0<\theta<\frac{\pi}{2} \\ G_{Ic} & \theta=\frac{\pi}{2} \end{cases}$$

$$G_{II} = \begin{cases} G_{IIc} & \theta = 0 \\ G_{IIc}\dfrac{\arctan\left(\frac{\overline{u}_{tp}}{r_c\overline{u}_{np}}\tan\theta\right)-\arctan\left(\frac{1}{r_c}\tan\theta\right)}{\frac{1}{r_c}\left(\frac{\overline{u}_{tp}}{\overline{u}_{np}}-1\right)}\cot\theta & 0<\theta<\frac{\pi}{2} \\ 0 & \theta=\frac{\pi}{2} \end{cases}$$

for $\overline{u}_{np} \neq \overline{u}_{tp}$, but uses the form that depends only on r_c when they are equal.

A usual method to represent mixed-mode failure criteria is in a plot of G_{II}/G_{IIc} *vs.* G_I/G_{Ic}. Using the above results, a few sample plots for $r_e = 1$ are in Fig. 6.4 for various values of r_c. All curves are concave up and all can be fit fairly well with

$$\left(\frac{G_I}{G_{Ic}}\right)^n + \left(\frac{G_{II}}{G_{IIc}}\right)^n = 1 \tag{6.38}$$

Sample fits are in Fig. 6.4. Figure 6.5 plots the fitting n as a function of r_c for $r_e = 0.5$. 1, or 2. For all values, the curve peaks at $n = 1$ when $r_e = r_c$ and the exponent is always $n \leq 1$ for all combinations of r_c and r_e. Thus, a sawtooth strength model can never model a material with mixed-mode failure law having $n > 1$. Experimental reports that claim $n > 1$, however, might be questionable or perhaps should be re-evaluated to see if they correctly calculated mode I and mode II components. Alternatively, CZM model might be questionable.

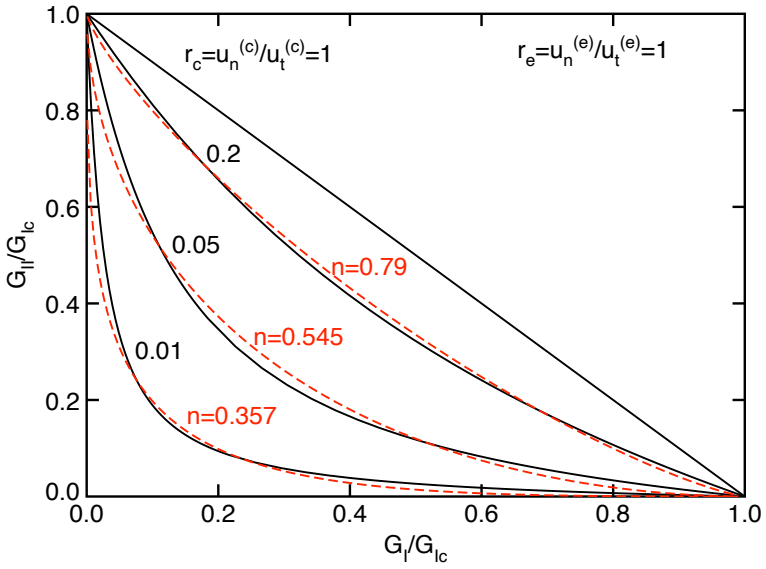

Figure 6.4: Four sample mixed-mode failure envelops for linear softening for $r_e = 1$ and various values of r_c. The dashed lines are fits to each curve using Eq. (6.38)

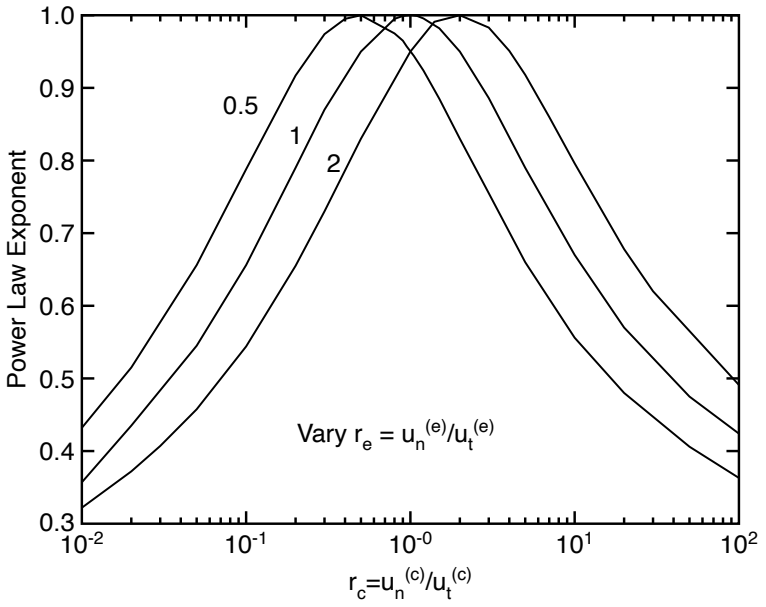

Figure 6.5: Best fit exponent, n, use Eq. (6.38) as a function of r_c for three values of r_e.

The cubic law also has analytical results:

$$G_I = \begin{cases} 0 & \theta = 0 \\ \dfrac{G_{Ic}}{1+\left(\frac{u_n^{(c)}}{u_t^{(c)}}\right)^2 \cot^2\theta} & 0 < \theta < \frac{\pi}{2} \\ G_{Ic} & \theta = \frac{\pi}{2} \end{cases} \qquad G_{II} = \begin{cases} G_{IIc} & \theta = 0 \\ \dfrac{G_{IIc}}{1+\left(\frac{u_t^{(c)}}{u_n^{(c)}}\right)^2 \tan^2\theta} & \\ 0 & \theta = \frac{\pi}{2} \end{cases}$$

This result is identical to the saw tooth law when $r_e = r_c$ (is it a universal result independent of the strength model?) or it has linear relation (*i.e.*, Eq. (6.38) with $n = 1$). In other words, using these cubic strength models imposes this linear relation on the mixed mode failure criterion. Furthermore, plots of G_{II} *vs.* G_I will be linear for any relative normal and tangential failure properties. Conversely, if experiments convincingly show that this linear law does not apply for some material, then that material should not be modeled with a cubic traction law. A law the does not impose similar shapes on normal and tangential loading should be used instead. So far, all laws have linear or concave up. What about experiments that show concave down (*e.g.*, and elliptical shape of $n > 1$).

Preload Under Some Mixed Mode followed by New Mixed Mode

Imagine preloading in pure mode I up to a certain value of D (could use mixed mode preloading too). The energy released (by integrating pure mode I loading dissipated energy to $\delta_n(D)$) to that point is:

$$G_I = G_{Ic}\frac{D\overline{u}_{np}}{1-D(1-\overline{u}_{np})} \qquad G_{II} = 0$$

Next unload, and then reload in pure mode II (could use mixed mode here too) until failure. The energy dissipated in this step (by integrating from $\delta_t(D)$ to $\delta_t^{(c)}$) is

$$G_I = 0 \qquad G_{II} = G_{IIc}\frac{(1-D)r_e}{(1-D)r_e + Dr_c\overline{u}_{np}} = G_{IIc}\frac{1-D}{1-D(1-\overline{u}_{tp})}$$

The mixed-mode failure curve for a series of such experiments is obtained as a parametric plot in D. Eliminating D gives

$$\frac{G_{II}}{G_{IIc}} = \frac{(G_{Ic}-G_I)\overline{u}_{np}}{(G_{Ic}-G_I)\overline{u}_{np} + G_I\overline{u}_{tp}}$$

Note that if $\overline{u}_{np} = \overline{u}_{tp}$, the mixed mode curve is a straight line (same as for constant mode mixity experiments):

$$\frac{G_{II}}{G_{IIc}} = 1 - \frac{G_I}{G_{Ic}}$$

The complementary experiment to preload in mode II followed by unloading and then loading in mode I is found by interchanging I and II and n and t in above expressions.

6.4 Decoupled Cohesive Zone Modeling

The previous sections derive methods to couple damage parameters in mixed-mode loading. Another option, which is common in the literature (see work for Thouless, *et al.*) is assume no coupling. This methods is simple to simple to implement. The now-independent normal and tangential laws separately track independent damage parameters (D_n, δ_n, D_t, and δ_t) and each direction evolves by 1D methods whenever normal or tangential traction component exceeds the current normal or tangential

strength model. Because decoupled strength models do not reach zero at the same time, failure has to be predicted by supplementing the strength models with a mixed-mode failure criterion such as:

$$\left(\frac{G_I}{G_{IIc}}\right)^p + \left(\frac{G_{II}}{G_{IIc}}\right)^q = 1$$

where p and q are material properties and the implementation tracks mode I and mode II energy during deformation. Because failure will occur by this criterion and not by D_n and D_t reaching zero, failure will occur, in general, with non-zero normal and tangential tractions. The failure will thus cause a sudden drop in tractions.

6.5 Assume Equal D at the Start

What if we started by assuming the D values are coupled and derive evolution equation directly? The traction magnitude as function of COD magnitude is

$$\|\boldsymbol{T}\| = \|\boldsymbol{u}\|\sqrt{k_n^2(1-D)^2\sin^2\theta + k_t^2(1-D)^2\cos^2\theta} \tag{6.39}$$

This loading causes damage when the elliptical surface is reached and that happens when

$$\begin{aligned} 1 &= \left(\frac{T_n}{S_n(D)}\right)^2 + \left(\frac{T_t}{S_t(D)}\right)^2 = \|\boldsymbol{u}_d\|^2(1-D)^2\left(\frac{k_n^2\sin^2\theta}{S_n(D)^2} + \frac{k_t^2\cos^2\theta}{S_t(D)^2}\right) \\ \|\boldsymbol{u}_d\| &= \delta_d = \frac{1}{(1-D)\sqrt{\frac{k_n^2\sin^2\theta}{S_n(D)^2} + \frac{k_t^2\cos^2\theta}{S_t(D)^2}}} \end{aligned} \tag{6.40}$$

Using the $d\sigma_d = d\|\boldsymbol{u}\|$ methods with full differential leads to

$$\begin{aligned} &(1-D)\delta_d^3\left(\frac{k_n^2\sin^2\theta}{S_n(D)^3}\left(S_n(D)+(1-D)S_n'(D)\right) + \frac{k_t^2\cos^2\theta}{S_t(D)^3}\left(S_t(D)+(1-D)S_t'(D)\right)\right)dD \\ &= d\|\boldsymbol{u}\| + (1-D)^2\delta_d^3\left(\frac{k_n^2}{S_n(D)^2} - \frac{k_t^2}{S_t(D)^2}\right)\sin\theta\cos\theta\, d\theta \end{aligned}$$

Converting the right hand side from using $d\|\boldsymbol{u}\|$ and $d\theta$ to du_n and du_t using Eq. (6.24) gives

$$\begin{aligned} &(1-D)\delta_d^3\left(\frac{k_n^2\sin^2\theta}{S_n(D)^3}\left(S_n(D)+(1-D)S_n'(D)\right) + \frac{k_t^2\cos^2\theta}{S_t(D)^3}\left(S_t(D)+(1-D)S_t'(D)\right)\right)dD \\ &= \left(1 + (1-D)^2\delta_d^2\left(\frac{k_n^2}{S_n(D)^2} - \frac{k_t^2}{S_t(D)^2}\right)\cos^2\theta\right)\sin\theta\, du_n \\ &+ \left(1 - (1-D)^2\delta_d^2\left(\frac{k_n^2}{S_n(D)^2} - \frac{k_t^2}{S_t(D)^2}\right)\sin^2\theta\right)\cos\theta\, du_t \end{aligned}$$

Using Eq. (6.23):

$$dD = \frac{\frac{\sin\theta}{\delta_n^2}du_n + \frac{\cos\theta}{\delta_t^2}du_t}{(1-D)\delta_d\left(\frac{k_n^2\sin^2\theta}{S_n(D)^3}\left(S_n(D)+(1-D)S_n'(D)\right) + \frac{k_t^2\cos^2\theta}{S_t(D)^3}\left(S_t(D)+(1-D)S_t'(D)\right)\right)}$$

or

$$dD = \frac{\frac{u_n}{\delta_n^2}du_n + \frac{u_t}{\delta_t^2}du_t}{(1-D)\left(\frac{k_n^2u_n^2}{S_n(D)^3}\left(S_n(D)+(1-D)S_n'(D)\right)+\frac{k_t^2u_t^2}{S_t(D)^3}\left(S_t(D)+(1-D)S_t'(D)\right)\right)}$$

The numerator matches the update in Eq. (6.33). The denominator can be reduced to Eq. (6.33) (or Eq. (6.34)) by using $S'(D) = S'(\delta)/\mathbb{R}$ and $1-D = S/(k\delta)$. The first term, for example, becomes

$$\frac{S_n}{k_n\delta_n}\frac{k_n^2u_n^2}{S_n^3}\left(S_n+\frac{S_nS'(\delta)}{\mathbb{R}_nk_n\delta_n}\right) = \frac{k_nu_n^2}{S_n\delta_n}\left(1+\frac{S'(\delta)}{\mathbb{R}_nk_n\delta_n}\right) = \frac{k_nu_n^2}{S_n\delta_n} = \frac{k_nu_n^2}{\varphi_n\delta_n}$$

The last step used $\mathbb{R} = \varphi/(k\delta^2)$. This analysis is thus identical to the previous one.

6.6 Example Strength Models

6.6.1 Linear Sawtooth Strength Model

A saw-tooth strength law is linear, with slope k up to peak $\sigma_c = ku^{(e)}$ cohesive stress at the end of the elastic region. After the peak, the traction decreases linearly until critical COD $u^{(c)}$. The full function is

$$S(\delta) = \sigma_c\frac{u^{(c)}-\delta}{u^{(c)}-u^{(e)}} \quad \text{and} \quad S'(\delta) = -\frac{\sigma_c}{u^{(c)}-u^{(e)}} \qquad \text{for } \delta > u^{(e)}$$

The area under elastic and damage regions is

$$G_c = \frac{1}{2}\sigma u^{(c)}$$

The energy dissipation and ratio functions in the only valid region are

$$\varphi(\delta) = \frac{\sigma_cu^{(c)}}{u^{(c)}-u^{(e)}} \qquad \text{and} \qquad \mathbb{R}(\delta) = \frac{\sigma_cu^{(c)}}{k\delta^2(u^{(c)}-u^{(e)})} = \frac{u^{(e)}u^{(c)}}{\delta^2(u^{(c)}-u^{(e)})}$$

Using dimensionless variables

$$\varphi(\delta) = \frac{\sigma_c}{1-\overline{u}_p}, \quad \mathbb{R}(\delta)u^{(c)} = \frac{\overline{u}_p}{\overline{\delta}^2(1-\overline{u}_p)}, \quad \overline{\delta} = \frac{\delta}{u^{(c)}}, \quad \overline{u}_p = \frac{u^{(e)}}{u^{(c)}}$$

Note that $\varphi(\delta)$ is a constant. Its increment and integral during damage evolution are:

$$d\Omega = \frac{1}{2}\varphi(\delta)d\delta = \frac{G_c}{u^{(c)}-u^{(e)}}d\delta \quad \text{and} \quad \int_{u^{(e)}}^{\delta} d\Omega = G_c\frac{\delta-u^{(e)}}{u^{(c)}-u^{(e)}}$$

where $G_c = \sigma_cu^{(c)}/2$ is area under the sawtooth tractions. The D damage parameter is related to δ by:

$$D(\delta) = 1-\frac{u^{(e)}}{\delta}\frac{u^{(c)}-\delta}{u^{(c)}-u^{(e)}} = 1-\frac{\overline{u}_p}{1-\overline{u}_p}\frac{1-\overline{\delta}}{\overline{\delta}}$$

Unlike most laws, this can be inverted to get

$$\delta(D) = D^{-1}(\delta) = \frac{u^{(e)}u^{(c)}}{u^{(c)}-D(u^{(c)}-u^{(e)})} \quad \text{and} \quad \overline{\delta}(D) = \frac{\overline{u}_p}{1-D(1-\overline{u}_p)}$$

The strength model in terms of D is

$$S(D) = \frac{ku^{(e)}u^{(c)}(1-D)}{u^{(c)}-D(u^{(c)}-u^{(e)})} \qquad \varphi(D) = \frac{\sigma_cu^{(c)}}{u^{(c)}-u^{(e)}} \qquad \mathbb{R}(D) = \frac{\left(u^{(c)}-D(u^{(c)}-u^{(e)})\right)^2}{u^{(c)}u^{(e)}(u^{(c)}-u^{(e)})}$$

6.6.2 Generalized Cubic Strength Law

We define a generalized cubic law such that loading is elastic until $u^{(e)}$ and $\sigma_0 = ku^{(e)}$ and thereafter has a cubic variation in $\delta - u^{(e)}$ with initial value σ_0, initial slope of cubic region being k_c, and stress and derivative both 0 at $\delta = u^{(c)}$. This strength function (for $\delta \geq u^{(e)}$) and its derivative are:

$$S(\delta) = \left(\sigma_0 + \left(2\sigma_0 + k_c\left(u^{(c)} - u^{(e)}\right)\right)\overline{\delta}\right)\left(1-\overline{\delta}\right)^2$$
$$S'(\delta) = \left(k_c - 3\left(2\sigma_0 + k_c\left(u^{(c)} - u^{(e)}\right)\right)\frac{\overline{\delta}}{u^{(c)} - u^{(e)}}\right)\left(1-\overline{\delta}\right)$$

where

$$\overline{\delta} = \frac{\delta - u^{(e)}}{u^{(c)} - u^{(e)}}$$

The area under elastic and damage regions is

$$G_c = \frac{\sigma_0 u^{(c)}}{2} + \frac{k_c\left(u^{(c)} - u^{(e)}\right)^2}{12}$$

If $k_c = k$, this law provides a smooth transition to damaged region where initial stiffness post damage equals the elastic stiffness. Note that when $k_c > 0$, σ_0 is not the maximum strength. The maximum strength is

$$\sigma_c = \max\left(S(\delta)\right) = \frac{4\left(3\sigma_0 + k_c\left(u^{(c)} - u^{(e)}\right)\right)^3}{27\left(2\sigma_0 + k_c\left(u^{(c)} - u^{(e)}\right)\right)^2} \qquad \text{for } k_c > 0$$

If $k_c = 0$, this function is cubic, smooth step function that monotonically decreases from $\sigma_c = \sigma_0$ to 0 as δ goes from $u^{(e)}$ to $u^{(c)}$:

$$S(\delta) = \sigma_0(1 + 2\overline{\delta})\left(1-\overline{\delta}\right)^2$$

Finally, if $u^{(e)} = 0$, $\sigma_0 = 0$, and $k_c = 27\sigma_c/(4u^{(c)})$, this law reduces to the Needleman cubic cohesive law of

$$S(\delta) = \frac{27}{4}\sigma_c\frac{\delta}{u^{(c)}}\left(1 - \frac{\delta}{u^{(c)}}\right)^2 = \frac{27}{4}\sigma_c\overline{\delta}\left(1-\overline{\delta}\right)^2 = k_c\delta\left(1-\overline{\delta}\right)^2 \quad \text{with} \quad \overline{\delta} = \frac{\delta}{u^{(c)}}$$

and with area

$$G_c = \frac{9}{16}\sigma_c u^{(c)}$$

The energy dissipation and ratio functions in the only valid region are

$$\varphi(\delta) = \left[k_c\left(u^{(e)}(3\overline{\delta} - 1) + 2(u^{(c)} - u^{(e)})\overline{\delta}^2\right) + \sigma_0\left((1 + 2\overline{\delta})^2 + 3\overline{\delta}\,\frac{3u^{(e)} - u^{(c)}}{u^{(c)} - u^{(e)}}\right)\right](1-\overline{\delta})$$
$$\mathbb{R}(\delta) = \frac{\left[k_c\left(u^{(e)}(3\overline{\delta} - 1) + 2(u^{(c)} - u^{(e)})\overline{\delta}^2\right) + \sigma_0\left((1 + 2\overline{\delta})^2 + 3\overline{\delta}\,\frac{3u^{(e)} - u^{(c)}}{u^{(c)} - u^{(e)}}\right)\right](1-\overline{\delta})}{k\left(u^{(e)} + (u^{(c)} - u^{(e)})\overline{\delta}\right)^2}$$

For cubic step function with $k_c = 0$:

$$\varphi(\delta) = \sigma_0\left((1 + 2\overline{\delta})^2 + 3\overline{\delta}\,\frac{3u^{(e)} - u^{(c)}}{u^{(c)} - u^{(e)}}\right)(1-\overline{\delta})$$
$$\mathbb{R}(\delta) = \frac{\sigma_0\left((1 + 2\overline{\delta})^2 + 3\overline{\delta}\,\frac{3u^{(e)} - u^{(c)}}{u^{(c)} - u^{(e)}}\right)(1-\overline{\delta})}{k\left(u^{(e)} + (u^{(c)} - u^{(e)})\overline{\delta}\right)^2}$$

In the limit of a Needleman cubic law, these reduce to

$$\varphi(\delta) = \frac{27}{2}\sigma_c\overline{\delta}^2\left(1-\overline{\delta}\right) = 2k_c u^{(c)}\overline{\delta}^2\left(1-\overline{\delta}\right), \quad \mathbb{R}(\delta)u^{(c)} = 2\left(1-\overline{\delta}\right) \quad \text{with} \quad \overline{\delta} = \frac{\delta}{u^{(c)}}$$

The D damage parameter is related to δ by:

$$D(\delta) = 1 - \frac{\left(k_c(u^{(c)}-u^{(e)})+2\sigma_0\right)\overline{\delta}+\sigma_0}{k\left(u^{(e)}+\overline{\delta}(u^{(c)}-u^{(e)})\right)}(1-\overline{\delta})^2$$

In the limit of a Needleman cubic law, this reduces to

$$D(\overline{\delta}) = 1-\left(1-\overline{\delta}\right)^2$$

$D(\delta)$ can be inverted by solving a cubic equation, but the result is lengthy. In the Needleman limit, a simple inversion is

$$\delta(D) = D^{-1}(\delta) = u^{(c)}\left(1-\sqrt{1-D}\right) \quad \text{and} \quad \overline{\delta}(D) = 1-\sqrt{1-D}$$

The Needleman strength model in terms of D becomes:

$$\begin{aligned} S(D) &= \frac{27}{4}\sigma_c\left(1-\sqrt{1-D}\right)(1-D) \\ \varphi(D) &= \frac{27}{2}\sigma_c\left(1-\sqrt{1-D}\right)^2\sqrt{1-D} \\ \mathbb{R}(D) &= \frac{2}{u^{(c)}}\sqrt{1-D} \end{aligned}$$

Special Case When Both Use Needleman Cubic Law

From the Special Case if No Elastic Regime section, use of laws with no initial elastic regime cannot use the general equation. But, if both directions using the Needleman cubic law and they are coupled, we can write

$$S_n(\overline{\delta}) = k_n u_n^{(c)}\overline{\delta}\left(1-\overline{\delta}\right)^2, \quad S_t(\overline{\delta}) = k_t u_t^{(c)}\overline{\delta}\left(1-\overline{\delta}\right)^2, \quad \text{where} \quad \overline{\delta} = \overline{\delta}_n = \frac{\delta_n}{u_n^{(c)}} = \overline{\delta}_t = \frac{\delta_t}{u_t^{(c)}}$$

The connection between δ_n and δ_t occurs when coupled to a single D value and using $1-D = (1-\overline{\delta}_n)^2 = (1-\overline{\delta}_t)^2$. We can then directly solve Eq. (6.28):

$$\begin{aligned} 1 &= \left(\frac{u_t+du_t}{u_t^{(c)}(\overline{\delta}+d\overline{\delta})}\right)^2 + \left(\frac{u_n+du_n}{u_n^{(c)}(\overline{\delta}+d\overline{\delta})}\right)^2 \\ \overline{\delta}+d\overline{\delta} &= \sqrt{\left(\frac{u_t+du_t}{u_t^{(c)}}\right)^2 + \left(\frac{u_n+du_n}{u_n^{(c)}}\right)^2} \end{aligned}$$

where u_t and u_n are the final displacement in the steps. Once $\overline{\delta}' = \overline{\delta}+d\overline{\delta}$ or the updated value of $\overline{\delta}$ is found, the update parameters are

$$\delta_t = u_t^{(c)}\overline{\delta}', \quad \delta_n = u_n^{(c)}\overline{\delta}', \quad \text{and} \quad D = 1-(1-\overline{\delta}')^2$$

Work, tractions, and released energy are then found by methods described above. In the compression half plane using Eq. (6.28): simplifies to

$$\overline{\delta}' = \overline{\delta} + d\overline{\delta} = \frac{|u_t|}{u_t^{(c)}}$$

A similar approach works when both laws are linear with $\overline{u}_{np} = \overline{u}_{tp}$, but not when these terms on unequal.

If one direction is cubic (say normal direction) while other is linear (say tangential direction), this simulation may proceed with no damage evolution provided du_n remains at zero. If the linear direction initiates damage first, that will cause damage in the cubic direction and things can proceed from there. But, if $du_n > 0$ before any linear direction damage occurs, we need special case again to get damage started. Substituting into Eq. (6.36) gives:

$$\left(\frac{du_n}{u_n^{(c)} d\overline{\delta}_n}\right)^2 + \left(\frac{u_t + du_t}{u_t^{(c)}(\overline{u}_{tp} + d\overline{\delta}_t)}\right)^2 = 1$$

Equation D in the two directions, leads to

$$\overline{\delta}_t = \frac{\overline{u}_{tp}}{1-(1-\overline{u}_{tp})\overline{\delta}_n(2-\overline{\delta}_n)} \quad \text{and} \quad d\overline{\delta}_t = \frac{2\overline{u}_{tp}(1-\overline{u}_{tp})(1-\overline{\delta}_n)d\overline{\delta}_n}{\left(1-(1-\overline{u}_{tp})\overline{\delta}_n(2-\overline{\delta}_n)\right)^2} \to 2\overline{u}_{tp}(1-\overline{u}_{tp})d\overline{\delta}_n$$

that correctly goes from $\overline{u}_{tp}$ to 1 as $\overline{\delta}_n$ goes from 0 to 1. The general differential is shown with special case when $\delta_n = 0$. The equation to solve becomes:

$$\left(\frac{du_n}{u_n^{(c)} d\overline{\delta}_n}\right)^2 + \left(\frac{u_t + du_t}{u_t^{(e)}(1 + 2(1-\overline{u}_{tp})d\overline{\delta}_n)}\right)^2 = 1$$

Alternatively, solving for $\overline{\delta}_n$ gives:

$$\overline{\delta}_n = 1 - \sqrt{\frac{\overline{u}_{tp}(1-\overline{\delta}_t)}{\overline{\delta}_t(1-\overline{u}_{tp})}} \quad \text{and} \quad d\overline{\delta}_n = \frac{\overline{u}_{tp} d\overline{\delta}_t}{2\overline{\delta}_t\sqrt{(1-\overline{\delta}_t)(1-\overline{u}_{tp})\overline{u}_{tp}\overline{\delta}_t}} \to \frac{d\overline{\delta}_t}{2\overline{u}_{tp}(1-\overline{u}_{tp})}$$

that goes from 0 to 1 as $\overline{\delta}_t$ goes from $\overline{u}_{tp}$ to 1. The general differential is shown with special case when $\delta_t = \overline{u}_{tp}$. The equation to solve becomes

$$\left(\frac{2\overline{u}_{tp}(1-\overline{u}_{tp})du_n}{u_n^{(c)} d\overline{\delta}_t}\right)^2 + \left(\frac{u_t + du_t}{u_t^{(c)}(\overline{u}_{tp} + d\overline{\delta}_t)}\right)^2 = 1$$

Both of these equations are quartic equations in the first differential. The code currently does not allow Needleman cubic law unless both direction use that law.

6.6.3 Exponential Strength Model

A exponential strength law is linear, with slope k up to peak $\sigma_c = ku^{(e)}$ cohesive stress at the end of the elastic region. After the peak, the traction decreases exponentially

$$S(\delta) = \sigma_c e^{-\xi(\delta - u^{(e)})} \quad \text{and} \quad S'(\delta) = -\sigma_c \xi e^{-\xi(\delta - u^{(e)})} \qquad \text{for } \delta > u^{(e)}$$

Unless a minimum strength is specified, this law extends to infinite deformation. The area under elastic and damage regions is

$$G_c = \frac{\sigma}{2}\left(u^{(e)} + \frac{2}{\xi}\right)$$

The energy dissipation and ratio functions in the only valid region are

$$\varphi(\delta) = \sigma_c(1+\delta\xi)e^{-\xi(\delta-u^{(e)})} \qquad \text{and} \qquad \mathbb{R}(\delta) = \frac{u^{(e)}(1+\delta\xi)e^{-\xi(\delta-u^{(e)})}}{\delta^2}$$

The D damage parameter is related to δ by:

$$D(\delta) = 1 - \frac{u^{(e)}e^{-\xi(\delta-u^{(e)})}}{\delta}$$

This law can only be inverted using inverse functions

$$\delta(D) = D^{-1}(\delta) = \frac{1}{\xi}\text{ProductLog}\left(\frac{\xi u^{(e)}e^{\xi u^{(e)}}}{1-D}\right)$$

6.6.4 Abaqus Exponential Damage Law

Abaqus provides a cohesive zone model based on an effective displacement. It is linear elastic with slope k until failure initiation. Thereafter, the model proposes an evolution of damage parameter D based on unweighted *effective* displacement maximum, δ. By reverse engineering, this model corresponds to a uniaxial strength model of

$$S(\delta) = \sigma_c\frac{e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}} - e^{-\alpha}}{1-e^{-\alpha}} \quad \text{and} \quad S'(\delta) = -\sigma_c\alpha\frac{e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{(1-e^{-\alpha})(u^{(c)}-u^{(e)})}$$

which is basically exponential decay renormalized and shifted to go from σ_c at $u^{(e)}$ to 0 at $u^{(c)}$. The area under elastic and damage regions is

$$G_c = \frac{\sigma_c}{2}\left(u^{(e)} + 2\left(\frac{1}{\alpha} - \frac{e^{-\alpha}}{1-e^{-\alpha}}\right)\left(u^{(c)}-u^{(e)}\right)\right)$$

Note that the α term decays from 1 when $\alpha = 0$ toward zero as α increases. In other words, small α reverts to linear softening (with $G_c = \sigma_c u^{(c)}/2$) and large α is very brittle (and likely unstable with $G_c \approx \sigma_c u^{(e)}/2$). Any finite α is a material with toughness $\sigma_c u^{(e)}/2 \le G_c \le \sigma_c u^{(c)}/2$. The energy dissipation and ratio functions in the only valid region are

$$\varphi(\delta) = \frac{\sigma_c}{1-e^{-\alpha}}\left(e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}} - e^{-\alpha} + \frac{\alpha\delta e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{u^{(c)}-u^{(e)}}\right) \tag{6.41}$$

$$\mathbb{R}(\delta) = \frac{u^{(e)}}{\delta^2(1-e^{-\alpha})}\left(e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}} - e^{-\alpha} + \frac{\alpha\delta e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{u^{(c)}-u^{(e)}}\right) \tag{6.42}$$

The D damage parameter is related to δ by:

$$D(\delta) = 1 - \frac{u^{(e)}}{\delta}\frac{e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}} - e^{-\alpha}}{1-e^{-\alpha}} = 1 - \frac{u^{(e)}}{\delta}\left(1 - \frac{1-e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{1-e^{-\alpha}}\right)$$

The second form is as provided in Abaqus documentation. This law can only be inverted using inverse functions

$$\delta(D) = \frac{u^{(c)} - u^{(e)}}{\alpha} \text{ProductLog}\left(\frac{\alpha g(\alpha)}{u^{(c)} - u^{(e)}} e^{\frac{\alpha((u^{(c)}+g(\alpha))}{u^{(c)}-u^{(e)}}} \right) - g(\alpha)$$

where

$$g(\alpha) = \frac{u^{(e)} e^{-\alpha}}{(1-D)(1-e^{-\alpha})}$$

Again, all these results pass to the limit of linear softening as $\alpha \to 0$ (although limiting results fo $\delta(D)$ is hard to evaluate).

The mixed-mode implementation in Abaqus is only valid (in my mixed mode view) when normal and tangential elastic and critical displacements are equal. In other words, the model requires $\sigma_{nc}/k_n = \sigma_{tc}/k_t$ and $G_{Ic}/\sigma_{nc} = G_{IIc}/\sigma_{tc}$. Because Abaqus does not restrict the modeling to these values, the implementation will not be valid whenever mode mixity changes.

6.6.5 Bilinear Strength Model

A bilinear strength law is linear, with slope k up to peak $\sigma_c = ku^{(e)}$ cohesive stress at the end of the elastic region. After the peak, the traction decreases by piecewise (two pieces) linear decay through σ_2 and $u^{(2)}$. The full functions is

$$S(\delta) = \begin{cases} \frac{\sigma_c(u^{(2)}-\delta)+\sigma_2(\delta-u^{(e)})}{u^{(2)}-u^{(e)}} & u^{(e)} \le \delta \le u^{(2)} \\ \frac{\sigma_2(u^{(c)}-\delta)}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

with derivative

$$S'(\delta) = \begin{cases} -\frac{\sigma_c-\sigma_2}{u^{(2)}-u^{(e)}} & u^{(e)} \le \delta \le u^{(2)} \\ -\frac{\sigma_2}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

The area under elastic and damage regions is

$$G_c = \frac{1}{2}\big(\sigma_c u^{(2)} + \sigma_2(u^{(c)} - u^{(e)})\big)$$

This area can be divided into two mechanisms by dividing the area by a line from the origin to $(u^{(2)}, \sigma_2)$ as

$$G_{1c} = \frac{1}{2}\big(\sigma_c u^{(2)} - \sigma_2 u^{(e)}\big) \quad \text{and} \quad G_{2c} = \frac{1}{2}\sigma_2 u^{(2)}$$

are areas above and below that line The energy dissipation function is:

$$\varphi(\delta) = \begin{cases} \frac{\sigma_c u^{(2)}-\sigma_2 u^{(e)}}{u^{(2)}-u^{(e)}} & u^{(e)} \le \delta \le u^{(2)} \\ \frac{\sigma_2 u^{(c)}}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

Its integral during damage evolution is:

$$\int_{u^{(e)}}^{\delta} \frac{1}{2}\varphi(\delta)d\delta = \begin{cases} G_{1c}\frac{\delta-u^{(e)}}{u^{(2)}-u^{(e)}} & u^{(e)} \le \delta \le u^{(2)} \\ G_{1c} + G_{2c}\frac{\delta-u^{(2)}}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

The D to δ ratio function is

$$\mathbb{R}(\delta) = \begin{cases} \frac{\sigma_c u^{(2)}-\sigma_2 u^{(e)}}{k\delta^2(u^{(2)}-u^{(e)})} & u^{(e)} \le \delta \le u^{(2)} \\ \frac{\sigma_2 u^{(c)}}{k\delta^2(u^{(c)}-u^{(2)})} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

In dimensionless form:

$$\varphi(\delta) = \begin{cases} \sigma_c \frac{\overline{u}^{(2)} - \frac{\sigma_2}{\sigma_c}\overline{u}_p}{\overline{u}^{(2)} - \overline{u}_p} & \overline{u}_p \le \xi \le \overline{u}^{(2)} \\ \frac{\sigma_2}{1-\overline{u}^{(2)}} & \overline{u}^{(2)} \le \xi \le 1 \end{cases} \qquad \mathbb{R}(\delta)u^{(c)} = \begin{cases} \frac{\overline{u}_p\left(\overline{u}^{(2)} - \frac{\sigma_2}{\sigma_c}\overline{u}_p\right)}{\xi^2(\overline{u}^{(2)} - \overline{u}_p)} & \overline{u}_p \le \xi \le \overline{u}^{(2)} \\ \frac{\sigma_2}{\sigma_c}\frac{\overline{u}_p}{\xi^2(1-\overline{u}^{(2)})} & \overline{u}^{(2)} \le \xi \le 1 \end{cases}$$

The D damage parameter is related to δ by:

$$D = \begin{cases} 1 - \frac{u^{(e)}}{\sigma_c \delta}\left(\sigma_2 + \frac{(\sigma_c - \sigma_2)(u^{(2)} - \delta)}{u^{(2)} - u^{(e)}}\right) & u^{(e)} \le \delta \le u^{(2)} \\ 1 - \frac{u^{(e)}}{\sigma_c \delta}\left(\frac{\sigma_2(u^{(c)} - \delta)}{u^{(c)} - u^{(2)}}\right) & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

At the junction of the two pieces where $\delta = u^{(2)}$, $D = 1 - \sigma_2 u^{(e)}/(\sigma_c u^{(2)})$. Each region can be invert to a piecewise non-linear function

$$\delta(D) = D^{-1}(\delta) = \begin{cases} \frac{u^{(e)}(\sigma_c u^{(2)} - \sigma_2 u^{(e)})}{\sigma_c(1-D)u^{(2)} + u^{(e)}(D\sigma_c - \sigma_2)} & 0 \le D \le 1 - \frac{\sigma_2 u^{(e)}}{\sigma_c u^{(2)}} \\ \frac{u^{(e)}u^{(c)}\sigma_2}{\sigma_c(1-D)(u^{(c)} - u^{(2)}) + u^{(e)}\sigma_2} & 1 - \frac{\sigma_2 u^{(e)}}{\sigma_c u^{(2)}} \le D \le 1 \end{cases}$$

At the junction of the two pieces, $\delta = u^{(2)}$.

6.7 Numerical Implementation

In `NairnMPM`, cohesive zones are implement by adding that to explicit crack surfaces. They can be created at the beginning, or a propagating cracks can dynamically insert a cohesive zone each to the crack tip propagates. This sections describes task handle by `TractionLaw` material types.

- `CrackTractionLaw(*cs,`$u_n, u_t, \hat{\boldsymbol{n}}, \hat{\boldsymbol{t}}, A$`)`

  This methods is called once each time step for each crack segment (`*cs`) with a traction law. It is called from `CrackSegment::UpdateTractions()` which is called from `CrackHeader::UpdateCrackTractions()`, which is called in the `MoveCracksTask` task near the end of each time step. The inputs to `CrackTractionLaw()` are the normal (u_n) and tangential (u_t) opening displacements (if the traction law needs du_n and du_t, it will need to track them in history variables for that crack segment), unit vectors in the normal ($\hat{\boldsymbol{n}}$) and tangential ($\hat{\boldsymbol{t}}$) directions, and area (A) associated with the crack segment. This method should calculate the current normal (T_n) and tangential tractions (T_t) and return a force vector due to the cohesive zone using:

$$\boldsymbol{F} = -A\left(T_n\hat{\boldsymbol{n}} + T_t\hat{\boldsymbol{t}}\right)$$

- `CrackWorkEnergy(*cs,`u_n, u_t`)`

  This methods is only called for J integral calculations and then is called as needed for crack segments (`*cs`) involved in the J contour. It should calculate and return total work required to load cohesive zone up to current COD.

$$W = \int \boldsymbol{T}(\boldsymbol{u}) \cdot d\boldsymbol{u}$$

  This calculations is area under the strength model plus any initial crack loading. It might only be correct for J integral during monotonic loading. It is clear, however, that just getting current strain energy in the zone does not give useful reults.

- `CrackDissipatedEnergy(*cs,GI,GII)`

  This method calculates to total amount of energy that has been dissipated by the cohesive zone. It is only called in J-integral calculations and is output during crack propagation. It has no affect on J integral or any other calculations. In 1D (or decoupled traction laws), it can be found from:

$$\Omega = \int_{\delta^{(e)}}^{\delta} \frac{1}{2}\varphi(\delta)d\delta$$

  Mixed-mode traction laws should track increments in G_I and G_{II} and return their sum when called

6.8 Triangular Traction Law

This traction law implements a decoupled cohesive zone where both normal and tangential laws use a Linear Sawtooth Strength Model. The crack segments track δ_n and δ_t in history variables 1 and 2. When finding tractions, the effective stiffness (for n or t directions) is

$$k_{eff} = \begin{cases} \frac{\sigma_c}{u^{(e)}} & \delta \le u^{(e)} \\ \frac{S(\delta)}{\delta} = \frac{\sigma_c}{\delta}\frac{u^{(c)}-\delta}{u^{(c)}-u^{(e)}} & \text{otherwise} \end{cases}$$

and the traction is $T = k_{eff}u$. The strain energy and work energy of each component is found from

$$U = \frac{1}{2}k_{eff}u \quad \text{and} \quad W = \frac{\sigma_c}{2}\frac{u(u^{(c)}-u)+u^{(c)}(u-u^{(e)})}{u^{(c)}-u^{(e)}}$$

but in elastic regime, they are $U = W = ku/2$. The cumulative dissipated energy is

$$\Omega = W(\delta) - \frac{1}{2}\delta S(\delta) = \frac{\sigma_c u^{(c)}(\delta - u^{(e)})}{2(u^{(c)}-u^{(e)})}$$

Failure is predicted by mixed mode failure law based on G_I and G_{II} (from Ω for each mode) and then using

$$\left(\frac{G_I}{G_{Ic}}\right)^{\texttt{nmix}} + \left(\frac{G_{II}}{G_{IIc}}\right)^{\texttt{nmix}} = 1$$

All equations above would work be $u^{(e)} = 0$ that corresponds to infinite initial stiffness, $k \to \infty$. The implementation in this case, however, would then treat any opening displacement as causing damage (*i.e.*, no amount of initial loading would be elastic). This situation could be resolved by implementing a pre-damage phase where crack is modeled as in perfect contact until traction reaches the peak stress. This approach would be like damage mechanics and opening would evolve by properties of the underlying material. Because this option is not implemented, the model prohibits use of infinite initial stiffness.

6.9 Exponential Traction Law

This traction law implements a decoupled cohesive zone where both normal and tangential laws use a Abaqus Exponential Damage Law. The crack segments track δ_n and δ_t in history variables 1 and 2. When finding tractions, the effective stiffness (for n or t directions) is

$$k_{eff} = \frac{S(\delta)}{\delta} = \frac{\sigma_c}{\delta}\frac{e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}} - e^{-\alpha}}{1-e^{-\alpha}}$$

and the traction is $T = k_{eff}u$. The strain energy and work energy of each component is found from

$$U = \frac{1}{2}k_{eff}u \quad \text{and} \quad W = \frac{\sigma_c}{2}\left(u^{(e)} + 2\left(\frac{(u^{(c)}-u^{(e)})}{\alpha}\frac{1-e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{1-e^{-\alpha}} - \left(u-u^{(e)}\right)\frac{e^{-\alpha}}{1-e^{-\alpha}}\right)\right)$$

but in elastic regime, they are $U = W = ku/2$. The cumulative dissipated energy is

$$\Omega = \frac{\sigma_c}{2}\left(u^{(e)} + \frac{2(u^{(c)}-u^{(e)})}{\alpha}\frac{1-e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}}{1-e^{-\alpha}} - \frac{\delta\left(e^{-\alpha}+e^{-\frac{\alpha(\delta-u^{(e)})}{u^{(c)}-u^{(e)}}}\right)-2u^{(e)}e^{-\alpha}}{1-e^{-\alpha}}\right)$$

which reaches G_c and $\delta = u^{(c)}$.

Failure is predicted by mixed mode failure law based on G_I and G_{II} (from Ω for each mode) and then using

$$\left(\frac{G_I}{G_{Ic}}\right)^{\texttt{nmix}} + \left(\frac{G_{II}}{G_{IIc}}\right)^{\texttt{nmix}} = 1$$

All equations above would work be $u^{(e)} = 0$ and infinite initial stiffness, but as for Triangular Traction Law, this model prohibits use of infinite initial stiffness.

6.10 Linear Traction Law

This traction law increases linearly with displacement and slope k. The normal and tangential directions are decoupled and the zone never fails. The tractions and strain energy (for each direction) are:

$$T = ku \quad \text{and} \quad U = \frac{1}{2}ku^2$$

Because it is linear and never fails, this law dissipates no energy (and tracks no damage history variables).

6.11 Cubic Traction Law

This traction law implements a decoupled cohesive zone where both normal and tangential laws use a Generalized Cubic Strength Law with $u^{(e)} = 0$, $\sigma_0 = 0$, and $k_c = 27\sigma_c/(4u^{(c)})$ leading to:

$$S(\delta) = \frac{27}{4}\sigma_c\frac{\delta}{u^{(c)}}\left(1-\frac{\delta}{u^{(c)}}\right)^2$$

The crack segments track δ_n and δ_t in history variables 1 and 2. Because this law has no initial elastic region, the tractions (for each direction) are give by

$$T = \frac{S(\delta)}{\delta}u = k_{eff}u \quad \text{where} \quad k_{eff} = \frac{27\sigma_c}{4\left(u^{(c)}\right)^3}\left(u^{(c)}-\delta\right)^2$$

The strain energy is

$$U = \frac{1}{2}k_{eff}u^2$$

for each direction. The work energy up to displacement u is:

$$W = G_c \left(\frac{u}{u^{(c)}}\right)^2 \left(6 - 8\frac{u}{u^{(c)}} + 3\left(\frac{u}{u^{(c)}}\right)^2\right)$$

The cumulative dissipated energy for each component is

$$\Omega = \int_{\delta^{(e)}}^{\delta} \frac{27\sigma_c}{4\left(u^{(c)}\right)^3}\delta^2\left(u^{(c)} - \delta\right) = G_c\left(4 - 3\frac{\delta}{u^{(c)}}\right)\left(\frac{\delta}{u^{(c)}}\right)^3 \quad \text{where} \quad G_c = \frac{9\sigma_c u^{(c)}}{16}$$

Failure is predicted by mixed mode failure law based on G_I and G_{II} (from Ω for each mode) and then using

$$\left(\frac{G_I}{G_{Ic}}\right)^{\texttt{nmix}} + \left(\frac{G_{II}}{G_{IIc}}\right)^{\texttt{nmix}} = 1$$

6.12 Pressure Traction Law

This traction law is not an elastic/damage model. Instead, it applies constant stress, σ, to the crack surfaces whenever the crack is opened. Is main use is when the stress in negative and it then models injecting a pressurized fluid into a crack. By default, the stress is applied whenever $u_n > 0$, but a parameter lets that change to requiring some opening. The total force on the crack is thus zero for $u_n < u_n^{(min)}$ but changes to $F_n = -\sigma A\hat{\boldsymbol{n}}$ when $u_n > u_n^{(min)}$. The strain energy for J integral calculations is

$$U = \max\left(0, \sigma(u_n - u_n^{(min)})\right)$$

When unloaded, the stress does not return to the origin, but rather returns along the constant stress loading law. The dissipated energy is always zero.

Note that this law could be converted to Dugdale's initial rigid-plastic law by setting σ to a positive yield stress, $u_n^{(min)} = 0$, the strain energy to zero, and the dissipated energy to σu_n. In other words, the loading traction is constant, but unloading returns vertically to zero. This option may be added in the future.

6.13 Trilinear Traction Law

This traction law implements a decoupled cohesive zone where both normal and tangential laws use a Bilinear Strength Model. The crack segments track δ_n and δ_t in history variables 1 and 2. When finding tractions, the effective stiffness (for n or t directions) is

$$k_{eff} = \begin{cases} \frac{\sigma_c}{u^{(e)}} & \delta \le u^{(e)} \\ \frac{\sigma_c(u^{(2)} - \delta) + \sigma_2(\delta - u^{(e)})}{\delta(u^{(2)} - u^{(e)})} & u^{(e)} < \delta \le u^{(2)} \\ \frac{\sigma_2(u^{(c)} - \delta)}{\delta(u^{(c)} - u^{(2)})} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

Note that this equation works even when $u^{(2)} - u^{(e)}$, which corresponds to sudden change in traction from σ_c to σ^2 at $u^{(e)}$. For this special case, the second from of k_{eff} is never used and therefore the zero in denominator does not cause a problem. As explained for the Triangular Traction Law, this law does not allow the initial stiffness to be infinite. Note that initial stifness can be zero fo $\sigma_c = 0$, but not clear if this option corresponds to any realistic cohesive zone.

The work energy of each component is found from

$$W = \begin{cases} \frac{1}{2}ku^2 & u \le u^{(e)} \\ \frac{1}{2}\left(\sigma_c u + \sigma_u(u-u^{(e)})\right) & u^{(e)} < \delta \le u^{(2)} \\ \frac{1}{2}\left(\sigma_c u^{(2)} + \sigma_2(u-u^{(e)}) + \sigma_u(u-u^{(2)})\right) & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

where σ_u is strength for u or:

$$\sigma_u = \begin{cases} \frac{\sigma_2(u-u^{(e)})+\sigma_c(u^{(2)}-u)}{u^{(2)}-u^{(e)}} & u^{(e)} < \delta \le u^{(2)} \\ \frac{\sigma_2(u^{(c)}-u)}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

The cumulative dissipated energy is

$$\Omega = \begin{cases} G_{1c}\frac{\delta-u^{(e)}}{u^{(2)}-u^{(e)}} & u^{(e)} \le \delta \le u^{(2)} \\ G_{1c} + G_{2c}\frac{\delta-u^{(2)}}{u^{(c)}-u^{(2)}} & u^{(2)} \le \delta \le u^{(c)} \end{cases}$$

Failure is predicted by mixed mode failure law based on G_I and G_{II} (from Ω for each mode) and then using

$$\left(\frac{G_I}{G_{Ic}}\right)^{\texttt{nmix}} + \left(\frac{G_{II}}{G_{IIc}}\right)^{\texttt{nmix}} = 1$$

6.14 Coupled Triangular Traction Law

This traction law is implementation of model proposed by Höberg ("Mixed-Mode Cohesive Law," 2006), but that model has some inconsistencies — some are corrected; others are left in place. As a result, this model should only be used under specific property settings or to compare to other models. This model assumes both normal and shear tractions follow a Linear Sawtooth Strength Model, but unlike the Triangular Traction Law, the two directions are coupled such that normal and shear tractions both decay to zero at failure.

The numerical algorithm used to implement the Höberg model as closely as possible (and correcting some issues)is as follows:

1. *Initialization*: we define 6 history variables for $h[0] = -1$ (to indicate damage not yet initiated), $h[1]$ and $h[2]$ for mode I and II energy released (incremented during damage evolution), $h[3]$ for total work (incremented all time steps), and $h[4]$ and $h[5]$ to store normal and tangential crack opening displacement (needed to find their increments in each time step, which is needed for work increment $\boldsymbol{T} \cdot d\boldsymbol{u}$).

2. *Mixed-Mode Loading*: during the analysis, the current deformation state is characterized by

$$\tan\theta_h = \frac{u_n u_t^{(c)}}{u_t u_n^{(c)}} = \frac{\overline{u}_n}{\overline{u}_t} \quad \Longrightarrow \quad \frac{u_n}{u_n^{(c)}} = \overline{u}_n = \lambda \sin\theta_h \quad \text{and} \quad \frac{u_t}{u_t^{(c)}} = \overline{u}_t = \lambda\cos\theta_h$$

   where $\boldsymbol{u} = (u_n, u_t)$ is the crack-opening displacement vector and the Höberg model defines an *effective* displacement as

$$\lambda = \sqrt{\overline{u}_n^2 + \overline{u}_t^2} = \sqrt{\left(\frac{u_n}{u_n^{(c)}}\right)^2 + \left(\frac{u_t}{u_t^{(c)}}\right)^2}$$

3. *Deformation up to Damage Initiation*: prior to initiation of damage ($h[0] < 0$), the tractions are linear elastic. Usual decoupling of normal and tangential loads would suggest $T_n = k_n u_n$ and $T_t = k_t u_t$, but Höberg revises elastic loading such that:

$$(T_n, T_t) = \frac{1}{\lambda_p(\theta)}(k_n \overline{u}_{np} u_n, k_t \overline{u}_{tp} u_t) = \frac{1}{\lambda_p(\theta)}(\sigma_c \overline{u}_n, \tau_c \overline{u}_t)$$

where $\lambda_p(\theta)$ is the value of λ at which damage initiates and $\overline{u}_{ip} = u_i^{(e)}/u_i^{(c)}$ (ratio of displacement at the peak to the critical displacement). Assuming an elliptical failure criterion, pre-damage loading ends when

$$\left(\frac{u_n}{u_n^{(e)}}\right)^2 + \left(\frac{u_t}{u_t^{(e)}}\right)^2 = \lambda\sqrt{\frac{\sin^2\theta_h}{\overline{u}_{np}^2} + \frac{\cos^2\theta_h}{\overline{u}_{tp}^2}} = 1$$

which occurs when λ first reaches:

$$\lambda \to \lambda_p(\theta) = \frac{1}{\sqrt{\frac{\sin^2\theta_h}{\overline{u}_{np}^2} + \frac{\cos^2\theta_h}{\overline{u}_{tp}^2}}} \tag{6.43}$$

Once initiation occurs, a damage variable, λ_ω is set equal to $\lambda_p(\theta)$ and the completion of this time step (as well as all subsequent times steps) uses the post-initiation methods. Prior to damage initiation, this phases uses the Högberg tractions above. Note that these tractions have a stiffness that depends on θ and therefore is not describing linear elastic deformation. The associated energy errors are ignored. The go away if and only if $\overline{u}_{np} = \overline{u}_{tp}$.

4. *After Damage Initiation*: the analysis begins by finding θ, λ, and $\lambda_p(\theta)$. If $\lambda \le \lambda_\omega$, this step is elastic, but if $\lambda > \lambda_\omega$, this step evolves the damage state:

   - *Elastic Unloading*: The tractions assume elastic unloading from the current damage state resulting in:

$$\begin{aligned}(T_n, T_t) &= \min\left(\frac{1-\lambda_\omega}{\lambda_\omega\big(1-\lambda_p(\theta)\big)}, \frac{1}{\lambda_p(\theta)}\right)\big(k_n \overline{u}_{np} u_n, k_t \overline{u}_{tp} u_t\big) \\ &= \frac{\min(1-\omega, 1)}{\lambda_p(\theta)}(\sigma_c \overline{u}_n, \tau_c \overline{u}_t)\end{aligned}$$

   where

$$\omega = 1 - \frac{(1-\lambda_\omega)\lambda_p(\theta)}{\lambda_\omega\big(1-\lambda_p(\theta)\big)}$$

   is an alternate damage parameter (it is defined in Höberg, but because it depends on θ it is not a damage state variable). These tractions match Höberg provided $\lambda_\omega > \lambda_p(\theta)$. The min() function is needed to guarantee that the stiffness does not exceed the stiffness of the undamaged material (and implements a correction not mentioned in Höberg). The problem with the Höberg approach is that changes in mode mixity will cause non-physical changes in elastic stiffness and could result in $\lambda_\omega < \lambda_p(\theta)$ (causing the excessive stiffness error). As a result, whenever θ changes during a simulation, the elastic unloading and reloading steps may gain or lose energy. In this implementation, such erroneous energy changes are ignored. In other words, the model is implemented as stated, but energy during elastic loading is not properly modeled. These errors go away if and only if $\overline{u}_{np} = \overline{u}_{tp}$.

- *Damage Evolution*: For damage evolution, λ_ω evolves to $\lambda_\omega = \min(\lambda, 1)$ (*i.e.*, $\lambda_\omega = \max(\lambda)$ with failure occurring when it reaches 1. For this time step, $d\lambda_\omega = \lambda_\omega - \lambda_\omega^{(0)}$ or increment from prior value of λ_ω). The tractions are set to the same values used for elastic loading based on the updated value for λ_ω. The mode I and mode II energy increments are given by

$$dG_I = \frac{G_{Ic} u_n^2}{{u_n^{(c)}}^2 \lambda_\omega^2 \big(1-\lambda_p(\theta)\big)} d\lambda_\omega \qquad \text{and} \qquad \frac{G_{IIc} u_t^2}{{u_t^{(c)}}^2 \lambda_\omega^2 \big(1-\lambda_p(\theta)\big)} d\lambda_\omega$$

  or using Höberg θ_h:

$$dG_I = \frac{G_{Ic} \sin^2\theta_h}{1-\lambda_p(\theta)} d\lambda_\omega \qquad \text{and} \qquad \frac{G_{IIc} \cos^2\theta_h}{1-\lambda_p(\theta)} d\lambda_\omega$$

  For pure mode loading, these both integrate to $G_I = G_{Ic}$ and $G_{II} = G_{IIc}$. The cohesive zone fails when λ_ω reaches 1 and the prior tracked G_I and G_{II} are output to define the mixed mode energy released at failure. Note that these incremental energy release rates differ from Högberg because he misinterprets area under is traction law as an energy release rate. The full area does equal energy released by final failure, but the energy release up to current λ_ω must subtract off remaining elastic energy (which he did not do). This implementation finds the correct incremental energy release rates.

The Höberg model is not always valid and should be avoided except under conditions were it is valid or for comparison to other models. The thermodynamic problem is that neither ω nor λ_ω are damage state variables. For example, when θ varies, the stiffness during elastic unloading is not constant, because it depends on $\lambda_p(\theta)$. When stiffness changes, the elastic unloading and reloading may gain or lose energy, and that does not correspond to the physical model of an elastic material with damage.

Under two situations, the Höberg model does provide valid mixed mode loading — uniform loading at constant θ or for materials in which $\lambda_p(\theta)$ is independent of θ. The first is not interesting, because it limits use of this model to trivial problems such as analysis of constant-mode, mixed-mode fracture tests (note that all validation examples given in Höberg were for constant θ loading). Even in such simulations, different parts of the cohesive zone may see different θ values. A cohesive zone for modeling general mixed-mode failure must be able to handle variable θ. For the second valid conditions, the second form of $\lambda_p(\theta)$ in Eq. (6.43) shows that it will be independent of θ if $\overline{u}_{np} = \overline{u}_{tp}$ and this special case corresponds to

$$\lambda_p(\theta) = \overline{u}_{np}$$

Although Höberg claims it can handle different normal and shear traction laws, for his approach to be valid, the ratio of elastic deformation to total deformation in normal and shear traction laws must be the same. In this special case, we can define a valid damage parameter, D, by

$$D = 1 - \frac{1-\lambda_\omega}{\lambda_\omega} \frac{\overline{u}_{np}}{1-\overline{u}_{np}}$$

and the tractions are always given by

$$(T_n, T_t) = (1-D)(k_n u_u, k_t u_t)$$

This damage parameter is a damage state variable and is independent of changes in mode mixity during the simulation. By initialized with $\lambda_\omega = \overline{u}_{np}$ (*i.e.*, $D = 0$), this traction applies before and after damage

initiation and during elastic loading and unloading and damage evolution. No damage is evolved during elastic phases, while energy dissipation during damage evolution becomes:

$$dG_I = \frac{1}{2}k_n u_n^2 dD = \frac{1}{2}\frac{k_n u_n^2 \overline{u}_{np}}{\lambda_\omega^2(1-\overline{u}_{np})}d\lambda_\omega = \frac{G_{Ic}u_n^2}{{u_n^{(c)}}^2\lambda_\omega^2(1-\overline{u}_{np})}d\lambda_\omega$$

where $G_{Ic} = (1/2)k_n u_n^{(e)} u_n^{(c)}$. An analogous results holds for mode II. In brief, a Höberg analysis is identical to 1D damage modeling. It does not correctly extend that modeling to mixed-mode loading, unless $\overline{u}_{np} = \overline{u}_{tp}$. The normal and tangential peak stresses and initial stiffnesses can vary, but the ratios of peak displacement to critical displacement must be the same.

6.14.1 Högberg in Mixed Mode Simulations

If θ_h is kept constant during a simulations (for example to initiation debonding), integrations λ_ω from $\lambda_p(\theta)$ to 1 results is

$$\frac{G_I}{G_{Ic}} + \frac{G_{II}}{G_{IIc}} = 1$$

In other words, the mixed-mode-failure envelope is always linear. This result is correct when $\overline{u}_{np} = \overline{u}_{tp}$, but a consequence of the model errors for other conditions.

If we preload in mode I from $\lambda_p(\pi/2)$ to $\lambda = \lambda_\omega$ and then reload in pure mode II from λ_ω to 1, the total energies released are

$$\frac{G_I}{G_{Ic}} = \frac{\lambda_\omega - \lambda_p(\pi/2)}{1-\lambda_p(\pi/2)} = \frac{\lambda_\omega - \overline{u}_{np}}{1-\overline{u}_{np}} \quad \text{and} \quad \frac{G_{II}}{G_{IIc}} = \frac{1-\lambda_\omega}{1-\lambda_p(0)} = \frac{1-\lambda_\omega}{1-\overline{u}_{tp}}$$

Eliminating λ_ω, the mixed mode failure envelop in this test becomes

$$\frac{G_{II}}{G_{IIc}} = \frac{1-\overline{u}_{np}}{1-\overline{u}_{tp}}\left(1-\frac{G_I}{G_{Ic}}\right)$$

The result for preload in mode II followed by reload in mode I is found by interchanging n and t and I nd II. Note that this equation assumes $\lambda_\omega > 0$. For $\lambda_\omega = 0$ (*i.e.*, the preload causes no damage), the result is trivially $G_{II} = G_{IIc}$.

6.15 Mixed-Mode Traction Law

This traction law implements the Nairn model for coupled, mixed-mode traction laws in cohesive zone modeling. In brief, this law postulates a normal strength model, $S_n(\delta_n)$, and a tangential strength model, $S_t(\delta_t)$ where δ_n and δ_t are two damage parameters. They are interrelated by a single damage parameter D that causes the coupling. The cohesive zone fails when $D \to 1$, $\delta_n \to u_n^{(c)}$, and $\delta_t \to u_t^{(c)}$, which all happen simultaneously. The critical displacements in the strength models correspond to the strength dropping to zero or $S_n(u_n^{(c)}) = S_t(u_t^{(c)}) = 0$. Details on this model are in the Mixed-Mode Cohesive Zone Modeling section.

The numerical implementation is as follows:

1. *Initialization*: the modeling is initialized with $D = 0$, $\delta_n = u_n^{(e)}$, and $\delta_t = u_t^{(e)}$ and defines eight history variables: $h[0] = D$, $h[1] = \delta_n$, $h[2] = \delta_t$, $h[3]$ and $h[4]$ for mode I and II energy released (incremented during damage evolution), $h[5]$ for total work (incremented all time steps), and $h[6]$ and $h[7]$ to store normal and tangential crack opening displacement (needed to find their increments in each time step.

2. *Mixed-Mode Loading*: during the analysis, the current deformation state is characterized by

$$\tan\theta = \frac{u_n}{u_t} \quad \Longrightarrow \quad u_n = \|\boldsymbol{u}\|\sin\theta \quad \text{and} \quad u_t = \|\boldsymbol{u}\|\cos\theta$$

where $\boldsymbol{u} = (u_n, u_t)$ is the crack-opening displacement vector.

3. *Trial Update*: for displacement increments du_n and du_t, the initial and trial traction vectors are found from

$$\boldsymbol{T}_0 = (1-D)(k_t u_t, k_n u_n) \quad \text{and} \quad \boldsymbol{T}^{(trial)} = (1-D)(k_t(u_t + du_t), k_n(u_n + du_n))$$

Find elliptical failure condition

$$t = \left(\frac{T_n^{(trial)}}{S_n(\delta_n)}\right)^2 + \left(\frac{T_t^{(trial)}}{S_t(\delta_n)}\right)^2$$

If $t \leq 1$, the deformation is elastic — the trial tractions are accepted and no changes are made to D, δ_n, or δ_t and no energy is dissipated and the step is done, but work increment is calculated using midpoint rule:

$$dW = \frac{1}{2}\left((T_{n,0} + T_n^{(trial)})du_n + (T_{t,0} + T_t^{(trial)})du_t\right)$$

4. *Partition Increment*: when not elastic, first task is to partition the step into elastic deformation and damage evolution by moving to ellipse along the current traction vector by increment $d\boldsymbol{T}_0 = \phi\hat{\boldsymbol{T}}_0\|\boldsymbol{T}_0\|$ until reaching the failure surface via:

$$(1+\phi)^2\|\boldsymbol{T}_0\|^2\left[\left(\frac{\hat{T}_{n,0}}{S_n(\delta_n)}\right)^2 + \left(\frac{\hat{T}_{t,0}}{S_t(\delta_n)}\right)^2\right] = 1 \implies \phi\|\boldsymbol{T}_0\| = \frac{1}{\sqrt{\left(\frac{\hat{T}_{n,0}}{S_n(\delta_n)}\right)^2 + \left(\frac{\hat{T}_{t,0}}{S_t(\delta_n)}\right)^2}} - \|\boldsymbol{T}_0\|$$

The total displacement increment is then be partitioned into elastic and damage evolution increments defined by

$$d\boldsymbol{u}^{(e)} = (du_n^{(e)}, du_t^{(e)}) = \frac{\phi\|\boldsymbol{T}_0\|}{1-D}\left(\frac{\hat{T}_{n,0}}{k_n}, \frac{\hat{T}_{t,0}}{k_t}\right) \quad \text{and} \quad d\boldsymbol{u}^{(d)} = d\boldsymbol{u} - d\boldsymbol{u}^{(e)}$$

The elastic increment contributes to work

$$dW = \left(1 + \frac{\phi}{2}\right)(T_{n,0}du_n^{(e)} + T_{t,0}du_t^{(e)})$$

The damage increment with new initial tractions and then input to the damage evolution step.

5. *Damage Evolution*: when $u_n > 0$, damage evolves and energy is dissipated. The updates for the three damage parameters are interrelated. For maximum stability, it is best to use an explicit update on the parameter than has the smallest proportional change. The algorithm is:

   - If $\max\left(\mathbb{R}_n u_n^{(c)}, \mathbb{R}_t u_t^{(c)}\right) < 1$, then update D.
   - else if $\mathbb{R}_n u_n^{(c)} > \mathbb{R}_t u_t^{(c)}$, then update δ_n

- else update δ_t

The update equations are given in the Selection of the Best Method section. After updating one damage variable, calculate the other two. Calculation of δ from D may require numerical methods, but analytical equations are available for Linear Sawtooth Strength Model, Needleman form of Generalized Cubic Strength Law, and Bilinear Strength Model.

6. *Compression Damage Evolution*: when $u_n \leq 0$ the cohesive zone is in compression, $u_n = du_n = 0$. The step partitioning simplifies to:

$$|du_t^{(e)}| = \frac{S_t - |T_{t,0}|}{k_t(1-D)} \qquad du_t^{(d)} = du_t - \text{sign}(T_{t,0})|du_t^{(e)}|$$

and this calculations allows for damage at positive or negative $T_{t,0}$. The update simplifies to

$$d\delta_t = |du_t^{(d)}|$$

Once this update if found, calculate D and δ_n that continue to be coupled into the damage process. Note this this MPM modeling treats compression as a contact problem and not as normal stress with stiffness equal to the tensile stiffness.

7. *Evolved Tractions and Energy Dissipation*: after updating the damage parameters, the tractions are found using the new fracture surface properties. Increments in mode I and mode II energies by midpoint rule using $\boldsymbol{u}$ and $\boldsymbol{\delta}$ at the start of the time step:

$$dG_I = \frac{1}{4}\left[\left(\frac{u_n}{\delta_n}\right)^2 \varphi_n(\delta_n) + \left(\frac{u_n + du_n}{\delta_n + d\delta_n}\right)^2 \varphi_n(\delta_n + d\delta_n)\right] d\delta_n$$
$$dG_{II} = \frac{1}{4}\left[\left(\frac{u_t}{\delta_t}\right)^2 \varphi_t(\delta_t) + \left(\frac{u_t + du_t}{\delta_t + d\delta_t}\right)^2 \varphi_t(\delta_t + d\delta_t)\right] d\delta_t$$

Note that in compression evolution only mode II energy is released.

Chapter 7

Poroelasticity Materials

7.1 Introduction

As pointed out by Rice (1973), poroelasticity is equivalent to thermal elasticity where some constants defined by Biot (1941) replace thermal expansion coefficient, heat capacity, and thermal conductivity and the isoentropic heating term is replaced by a pore pressure coupling term. Although poroelasticy calculations can be done using this analogy, it would preclude doing simulations where both pore pressure and temperature vary.

An better alternative is to use diffusion code for poroelasticity and then poroelasticy could be done along with thermal calculations. Again, an analogy with diffusion equation means poroelasticity can be modeled by having Biot constants replace moisture expansion coefficient and diffusion tensor. The standard diffusion code, however, does not have a term to couple concentration to volume changes (maybe it should). To run poroelasticity with diffusion, each material type will need to account for change in pore pressure caused by global volume change. In analogy to isoentropic temperature change, this coupling term could be called isofluid-content pressure change. In poroelasticity theory, an increment that occurs without a change in fluid content is referred to an "undrained" increment. Modeling of poroelasticity therefore needs a coupling term in material constitutive laws to find undrained pressure change (dp_{ud}). This chapter describes Biot poroelasticty theory and how it can be implemented in any material that supports diffusion and adds a required undrained pressure change term.

7.2 Biot Poroelasticity Theory

Generalizing Biot (1941) poroelasticity theory to anisotropic materials, the strain and water increment, θ, are given by:

$$\boldsymbol{\varepsilon} = \mathsf{S}\boldsymbol{\sigma} + \boldsymbol{h}dp \tag{7.1}$$

$$\theta = \boldsymbol{h}\cdot\boldsymbol{\sigma} + \frac{dp}{R} \tag{7.2}$$

where S is compliance tensor, dp is increment in pore pressure, R is property defined by Biot (with units of stress), $\boldsymbol{h}$ is tensor of Biot constants (when generalized to anisotropic). The water volume and pressure increments over compared to some reference state:

$$\theta = dv = v - v_0 \qquad \text{and} \qquad dp = p - p_0 \tag{7.3}$$

When $v = v_0$ and $p = p_0$, total stress is zero: $\boldsymbol{\sigma} = 0$. For an orthotropic material in material axes:

$$\boldsymbol{h} = \left(\frac{1}{3H_x}, \frac{1}{3H_y}, \frac{1}{3H_z}, 0, 0, 0 \right) \tag{7.4}$$

where H_i have units of stress. Biot started with $\boldsymbol{h}$ in θ expression being a different property ($\boldsymbol{h}'$) but then showed by work arguments that $\boldsymbol{h}' = \boldsymbol{h}$. His proof extends to each anisotropic property as well (*i.e.*, the components of $\boldsymbol{h}$).

Inverting these equations

$$\boldsymbol{\sigma} = \mathsf{C}(\boldsymbol{\varepsilon} - \boldsymbol{h}dp) = \mathsf{C}\boldsymbol{\varepsilon} - \boldsymbol{\alpha}dp \tag{7.5}$$

$$\theta = \boldsymbol{h} \cdot (\mathsf{C}\boldsymbol{\varepsilon} - \boldsymbol{\alpha}dp) + \frac{dp}{R} = \boldsymbol{\alpha} \cdot \varepsilon + \frac{dp}{Q} \tag{7.6}$$

where

$$\boldsymbol{\alpha} = \mathsf{C}\boldsymbol{h} \text{ (or } \boldsymbol{h} = \mathsf{S}\boldsymbol{\alpha}) \qquad \text{and} \qquad \frac{1}{Q} = \frac{1}{R} - \boldsymbol{h} \cdot \boldsymbol{\alpha} \tag{7.7}$$

$\boldsymbol{\alpha}$ is a dimensionless tensor, often called the "Biot coefficient," and Q (also from Biot) is property with units of stress.

We consider two limiting cases. First, imagine "undrained" loading such that water volume does not change or that $\theta = 0$. In this loading, the pore pressure increment will be $dp = -R\boldsymbol{h} \cdot \Delta\boldsymbol{\sigma} = -Q\boldsymbol{\alpha} \cdot \varepsilon$. The change in strain becomes:

$$\Delta\boldsymbol{\varepsilon} = \mathsf{S}\Delta\sigma - \boldsymbol{h}R\boldsymbol{h} \cdot \Delta\sigma \tag{7.8}$$

The change in normal strains become

$$\begin{pmatrix} \Delta\varepsilon_{xx} \\ \Delta\varepsilon_{yy} \\ \Delta\varepsilon_{zz} \end{pmatrix} = \begin{pmatrix} \frac{\Delta\sigma_{xx} - \nu_{xy}\Delta\sigma_{yy} - \nu_{xz}\Delta\sigma_{zz}}{E_{xx}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_x} \\ \frac{\nu_{yx}\Delta\sigma_{xx} + \Delta\sigma_{yy} - \nu_{yz}\Delta\sigma_{zz}}{E_{yy}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_y} \\ \frac{\nu_{zx}\Delta\sigma_{xx} - \nu_{zy}\Delta\sigma_{yy} + \Delta\sigma_{zz}}{E_{zz}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_z} \end{pmatrix} \tag{7.9}$$

The total change in volumetric strain becomes:

$$\begin{aligned} \Delta\varepsilon_{ii} &= \frac{1}{3}\left(\frac{3(1 - \nu_{xy} - \nu_{xz})}{E_{xx}} - \frac{Rh_{ii}}{H_x} \right)\Delta\sigma_{xx} + \frac{1}{3}\left(\frac{3(1 - \nu_{yx} - \nu_{yz})}{E_{yy}} - \frac{Rh_{ii}}{H_y} \right)\Delta\sigma_{yy} \\ &\quad + \frac{1}{3}\left(\frac{3(1 - \nu_{zx} - \nu_{zy})}{E_{zz}} - \frac{Rh_{ii}}{H_z} \right)\Delta\sigma_{zz} \qquad (7.10) \\ &= \boldsymbol{k}_u \cdot \frac{1}{3}\left(\Delta\sigma_{xx}, \Delta\sigma_{yy}, \Delta\sigma_{yy} \right) \qquad (7.11) \end{aligned}$$

where $\boldsymbol{k}_u$ is an anisotropic compressibility tensor (components from terms above) and

$$h_{ii} = \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z} \right) \tag{7.12}$$

For an aniostropic material, we consider $\Delta\sigma_{xx} = \Delta\sigma_{yy} = \Delta\sigma_{zz} = -P$ and we can write

$$\Delta\varepsilon_{ii} = \left(\frac{1}{K} - \frac{Rh_{ii}}{3H_x} - \frac{Rh_{ii}}{3H_y} - \frac{Rh_{ii}}{3H_x} \right)P \quad \text{or} \quad \frac{1}{K_u} = \frac{1}{K} - Rh_{ii}^2 \tag{7.13}$$

is the undrained bulk modulus and

$$\frac{1}{K} = \frac{1-\nu_{xy}-\nu_{xz}}{E_{xx}} + \frac{1-\nu_{yx}-\nu_{yz}}{E_{yy}} + \frac{1-\nu_{zx}-\nu_{zy}}{E_{zz}} \tag{7.14}$$

The other limit is the "drained" limit where $dp = 0$. In this condition:

$$\boldsymbol{\varepsilon} = \mathsf{S}\boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = \mathsf{C}\boldsymbol{\varepsilon}, \quad \text{and} \quad \theta = \boldsymbol{h}\cdot\boldsymbol{\sigma} = \boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon} \tag{7.15}$$

For modeling and when allowing anisotropy, we need to specify H_i and Q or four poroelasticity properties. But perhaps more physical properties are to specify K_u (undrained bulk modulus in stress units) and components of $\boldsymbol{\alpha}$ (which are dimensionless). For input $\boldsymbol{\alpha}$ and K_u, find $\boldsymbol{h}$ from:

$$\boldsymbol{h} = \mathsf{S}\boldsymbol{\alpha} = \left(\frac{\alpha_x - \nu_{xy}\alpha_y - \nu_{xz}\alpha_z}{E_{xx}}, \frac{\alpha_y - \nu_{yx}\alpha_x - \nu_{yz}\alpha_z}{E_{yy}}, \frac{\alpha_z - \nu_{zx}\alpha_x - \nu_{zy}\alpha_y}{E_{zz}}, 0, 0, 0 \right) \tag{7.16}$$

and then find Q through R from

$$R = \frac{1}{h_{ii}^2}\left(\frac{1}{K} - \frac{1}{K_u}\right) \quad \text{and} \quad \frac{1}{Q} = \frac{1}{R} - \boldsymbol{h}\cdot\boldsymbol{\alpha} \tag{7.17}$$

which expands to:

$$Q = \frac{R}{1 - R\boldsymbol{h}\cdot\boldsymbol{\alpha}} = \frac{\left(\frac{1}{K} - \frac{1}{K_u}\right)}{h_{ii}^2 - \left(\frac{1}{K} - \frac{1}{K_u}\right)\boldsymbol{h}\cdot\boldsymbol{\alpha}} = \frac{K_u - K}{KK_u h_{ii}^2 - (K_u - K)\,\boldsymbol{h}\cdot\boldsymbol{\alpha}} \tag{7.18}$$

The code stores pore pressure capacity term as $C_T = 1/Q$ (see next section).

The modeling of poroelasticity is done by using moisture diffusion code by replacing concentration potential with pore pressure and changing standard diffusion properties. The first property changes are to set saturation concentration to $c_{sat} = 1$ and moisture expansion coefficients to $\boldsymbol{\beta} = \boldsymbol{h}$. In addition, the analysis will need a reference pore pressure or p_0 (and it replaces the reference concentration). Particles that do not start at that pressure will evolve until they represent the change in pore pressure. Unlike concentration modeling, pore pressure has a coupling term between volume change and undrained pressure change, which is

$$dp_{ud} = -Q\boldsymbol{\alpha}\cdot d\boldsymbol{\varepsilon} \tag{7.19}$$

If strain is in material axis system for orthotropic material, then

$$dp_{ud} = -Q(\alpha_x d\varepsilon_{xx} + \alpha_y d\varepsilon_{xx} + \alpha_z d\varepsilon_{xx}) \tag{7.20}$$

In other axis systems, need to rotate $\boldsymbol{\alpha}$ to the same axis system as the strain. Any material that supports poroelasticity will have to convert input properties to concentration modeling properties and also calculate dp_{ud} in constitutive law calculations. All other parts of poroelasticity are automatically handled by diffusion methods.

For an isotropic material, $\alpha_x = \alpha_y = \alpha_z = \alpha$ leading to:

$$\boldsymbol{\beta} = \boldsymbol{h} = \mathsf{S}\boldsymbol{\alpha} = \left(\frac{\alpha}{3K}, \frac{\alpha}{3K}, \frac{\alpha}{3K}, 0, 0, 0\right), \quad h_{ii} = \frac{\alpha}{K}, \quad \text{and} \quad \boldsymbol{h}\cdot\boldsymbol{\alpha} = \frac{\alpha^2}{K} \tag{7.21}$$

Then Q is found from:

$$Q = \frac{K_u - K}{\frac{K_u\alpha^2}{K} - \frac{(K_u - K)\alpha^2}{K}} = \frac{K_u - K}{\alpha^2} \tag{7.22}$$

Clearly, we need $\alpha > 0$ and $K_u > K$. Finally:

$$dp_{ud} = -Q\alpha\frac{\Delta V}{V} \tag{7.23}$$

For transversely isotropic material with axial direction in the y direction, $\alpha_x = \alpha_z = \alpha_T$, $\alpha_y = \alpha_A$ leading to

$$\boldsymbol{\beta} = \boldsymbol{h} = \mathsf{S}\boldsymbol{\alpha} = \left(\frac{(1-\nu_T)\alpha_T - \nu_T\alpha_A}{E_T}, \frac{\alpha_A - 2\nu_A\alpha_T}{E_A}, \frac{(1-\nu_T)\alpha_T - \nu_T\alpha_A}{E_T}, 0, 0, 0\right) \tag{7.24}$$

$$h_{ii} = \frac{2\big((1-\nu_T)\alpha_T - \nu_T\alpha_A\big)}{E_T} + \frac{\alpha_A - 2\nu_A\alpha_T}{E_A} \tag{7.25}$$

$$\boldsymbol{h}\cdot\boldsymbol{\alpha} = \frac{2\big((1-\nu_T)\alpha_T^2 - \nu_T\alpha_A\alpha_T\big)}{E_T} + \frac{\alpha_A^2 - 2\nu_A\alpha_A\alpha_T}{E_A} \tag{7.26}$$

7.2.1 Darcy's Law Flow

In a Darcy flow analysis, the fluid volume rate of change is

$$\frac{d\theta}{dt} = -\frac{1}{\eta}\nabla\cdot\mathsf{k}\nabla p \tag{7.27}$$

where k is Darcy tensor (units length^2) and η is viscosity of permeating fluid. Substituting equation for θ leads to:

$$\frac{1}{Q}\frac{dp}{dt} = -\frac{1}{\eta}\nabla\cdot\mathsf{k}\nabla p - \boldsymbol{\alpha}\cdot\frac{d\boldsymbol{\varepsilon}}{dt} \tag{7.28}$$

The poroelasticity transport law is modeled by using diffusion code where diffusion tensor is replaced by the Darcy tensor divided by viscosity (k/η) and the transport capacity is:

$$C_T = \frac{1}{Q} \tag{7.29}$$

instead of 1. The second term is a coupling term where volumetric change (increment in $\boldsymbol{\varepsilon}$) causes a change in pore pressure. A physical interpretation of this term is that is it the pore pressure change caused by a change in strains under conditions where $d\theta/dt = 0$. In other words, it is the "undrained" pressure increment. In thermoelastic analysis, this pressure change is analog of adiabatic temperature change in a material. The explicit form for pressure change in one time step is

$$\Delta p_{ud} = -Q\boldsymbol{\alpha}\cdot\Delta\boldsymbol{\varepsilon} \tag{7.30}$$

where $\Delta\boldsymbol{\varepsilon}$ is strain increment in the time step.

The time steps needed for stress wave and pore pressure transport and their ratio are:

$$\Delta t_\sigma = \frac{\Delta x}{v_{max}}, \qquad \Delta t_p = \frac{\eta\Delta x^2}{2Qk_{max}}, \qquad \text{and} \qquad \frac{\Delta t_p}{\Delta t_\sigma} = \frac{\eta v_{max}\Delta x}{2Qk_{max}} \tag{7.31}$$

where Δx is cell size, v_{max} is maximum wave speed, and k_{max} is maximum permeability. For an isotropic material:

$$v_{max} = \sqrt{\frac{2G(1-\nu)}{\rho(1-2\nu)}} = \sqrt{\frac{3K(1-\nu)}{\rho(1+\nu)}} \quad \text{and} \quad \frac{\Delta t_p}{\Delta t_\sigma} = \frac{\eta\alpha^2\Delta x}{2k(K_u - K)}\sqrt{\frac{3K(1-\nu)}{\rho(1+\nu)}} \tag{7.32}$$

Nothing in the flow analysis prevents p from going negative. An actual pressure cannot be negative (tension on fluid), but a negative p can be used to track transition between fully saturated ($p \geq 0$) and partially saturated ($p < 0$). A negative p can be used in modeling with the following algorithm:

1. The Darcy flow equation continues regardless of the sign of p
2. Whenever $p > 0$, p corresponds to pore pressure and dp due to transport (∇p term) or "undrained" pressure increment (second term) is input to constitutive law modeling and affects global stresses.
3. Whenever $p < 0$, Darcy flow analysis continues to evolve, but $dp = 0$ for constitutive law modeling. The material acts as if there is zero pore pressure.
4. When p changes sign, adjust dp for constitutive law to be change to stop at zero (if p now less than zero) to become new value (if p now greater than 0).
5. `OSParticulas` tracks p in particle concentration using `pConcentration`. The `pPrevious-Concentration` tracks pore pressure smoothed by extrapolating to the grid, but it tracks an actual pressure and therefore never becomes negative. These two values are the same (except for numerical issues that might cause some differences) when $p > 0$, but will mean different things when $p < 0$.

By this algorithm, a negative p is not pore pressure, but the value $-p/Q$ is a measure of the amount of empty pore space (pore volume not filled with fluid) that has opened due to mechanical loading. When there is empty pore volume ($p < 0$), mechanical loading does not induce pore pressure. Once the empty volume (and p) return to zero, further mechanical loading can induce pore pressure.

7.2.2 Biot Example for Uniaxial Compression

Imagine a soil compressed in uniaxial direction and confined in lateral direction such that $\varepsilon_{yy} = \varepsilon_{xx} = 0$ and water can flow out through a porous slab used to apply the pressure. In this "drained" limit, $\boldsymbol{\sigma} = \mathsf{C}\boldsymbol{\varepsilon}$, leading to trivial result of:

$$\sigma_{zz} = (\lambda + 2G)\varepsilon_{zz} = \frac{\varepsilon_{zz}}{a} \tag{7.33}$$

where a defined in Biot's paper is

$$a = \frac{1}{\lambda + 2G} = \frac{1}{C_{zz}} = \frac{(1+\nu)(1-2\nu)}{E(1-\nu)} = \frac{(1-2\nu)}{2G(1-\nu)} \tag{7.34}$$

For generalizations here to an orthotropic material:

$$a = \frac{1}{C_{zz}} = \frac{1 - \nu_{yz}\nu_{zy} - \nu_{xz}\nu_{zx} - \nu_{xy}\nu_{yx} - 2\nu_{xz}\nu_{yx}\nu_{zy}}{E_{zz}(1 - \nu_{xy}\nu_{yx})} \tag{7.35}$$

7.2.3 2D Problems

The 2D constitutive law in plane strain is

$$\boldsymbol{\sigma} = \mathsf{C}(\boldsymbol{\varepsilon} - \mathsf{S}^{(r)}\boldsymbol{\alpha}dp) \tag{7.36}$$

where $\mathsf{S}^{(r)}$ is the reduced compliance tensor for plane strain. This form gives the usual reduced expansion coefficients to find in-plane stress. For example, an isotropic material would use $\beta_x = \beta_y = \beta_z = \alpha(1+\nu)/(3K)$. The out-of-plane stress is

$$\sigma_{zz} = C_{13}(\varepsilon_{xx} - \beta_x dp) + C_{23}(\varepsilon_{yy} - \beta_y dp) - C_{33}(\varepsilon_{zz} - \beta_z dp) \tag{7.37}$$

where inclusion of ε_{zz} is when implementing generalized plane strain (normally it is zero). The coupling term

$$\Delta p_{ud} = -Q\boldsymbol{\alpha} \cdot \Delta\boldsymbol{\varepsilon} \tag{7.38}$$

remains the same, although $d\varepsilon_{zz} = 0$ in standard plane strain (may be non-zero in generalized plane strain).

The 2D constitutive law in plane stress is

$$\boldsymbol{\sigma} = \mathsf{Q}(\boldsymbol{\varepsilon} - \boldsymbol{\beta} dp) \tag{7.39}$$

where Q is the reduced plane stress stiffness matrix. The out-of-plane strain is

$$\varepsilon_{zz} = \frac{1}{C_{33}}\sigma_{zz} - \frac{C_{13}}{C_{33}}(\varepsilon_{xx} - \beta_x dp) - \frac{C_{23}}{C_{33}}(\varepsilon_{yy} - \beta_y dp) + \beta_z dp \tag{7.40}$$

where inclusion of σ_{zz} is when implementing generalized plane stress (normally it is zero). The coupling term needs to use this ε_{zz} (in incremental form).

Axisymmetric equations are same as 3D and hoop strain in part of the solution. The only addition is to find hoop stress.

7.3 Effective and Solid Stress

Biot poroelasticity is finding an *effective* stress that combines stress on the solid and stress due to pore pressure. Taking Eq. (7.5) as definition of effective stress, that stress is composed of stress on the solid and pore pressure stress:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^p \quad \text{where} \quad \boldsymbol{\sigma}^s = \mathsf{C}\boldsymbol{\varepsilon} \quad \text{and} \quad \boldsymbol{\sigma}^p = -\boldsymbol{\alpha} dp \tag{7.41}$$

In other words, the stress on the solid is

$$\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\alpha} dp \tag{7.42}$$

We can partition the stress update into:

$$d\boldsymbol{\sigma} = d\boldsymbol{\sigma}^s + d\boldsymbol{\sigma}^p \quad \text{where} \quad d\boldsymbol{\sigma}^s = \mathsf{C}d\varepsilon^* \quad \text{and} \quad d\boldsymbol{\sigma}^p = -\boldsymbol{\alpha}\Delta dp \tag{7.43}$$

where $d\varepsilon^*$ includes residual strains (if present), but not residual pore pressure terms. After finding $d\boldsymbol{\sigma}^s$ ignoring pore pressure, final *e*ffective stress update is:

$$d\boldsymbol{\sigma} = d\boldsymbol{\sigma}^p - \boldsymbol{\alpha}\Delta dp = \sigma^p + d\boldsymbol{\sigma}^p - \boldsymbol{\alpha}(dp + \Delta dp) \tag{7.44}$$

Dividing up these stress night be useful when modeling plasticity or damage where failure should focus only on σ^s. For 2D plane strain, the out-of-plane stress increment is:

$$d\sigma_{zz} = C_{13}(d\varepsilon^*_{xx} - \beta_x \Delta dp) + C_{23}(d\varepsilon^*_{yy} - \beta_y \Delta dp) - C_{33}(d\varepsilon_{zz} - \beta_z \Delta dp) \tag{7.45}$$

For plane stress, the out-of-plane strain increment

$$d\varepsilon_{zz} = \frac{1}{C_{33}}d\sigma_{zz} - \frac{C_{13}}{C_{33}}(d\varepsilon^*_{xx} - \beta_x \Delta dp) - \frac{C_{23}}{C_{33}}(d\varepsilon^*_{yy} - \beta_y \Delta dp) + \beta_z \Delta dp \tag{7.46}$$

For axisymmetric, calculation of hoop stress needs to account for $\boldsymbol{\beta}\Delta dp$ terms.

7.3.1 Partitioning in Damage Mechanics

Modeling for damage should partition out pore pressure stress during damage evolution, but be sure to add it back before done and to correctly get volume change for undrained pore pressure calculation. The algorithm is:

1. For undamaged material, find current solid stress, rotate it to initial configuration, and then get trial solid stress using effective strain increment in the initial configuration

$$\boldsymbol{\sigma}^{(trial)} = (\mathsf{R}^0_{n-1})^T(\boldsymbol{\sigma}^{(p)}_{n-1} + \boldsymbol{\alpha} dp)\mathsf{R}^0_{n-1} + \mathsf{C} d\boldsymbol{\varepsilon}^*_0 \tag{7.47}$$

   where $d\boldsymbol{\varepsilon}^*_0$ includes residual thermal strains, but not pore-pressure strains. Note that for isotropic materials:

$$(\mathsf{R}^0_{n-1})^T \boldsymbol{\alpha} dp \mathsf{R}^0_{n-1} = \alpha dp \mathsf{I} \tag{7.48}$$

2. If no damage, then accept the above update by updating pore pressure increment and adding to the undated solid stress. In initial configuration:

$$\boldsymbol{\sigma}^{(final)} = \boldsymbol{\sigma}^{(trial)} + (\mathsf{R}^0_{n-1})^T \boldsymbol{\alpha}(dp + \Delta p)\mathsf{R}^0_{n-1} \tag{7.49}$$

   To calculate out-of-plane results correctly, update effective strains in initial configuration to

$$d\boldsymbol{\varepsilon}^* = d\boldsymbol{\varepsilon}^*_0 + (\mathsf{R}^0_{n-1})^T \boldsymbol{\alpha} \Delta p \mathsf{R}^0_{n-1} \tag{7.50}$$

   For isotropic materials, the pore pressure terms need not be rotated.

3. If damage occurs, record start of damage and crack-plane orientation and proceed to next step.

4. Find the initial solid stress in the crack axis system:

$$\boldsymbol{\sigma}^{(0)} = (\mathsf{R}_{n-1})^T(\boldsymbol{\sigma}^{(p)}_{n-1} + \boldsymbol{\alpha} dp)\mathsf{R}_{n-1} \tag{7.51}$$

   and find $d\boldsymbol{\varepsilon}^*_0$ including thermal stresses, but not pore pressure expansion stresses. Proceed with usual damage mechanics ending in calculations of $d\boldsymbol{\sigma}^s$ and changes in cracking strains. Before updating particle, add pore pressure increment to the stress increment by adding $\alpha\Delta dp$ to each normal stress increment. In code $d\sigma_{xx}$ is already found so add pore pressure terms. The remaining stress increments can subtract pore pressure expansion termss for effective strains inside. When needed, add pore pressure terms to constant used to find out-of-plane results.

7.4 Rice's Solid Stress Version?

Rice (1976) arranges the equation in a different, but seemingly equivalent, style. I think Rice's method is to focus on stress in the solid phase, $\boldsymbol{\sigma}_s = \boldsymbol{\sigma} + p\mathsf{I}$, instead of total stress on the volume element (which is $\boldsymbol{\sigma}$). Generalizing Rice's equations to anisotropic materials, the Biot equations become:

$$\boldsymbol{\varepsilon} = \mathsf{S}\sigma_s - \frac{\boldsymbol{k}'_s p}{3} \tag{7.52}$$

$$\theta - \theta_0 = \boldsymbol{h} \cdot \sigma_s - \frac{\theta_0}{K''_s} p \tag{7.53}$$

where

$$\boldsymbol{k}_s' = 3(\mathsf{S}\mathsf{I} - \boldsymbol{h}), \quad \frac{\theta_0}{K_s''} = h_{ii} - \frac{1}{R} \quad \text{and} \quad h_{ii} = \boldsymbol{h} \cdot \mathsf{I} = \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z}\right) \tag{7.54}$$

Note that θ is now pore volume (rather then increment as in Biot) and θ_0 is reference volume in the "unstressed state," which must mean stress when $\theta = \theta_0$. From above, this state occurs when:

$$p = \frac{K_s'' \boldsymbol{h} \cdot \sigma_s}{\theta_0} \tag{7.55}$$

In this "unstressed state", the total strain is

$$\boldsymbol{\varepsilon} = \mathsf{S}\sigma_s - \frac{\boldsymbol{k}_s' K_s'' \boldsymbol{h} \cdot \sigma_s}{3\theta_0} \tag{7.56}$$

Writing out expressions for an orthoropic material gives

$$\boldsymbol{k}_s' = \left(\frac{3(1-\nu_{xy}-\nu_{xz})}{E_{xx}} - \frac{1}{H_x}, \frac{3(1-\nu_{yx}-\nu_{yz})}{E_{yy}} - \frac{1}{H_y}, \frac{3(1-\nu_{zx}-\nu_{zy})}{E_{zz}} - \frac{1}{H_z}, 0, 0, 0\right) \tag{7.57}$$

$$\frac{\theta_0}{K_s'} = \left(\frac{1}{R} - \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z}\right)\right) \tag{7.58}$$

If the material is isotropic, the results become:

$$\boldsymbol{k}_s'' = \left(\frac{1}{K} - \frac{1}{H}\right)(1,1,1,0,0,0) = \frac{1}{K_s'}(1,1,1,0,0,0) \tag{7.59}$$

$$\frac{\theta_0}{3K_s''} = \frac{1}{R} - \frac{1}{H} \tag{7.60}$$

Here K_s' and K_s'' are terms defined by Rice (1976).

Chapter 8

Hyperelastic Materials

8.1 Introduction

Constitutive laws for hyperelastic materials always involve the deformation gradient, F. All hyperelastic materials store the full deformation gradient using the strain and rotation variables on the particles (named $\boldsymbol{\varepsilon}$ =ep and $\boldsymbol{\omega}$ =wrot) as follows:

$$\mathbf{F} = \begin{pmatrix} 1+\varepsilon_{xx} & \frac{1}{2}(\gamma_{xy}-\omega_{xy}) & \frac{1}{2}(\gamma_{xz}-\omega_{xz}) \\ \frac{1}{2}(\gamma_{xy}+\omega_{xy}) & 1+\varepsilon_{yy} & \frac{1}{2}(\gamma_{yz}-\omega_{yz}) \\ \frac{1}{2}(\gamma_{xz}+\omega_{xz}) & \frac{1}{2}(\gamma_{yz}+\omega_{yz}) & 1+\varepsilon_{zz} \end{pmatrix} \tag{8.1}$$

and should store the updated gradient back in strain and rotation tensors on each time step (*i.e.*, $\varepsilon_{ii} = F_{ii} - 1$, $\gamma_{ij} = F_{ij} + F_{ji}$, and $\omega_{ij} = F_{ji} - F_{ij}$ for $i < j$). Note that in large deformation, the stored particle strains and rotation are no longer equal to small-strain strains and rotations. To calculate strains and the rotation matrix, this $\mathbf{F}$ is decomposed to:

$$\mathbf{F} = \mathbf{RU} \quad \Longrightarrow \quad \boldsymbol{\varepsilon} = \mathbf{U} - \mathbf{I} \quad \text{and} \quad \mathbf{R} = \mathbf{F}\mathbf{U}^{-1}$$

This strain is known as the Biot strain (and note that $\mathbf{U}^{-1}$ can be found during decomposition using already-calculated terms and the Cayley-Hamilton theorem; it does not require and separate inversion process).

Hyperelastic materials with plasticity, still store full deformation gradient as above and thus unlike small-strain plasticity materials, the strain variables describe the total strain and not just the elastic deformation. To allow separation of elastic and plastic deformation, both elastic and plastic hyperelasic materials use the plastic strain variable on the particles ($\boldsymbol{\varepsilon}^{(p)}$ =eplast) to store the symmetric, *elastic*, left Cauchy-Green tensor ($\mathbf{B} = \mathbf{F}\mathbf{F}^T$). For convenience, hyperelastic materials can obtain a pointer to this variable using the particle accessor `GetAltStrainTensor()`. Because this just returns a pointer to `eplast`, that material cannot also use `GetAltStrainTensor()` expecting an option to store different particle state information.

Large deformation MPM requires calculation of specific Cauchy stress ($\boldsymbol{\sigma}$) on each time step, or the Cauchy stress divided by the current density (ρ) accounting for volume changes. This required quantity is equivalent to

$$\frac{\boldsymbol{\sigma}}{\rho} = \frac{\boldsymbol{\sigma} J}{\rho_0} = \frac{\boldsymbol{\tau}}{\rho_0} \tag{8.2}$$

where J is $\det \mathbf{F}$ and equal to the relative volume change ($J = V/V_0$), $\boldsymbol{\tau}$ is the Kirchoff stress, and ρ_0 is the initial volume (*i.e.*, $\rho_0 = J\rho$). In other words, all hyperelastic materials track the Kirchoff

stress normalized to the initial density, which is done by dividing all constitutive law properties by ρ_0 at the start of the calculation and then finding Kirchoff stress in constitutive laws. The output stresses, however, are converted to true Cauchy stress using particle J.

8.2 Incremental Deformation Gradient

Each MPM time step requires evaluation of deformation gradient rate defined by

$$\frac{d\mathbf{F}}{dt} = \nabla \boldsymbol{v}\mathbf{F} \tag{8.3}$$

where $\nabla \boldsymbol{v}$ is spatial gradient extrapolated from grid nodes to the particles. If $\nabla \boldsymbol{v}$ is constant for the time step, the exact solution is

$$\mathbf{F}(t+\Delta t) = \exp(\Delta t \nabla \boldsymbol{v})\mathbf{F}(t) = \mathbf{dF}\,\mathbf{F}(t) \tag{8.4}$$

where

$$\mathbf{dF} = \exp(\Delta t \nabla \boldsymbol{v}) = \mathbf{F}(t+\Delta t)\mathbf{F}(t)^{-1} \tag{8.5}$$

is the incremental deformation gradient. An interesting review article on finding the exponential of a matrix is "Nineteen Dubious Ways to Compute the Exponential of a Matrix. Twenty Five Years Later." (C. Moler and C. Van Loan, *SIAM Review*, **46**, 2003). They conclude no single way is stable and efficient for all problems, but in MPM with sufficiently small time steps, an expansion method should work well

$$\exp(\Delta t \nabla \boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \sum_{k=2}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{8.6}$$

where $\nabla u = \nabla \boldsymbol{v} \Delta t$ is the incremental displacement gradient. The first two terms are trivial, but have been noticed to have issues in rotational deformation fields. The question is how to evaluate extra terms as efficiently as possible.

Method 8 of the "Nineteen Dubious Ways" uses the Cayley-Hamilton theorem to find $(\nabla u)^k$ without any matrix multiplications in 2D and just one in 3D. In 2D (plane stress, plain strain, or axisymmetric), the displacement gradient can be partitioned as

$$\nabla u = \begin{pmatrix} \begin{bmatrix} du_{xx} & du_{xy} \\ du_{yx} & du_{yy} \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz} \end{pmatrix} \tag{8.7}$$

where $du_{ij} = \partial u_i / \partial x_j$ ($du_{zz} = 0$ for plain strain, but not for plane stress or axisymmetry). If A is the 2×2 partition, then

$$(\nabla u)^k = \begin{pmatrix} \mathsf{A}^k & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz}^k \end{pmatrix} \tag{8.8}$$

Let the characteristic polymer of A (of any dimension n) be

$$c(z) = \det(z\mathbf{I} - \mathsf{A}) = z^n - \sum_{k=0}^{n-1} c_k z^k \tag{8.9}$$

Because $c(\mathsf{A}) = 0$, the n^{th} power of A can be found from lower powers of A

$$\mathsf{A}^n = \sum_{k=0}^{n-1} c_k \mathsf{A}^k \tag{8.10}$$

For $n = 2$, these reduce to

$$c_0 = -\det(\mathsf{A}), \qquad c_1 = \mathrm{Tr}(\mathsf{A}), \qquad \text{and} \qquad \mathsf{A}^2 = c_0\mathbf{I} + c_1\mathsf{A} \tag{8.11}$$

Higher powers of A can be found by recursion to be

$$\mathsf{A}^k = \beta_{k,0}\mathbf{I} + \beta_{k,1}\mathsf{A} \tag{8.12}$$

where $\beta_{1,i} = \delta_{i1}$, $\beta_{k,0} = c_0\beta_{k-1,1}$, and $\beta_{k,1} = c_1\beta_{k-1,1} + \beta_{k-1,0}$. In other words, $\mathbf{I}$ and A are a basis for all powers of A. Finally, we can expand the incremental deformation gradient using k_{max} terms as

$$\mathbf{dF}(k_{max}) = \begin{pmatrix} [\alpha_0\mathbf{I} + \alpha_1\mathsf{A}] & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & 1 + du_{zz} + \sum_{k=2}^{k_{max}} \frac{du_{zz}^k}{k!} \end{pmatrix} \tag{8.13}$$

where

$$\alpha_0 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,0}}{k!} \qquad \text{and} \qquad \alpha_1 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,1}}{k!} \tag{8.14}$$

An efficient computer algorithm for all non-zero elements of the deformation gradient using k_{max} terms (which eliminates as many multiplications and divides as I think are possible and the factorial terms are scaled into the `beta` variables such that `betai`$= \beta_{k,i}/k!$) is:

```
double c0 = duxy*duyx - duxx*duyy, c1 = duxx + duyy;
double beta0 = 0., beta1 = 1., alpha0 = 1., alpha1 = 1.;
double betaz = duzz; dFzz = 1. + duzz
int k;
double factor, temp;;
for(k = 2; k <= kmax; k++)
{   factor = 1/(double)k;
    temp = beta1;
    beta1 = factor*(c1*temp + beta0);
    beta0 = factor*c0*temp;
    betaz *= factor*duzz;
    alpha0 += beta0;
    alpha1 += beta1;
    dFzz += betaz;
}
double dFxx = alpha0 + alpha1*duxx;
double dFxy = alpha1*duxy;
double dFyx = alpha1*duyx;
double dFyy = alpha0 + alpha1*duyyl
```

Each extra term included in the expansion costs 6 multiplications, 1 division, and 4 additions. Direct matrix multiplication would add 14 multiplcations/division and 13 additions for each term.

A similar approach can be done in 3D, but does require one matrix multiplication. The overall expansion is

$$\exp(\Delta t \nabla \boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \frac{1}{2}(\nabla u)^2 + \sum_{k=3}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{8.15}$$

which can be reduced to

$$\exp(\Delta t \nabla \boldsymbol{v}) = \alpha_0 \mathbf{I} + \alpha_1 \nabla u + \alpha_2 (\nabla u)^2 \tag{8.16}$$

$$\alpha_0 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,0}}{k!}, \qquad \alpha_1 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,1}}{k!}, \quad \text{and} \quad \alpha_2 = \frac{1}{2} + \sum_{k=3}^{k_{max}} \frac{\beta_{k,2}}{k!} \tag{8.17}$$

The required recursion relations are $\beta_{2,i} = \delta_{i2}$, $\beta_{k,0} = c_0\beta_{k-1,2}$, $\beta_{k,1} = c_1\beta_{k-1,2} + \beta_{k-1,0}$, and $\beta_{k,2} = c_2\beta_{k-1,2} + \beta_{k-1,1}$. For a 3×3 matrix, $c_0 = \det(\mathsf{M})$, $c_1 = -I_2$, and $c_2 = \mathrm{Tr}(\mathsf{M})$, where I_2 is the second invariant. Each extra term included in the expansion adds 6 multiplications, 1 division and 5 additions. Direct matrix multiplication would add about 36 multiplications, 1 division, and 27 additions for each term.

One MPM user suggested loading a single particle in tension to some value and then rotating. A plot of axial stress in the loading direction should increase linearly while loading and then oscillate around a constant mean during rotation. In 2D calculations with $k_{max} = 1$, the stress continues to increase while rotating, but using $k_{max} = 2$ appears to make it constant. Addition of extra terms beyond $k_{max} = 2$ does not seem to provide much benefit (at least in this example). A need for extra terms can be demonstrated by using a very large time step, such as 8 times the Courant-Friedrichs-Lewy (CFL) condition. Some results are in Fig. 8.1. With 1 term, the calculations are immediately bad once rotation starts. Each extra term improves the result. With 5 or more terms, the result is correct. When CFL is less than 1 (as it should be), terms beyond $k_{max} = 2$ might not have much benefit, but can be seen, for example, in pure shear examples.

8.3 General Hyperelastic Materials

This section is for Green-elastic materials, which means a scalar potential energy, $W(\mathbf{F})$, exists such that the energy differential is defined by:

$$dW = \frac{\partial W}{\partial \mathbf{F}} \cdot d\mathbf{F} = \mathrm{Tr}\left(\frac{\partial W}{\partial \mathbf{F}} d\mathbf{F}^T\right)$$

where $d\mathbf{F}$ is incremental deformation gradient.

8.3.1 Four Measures of Stress

Four different stresses are used — Cauchy stress ($\boldsymbol{\sigma}$), Kirchoff stress ($\boldsymbol{\tau} = J\boldsymbol{\sigma}$), the first Piola-Kirchoff stress ($\mathbf{P}$, not symmetric), and the second Piola-Kirchoff stress (symmetric) ($\mathbf{S}$). By equating Cauchy stress per unit deformed area to first Piola-Kirchoff stress per unit undeformed area and using Nanson's formula:

$$\boldsymbol{\sigma n}\, da = \mathbf{P}\boldsymbol{N} dA = J\sigma \mathbf{F}^{-T} \boldsymbol{N} dA \quad \Longrightarrow \quad \mathbf{P} = J\sigma \mathbf{F}^{-T} = \tau \mathbf{F}^{-T} \text{ or } \mathbf{P}^T = \mathbf{F}^{-1}\tau$$

In general, $\mathbf{P}$ is not symmetric. By transforming energy increment per unit deformed volume to energy per unit initial volumes, we can derive

$$dW = J\mathrm{Tr}\left(\sigma(\nabla \boldsymbol{u})^T\right) = \mathrm{Tr}\left(J\sigma \mathbf{F}^{-T} d\mathbf{F}^T\right) = \mathrm{Tr}\left(\mathbf{P} d\mathbf{F}^T\right) = \mathbf{P}\mathrm{d}\mathbf{F}$$

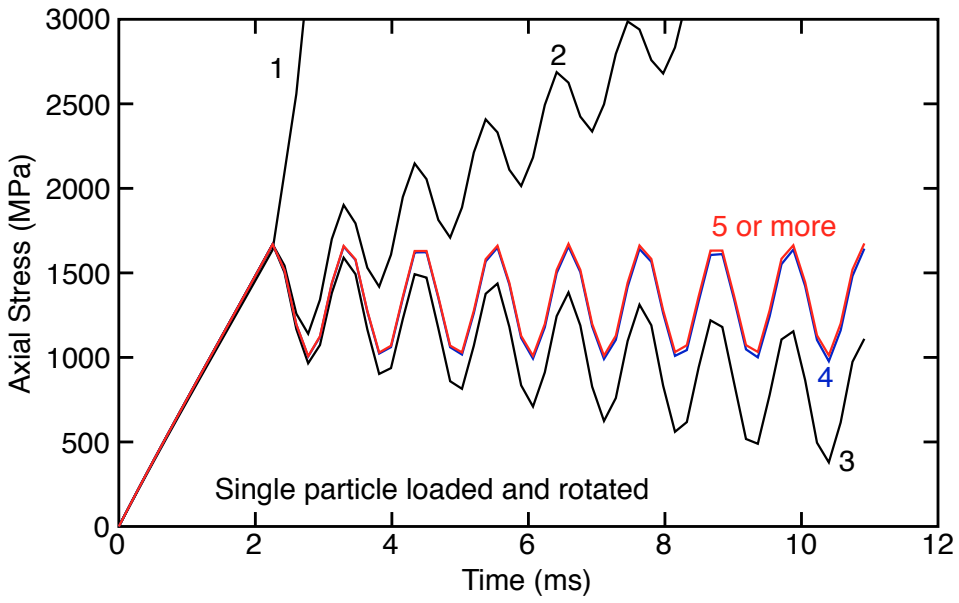

Figure 8.1: Calculation for a single particle loaded in tension, held, and then rotated. The different curves show k_{max} or the number of terms used to expand the matrix exponential in the incremental deformation gradient.

From the definition of Green-elastic material, we associate first Piola-Kirchoff stress with

$$\mathbf{P} = \frac{\partial W}{\partial \mathbf{F}} \quad \text{or} \quad \mathbf{P} = \mathbf{F}\frac{\partial W}{\partial \mathbf{E}} \quad \text{or} \quad \mathbf{P} = 2\mathbf{F}\frac{\partial W}{\partial \mathbf{C}}$$

where $\mathbf{E} = (\mathbf{C} - \mathbf{I})/2$ is the Green-Lagrange strains and $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the right-Cauchy strain tensor.

The second Piola-Kirchoff stress is given by

$$\mathbf{S} = \mathbf{F}^{-1}\mathbf{P} = \mathbf{F}^{-1}\boldsymbol{\tau}\mathbf{F}^{-T} = \mathbf{F}^{-T}\boldsymbol{\tau}\mathbf{F}^{-1} \quad \text{or} \quad \mathbf{P} = \mathbf{F}\mathbf{S}$$

Using $\mathbf{S} = \mathbf{F}^{-1}\mathbf{P} = \mathbf{P}^T\mathbf{F}^{-T}$, the relations for $\mathbf{S}$ are:

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{F}}\mathbf{F}^{-T} \quad \text{or} \quad \mathbf{S} = \frac{\partial W}{\partial \mathbf{E}} \quad \text{or} \quad \mathbf{S} = 2\frac{\partial W}{\partial \mathbf{C}}$$

Using $\tau = \mathbf{F}\mathbf{P}^T = \mathbf{F}\mathbf{S}\mathbf{F}^T$, the relations for τ are

$$\boldsymbol{\tau} = \mathbf{F}\frac{\partial W}{\partial \mathbf{F}} \quad \text{or} \quad \boldsymbol{\tau} = \mathbf{F}\frac{\partial W}{\partial \mathbf{E}}\mathbf{F}^T \quad \text{or} \quad \boldsymbol{\tau} = 2\mathbf{F}\frac{\partial W}{\partial \mathbf{C}}\mathbf{F}^T$$

The relations for $\boldsymbol{\sigma}$ divide each $\boldsymbol{\tau}$ relation by J:

$$\boldsymbol{\sigma} = \frac{1}{J}\mathbf{F}\frac{\partial W}{\partial \mathbf{F}} \quad \text{or} \quad \boldsymbol{\sigma} = \frac{1}{J}\mathbf{F}\frac{\partial W}{\partial \mathbf{E}}\mathbf{F}^T \quad \text{or} \quad \boldsymbol{\sigma} = \frac{2}{J}\mathbf{F}\frac{\partial W}{\partial \mathbf{C}}\mathbf{F}^T$$

8.3.2 Tangent Stiffness Tensor

The first Piola-Kirchoff stress increment is

$$\mathbf{P}^{n+1} - \mathbf{P}^n = \frac{\partial^2 W}{\partial \mathbf{F}^2}\delta\mathbf{F} \quad \text{where} \quad \delta\mathbf{F} = (d\mathbf{F} - \mathbf{I})\mathbf{F}$$

and the derivative is a fourth-rank tensor with elements

$$\left(\frac{\partial^2 W}{\partial \mathbf{F}^2}\right)_{ijkl} = \frac{\partial P_{ij}}{\partial F_{kl}}$$

The second Piola-Kirchoff stress increment is

$$\mathbf{S}^{n+1} - \mathbf{S}^n = 4\frac{\partial^2 W}{\partial \mathbf{C}^2} d\mathbf{C} = 2\frac{\partial^2 W}{\partial \mathbf{C}^2} d\mathbf{E} = \mathsf{C} d\mathbf{E}$$

where $\mathbf{E} = (1/2)(\mathbf{C} - \mathbf{I})$ is the Green-Lagrange strain and C is fourth-rank stiffness matrix for $\mathbf{S}$ and $\mathbf{E}$ with elements

$$C_{ijkl} = 2\frac{\partial S_{ij}}{\partial C_{kl}}$$

Defining incremental deformation $d\mathbf{F}$, this equation can be transformed to and update for Kirchoff stress:

$$\boldsymbol{\tau}^{n+1} = d\mathbf{F}\boldsymbol{\tau}^n d\mathbf{F}^T + \mathbf{F}^{n+1}\mathsf{C}(\mathbf{F}^{n+1})^T \frac{1}{2}(\mathbf{I} - d\mathbf{F}^{-T} d\mathbf{F}^{-1})\mathbf{F}^{n+1}(\mathbf{F}^{n+1})^T$$

For small increments:

$$d\mathbf{F} = \exp(\nabla \boldsymbol{u}) \text{ and } d\mathbf{F}^{-1} \approx \mathbf{I} - \nabla \boldsymbol{u} \quad \Longrightarrow \quad \frac{1}{2}(\mathbf{I} - d\mathbf{F}^{-T} d\mathbf{F}^{-1}) = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) = d\boldsymbol{\varepsilon}$$

where $\nabla \boldsymbol{u} = \nabla \boldsymbol{v} \Delta t$ is the displacement gradient for the time step given a constant velocity gradient and $d\boldsymbol{\varepsilon}$ is the strain increment. More directly:

$$\Delta \boldsymbol{\tau} = \mathsf{c} d\boldsymbol{\varepsilon} + \nabla \boldsymbol{u}\boldsymbol{\tau} + \boldsymbol{\tau}\nabla \boldsymbol{u}^T \quad \text{with} \quad \mathsf{c} d\boldsymbol{\varepsilon} = \mathbf{F}\mathsf{C}\mathbf{F}^T d\boldsymbol{\varepsilon}\mathbf{F}\mathbf{F}^T$$

Using notation with repeated indices summed

$$\begin{aligned} c_{ijkl} d\varepsilon_{kl} &= F_{ir}\left(\mathsf{C}\mathbf{F}^T d\boldsymbol{\varepsilon}\mathbf{F}\right)_{rs} F_{js} \\ &= F_{ir} C_{rsmn}\left(\mathbf{F}^T d\boldsymbol{\varepsilon}\mathbf{F}\right)_{mn} F_{js} \\ &= F_{ir} F_{js} F_{km} F_{ln} C_{rsmn} d\varepsilon_{kl} \end{aligned}$$

or with summations

$$c_{ijkl} = \sum_r \sum_s \sum_m \sum_n F_{ir} F_{js} F_{km} F_{ln} C_{rsmn}$$

An increment in Cauchy stress during a time step can be written as:

$$\boldsymbol{\sigma}^{n+1} = \frac{d\mathbf{F}\boldsymbol{\sigma}^n d\mathbf{F}^T}{\det(d\mathbf{F})} + \frac{1}{J}\mathsf{c} d\boldsymbol{\varepsilon}$$

with

$$\det(d\mathbf{F}) = \det\left(\exp(\nabla \boldsymbol{u})\right) = \exp(\mathrm{Tr}(\nabla \boldsymbol{u})) \approx 1 + d\epsilon \quad \text{where} \quad d\epsilon = \mathrm{Tr}(d\boldsymbol{\varepsilon}) = \mathrm{Tr}(\nabla \boldsymbol{u})$$

Keeping linear terms only gives

$$\Delta \boldsymbol{\sigma} = \frac{1}{J}\mathsf{c}\boldsymbol{\varepsilon} + \nabla \boldsymbol{u}\boldsymbol{\sigma} + \boldsymbol{\sigma}\nabla \boldsymbol{u}^T - \boldsymbol{\sigma} d\epsilon \tag{8.18}$$

8.3.3 Stress Power Density or Energy Increments

The energy change per unit initial volume due to incremental deformation gradient is

$$dW = \mathrm{Tr}\left(\frac{\partial W}{\partial \mathbf{F}} d\mathbf{F}^T\right) = \mathbf{P} \cdot d\mathbf{F}$$

Using other stresses, it is easy to how that

$$dW = \mathrm{Tr}(\mathbf{S} d\mathbf{E}) = \mathbf{S} \cdot d\mathbf{E} = \mathrm{Tr}(\boldsymbol{\tau} d\boldsymbol{\varepsilon}) = \boldsymbol{\tau} \cdot d\boldsymbol{\varepsilon} = J\boldsymbol{\sigma} \cdot d\boldsymbol{\varepsilon}$$

The conjugate variable pairs with respect to energy increments are $(\mathbf{P}, \mathbf{F})$, $(\mathbf{S}, \mathbf{E})$, and $(\boldsymbol{\tau}, \boldsymbol{\varepsilon})$. The energy increment per unit mass is found by dividing each by ρ_0 or

$$dW(\text{per unit mass}) = \frac{\boldsymbol{\tau}}{\rho_0} \cdot d\boldsymbol{\varepsilon} = \frac{\boldsymbol{\sigma}}{\rho} \cdot d\boldsymbol{\varepsilon}$$

where ρ is current density (and $J = V/V_0 = \rho_0/\rho$).

8.4 Isotopic, Hyperelastic Materials

These sections restrict attention to isotropic materials.

8.4.1 Stress Invariants

Isotropic, hyperelastic materials can be derived by defining an energy function in terms of invariants of $\mathbf{F}$ or other large-strain tensors. One approach is based on invariants of the left, Cauchy-Green tensor:

$$I_1 = \mathrm{Tr}(\mathbf{B}) = B_{11} + B_{22} + B_{33} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \tag{8.19}$$

$$I_2 = \frac{1}{2}\left(I_1^2 - \mathbf{B} \cdot \mathbf{B}\right) = \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2 \tag{8.20}$$

$$I_3 = \det(\mathbf{B}) = (\det(\mathbf{F}))^2 = J^2 = \lambda_1^2\lambda_2^2\lambda_3^2 \tag{8.21}$$

where λ_i are the principle stretches of the deformation. Note that $\mathbf{C}$ has the same invariants. Sometimes modified invariants are used instead, such as $\overline{I_1} = I_1/J^{2/3}$ and $\overline{I_2} = I_2/J^{4/3}$. Ogden (1972) suggests generlized invariants of the form

$$\left(\lambda_1^\alpha\left(\lambda_2^\beta + \lambda_3^\beta\right) + \lambda_2^\alpha\left(\lambda_1^\beta + \lambda_3^\beta\right) + \lambda_3^\alpha\left(\lambda_1^\beta + \lambda_2^\beta\right)\right)(\lambda_1\lambda_2\lambda_3)^\gamma - 6$$

For modeling isotropic materials, these invariants are chosen such that they are independent of permutation of the indices. For example

$$\begin{aligned}
\alpha = 2,\ \beta = \gamma = 0 &\implies 2(I_1 - 3) \\
\alpha = 2,\ \beta = 0,\ \gamma = -\frac{2}{3} &\implies 2(\overline{I_1} - 3) \\
\alpha = \beta = 2,\ \gamma = 0 &\implies 2(I_2 - 3) \\
\alpha = \beta = 2,\ \gamma = -\frac{4}{3} &\implies 2(\overline{I_2} - 3) \\
\alpha = \beta = 0,\ \gamma = 2 &\implies 6(I_3 - 1) \\
\alpha = \beta = 0,\ \gamma = 1 &\implies 6(J - 1) \\
\alpha = \beta = 2,\ \gamma = -2 &\implies 2\left(\frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2} + \frac{1}{\lambda_3^2}\right) = 2\left(\frac{I_2}{I_3} - 3\right) \\
\alpha = -2,\ \beta = \gamma = 0 &\implies 2\left(\frac{I_2}{I_3} - 3\right)
\end{aligned}$$

Next the strain energy is written as a function of three invariants, with the common forms being $W(I_1, I_2, J)$, $W(\overline{I_1}, \overline{I_2}, J)$ and $W(\lambda_1, \lambda_2, \lambda_3)$. The following sections find various stresses from this isotropic forms for energy.

8.4.2 First Piola-Kirchoff Stresses

The first Piola-Kirchoff stress expands in terms of invariants to:

$$\mathbf{P} = \frac{\partial W}{\partial \mathbf{F}} = \frac{\partial W}{\partial I_1}\frac{\partial I_1}{\partial \mathbf{F}} + \frac{\partial W}{\partial I_2}\frac{\partial I_2}{\partial \mathbf{F}} + \frac{\partial W}{\partial J}\frac{\partial J}{\partial \mathbf{F}}$$

The needed derivatives are:

$$I_1 = \sum_k \sum_l F_{kl}^2 = ||\mathbf{F}||_F^2, \quad I_2 = \frac{1}{2}\left(I_1^2 - \sum_k \sum_l B_{kl}^2\right), \quad B_{kl} = \sum_m F_{km}F_{lm} \tag{8.22}$$

$$\frac{\partial I_1}{\partial \mathbf{F}} = 2\mathbf{F}, \quad \frac{\partial I_2}{\partial \mathbf{F}} = 2\mathbf{F}\left(I_1\mathbf{I} - \mathbf{F}^T\mathbf{F}\right), \quad \frac{\partial J}{\partial \mathbf{F}} = J\mathbf{F}^{-T}, \quad \frac{\partial I_3}{\partial \mathbf{F}} = 2J^2\mathbf{F}^{-T} \tag{8.23}$$

$$\frac{\partial \overline{I_1}}{\partial \mathbf{F}} = \frac{2}{J^{2/3}}\left(\mathbf{F} - \frac{I_1\mathbf{F}^{-T}}{3}\right) = \frac{2\mathbf{F}}{J^{2/3}} - \frac{2\overline{I_1}\mathbf{F}^{-T}}{3} \tag{8.24}$$

$$\frac{\partial \overline{I_2}}{\partial \mathbf{F}} = \frac{2\overline{I_1}\mathbf{F}}{J^{2/3}} - \frac{2\mathbf{F}\mathbf{F}^T\mathbf{F}}{J^{4/3}} - \frac{4\overline{I_2}\mathbf{F}^{-T}}{3} \tag{8.25}$$

The final stresses from $W(I_1, I_2, J)$ are:

$$\mathbf{P} = \left(2\mathbf{F}, 2\mathbf{F}\left(I_1\mathbf{I} - \mathbf{F}^T\mathbf{F}\right), J\mathbf{F}^{-T}\right) \cdot \left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right)$$

The final stresses from $W(\overline{I_1}, \overline{I_2}, J)$ are

$$\mathbf{P} = \left(2\mathbf{F}\left(\frac{1}{J^{2/3}} - \frac{\overline{I_1}\mathbf{F}^{-1}\mathbf{F}^{-T}}{3}\right), 2\mathbf{F}\left(\frac{\overline{I_1}\mathbf{I}}{J^{2/3}} - \frac{\mathbf{F}^T\mathbf{F}}{J^{4/3}} - \frac{2\overline{I_2}\mathbf{F}^{-1}\mathbf{F}^{-T}}{3}\right), J\mathbf{F}^{-T}\right) \cdot \left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right)$$

If needed, derivatives of $\mathbf{B}$ and $\mathbf{C}$ with respect to $\mathbf{F}$ are

$$B_{ij} = \sum_k F_{ik}F_{jk}, \quad \frac{\partial B_{kl}}{\partial F_{ij}} = \delta_{ki}F_{lj} + \delta_{li}F_{kj}$$

$$C_{ij} = \sum_k F_{ki}F_{kj}, \quad \frac{\partial C_{kl}}{\partial F_{ij}} = \delta_{ki}F_{jl} + \delta_{li}F_{jk}$$

8.4.3 Second Piola-Kirchoff Stresses

The second Piola-Kirchoff stress from $W(I_1, I_2, J)$ are:

$$\mathbf{S} = \mathbf{F}^{-1}\mathbf{P} = 2\frac{\partial W}{\partial \mathbf{C}} = 2\left(\mathbf{I}, I_1\mathbf{I} - \mathbf{C}, \frac{J}{2}\mathbf{C}^{-1}\right) \cdot \left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right)$$

The second version used derivatives of $\mathbf{C}$ as

$$\frac{\partial I_1}{\partial \mathbf{C}} = \mathbf{I}, \qquad \frac{\partial I_2}{\partial \mathbf{C}} = I_1\mathbf{I} - \mathbf{C}, \quad \text{and} \quad \frac{\partial J}{\partial \mathbf{C}} = \frac{J}{2}\mathbf{C}^{-1}$$

The stresses from $W(\overline{I_1},\overline{I_2},J)$ are

$$\mathbf{S} = 2\left(\frac{1}{J^{2/3}} - \frac{\overline{I_1}\mathbf{C}^{-1}}{3}, \frac{\overline{I_1}\mathbf{I}}{J^{2/3}} - \frac{\mathbf{C}}{J^{4/3}} - \frac{2\overline{I_2}\mathbf{C}^{-1}}{3}, \frac{J}{2}\mathbf{C}^{-1}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right)$$

The version used new derivatives of $\mathbf{C}$ as

$$\frac{\partial \overline{I_1}}{\partial \mathbf{C}} = \frac{1}{J^{2/3}} - \frac{2\overline{I_1}\mathbf{C}^{-1}}{3}, \qquad \frac{\partial \overline{I_2}}{\partial \mathbf{C}} = \frac{\overline{I_1}\mathbf{I}}{J^{2/3}} - \frac{\mathbf{C}}{J^{4/3}} - \frac{4\overline{I_2}\mathbf{C}^{-1}}{3}$$

8.4.4 Cauchy and Kirchoff Stresses

The Kirchoff stress (and Cauchy stress is $\boldsymbol{\sigma} = \boldsymbol{\tau}/J$) using $W(I_1,I_2,J)$ is

$$\boldsymbol{\tau} = \mathbf{F}\mathbf{S}\mathbf{F}^T = 2\mathbf{F}\frac{\partial W}{\partial \mathbf{C}}\mathbf{F}^T = 2\left(\mathbf{B}, I_1\mathbf{B} - \mathbf{B}^2, \frac{J}{2}I\right)\cdot\left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right)$$

This result also follows from direct differentiation by:

$$\begin{aligned}
\frac{\partial W}{\partial \mathbf{C}} &= \frac{\partial W}{\partial I_1}\mathbf{I} + \frac{\partial W}{\partial I_2}(I_1\mathbf{I} - \mathbf{C}) + \frac{\partial W}{\partial J}\frac{J}{2}\mathbf{C}^{-1} \\
\mathbf{F}\frac{\partial W}{\partial \mathbf{C}}\mathbf{F}^T &= \mathbf{B}\left(\frac{\partial W}{\partial I_1}\mathbf{I} + \frac{\partial W}{\partial I_2}(I_1\mathbf{I} - \mathbf{B}) + \frac{\partial W}{\partial J}\frac{J}{2}\mathbf{B}^{-1}\right) \\
&= \mathbf{B}\frac{\partial W}{\partial \mathbf{B}}
\end{aligned}$$

where as for $\mathbf{C}$, the $\mathbf{B}$ derivatives are

$$\frac{\partial I_1}{\partial \mathbf{B}} = \mathbf{I}, \qquad \frac{\partial I_2}{\partial \mathbf{B}} = I_1\mathbf{I} - \mathbf{B}, \quad \text{and} \quad \frac{\partial J}{\partial \mathbf{B}} = \frac{J}{2}\mathbf{B}^{-1}$$

The stresses from $W(\overline{I_1},\overline{I_2},J)$ are

$$\boldsymbol{\tau} = 2\left(\frac{1}{J^{2/3}}\left(\mathbf{B} - \frac{I_1\mathbf{I}}{3}\right), \frac{1}{J^{4/3}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2\mathbf{I}}{3}\right), \frac{J}{2}\mathbf{I}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right)$$

Because $\mathbf{B}$ is symmetric (and therefore $\mathrm{Tr}(\mathbf{B}^2) = \mathbf{B}\cdot\mathbf{B}$ and $\mathrm{Tr}(I_1\mathbf{B} - \mathbf{B}^2) = I_1^2 - \mathbf{B}\cdot\mathbf{B} = 2I_2$), the second version can be written

$$\boldsymbol{\tau} = 2\left(\frac{1}{J^{2/3}}\mathrm{dev}(\mathbf{B}), \frac{1}{J^{4/3}}\mathrm{dev}(I_1\mathbf{B} - \mathbf{B}^2), \frac{J}{2}\mathbf{I}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right)$$

8.4.5 Cauchy Pressure and Deviatoric Stress

The pressure ($P = -\mathrm{Tr}(\boldsymbol{\sigma})/3$) can be found (making use of $\mathrm{Tr}(\mathrm{dev}(\cdot)) = 0$) from two types of invariants:

$$P = -\frac{\partial W}{\partial J} - \frac{2}{3J}\left[I_1\frac{\partial W}{\partial I_1} + 2I_2\frac{\partial W}{\partial I_2}\right] \tag{8.26}$$

$$P = -\frac{\partial W}{\partial J} \tag{8.27}$$

Thus the deviatoric Cauchy stresses are ($\mathbf{s} = \boldsymbol{\sigma} + P\mathbf{I}$):

$$\mathbf{s} = \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\text{dev}(\mathbf{B}) + \frac{\partial W}{\partial I_2}\text{dev}\left(I_1\mathbf{B} - \mathbf{B}^2\right)\right] \tag{8.28}$$

$$\mathbf{s} = \frac{2}{J^{5/3}}\left[\frac{\partial W}{\partial \overline{I}_1}\text{dev}(\mathbf{B}) + \frac{1}{J^{2/3}}\frac{\partial W}{\partial \overline{I}_2}\text{dev}(I_1\mathbf{B} - \mathbf{B}^2)\right] \tag{8.29}$$

The incremental bulk modulus is

$$\frac{1}{K(P)} = -\frac{d\ln V}{dP} = -\frac{d\ln J}{dP} \qquad \text{or} \qquad K = -J\frac{dP}{dJ} \tag{8.30}$$

For the two types of invariants:

$$K = J\frac{\partial^2 W}{\partial J^2} + \frac{2}{3}\left[I_1\left(\frac{\partial^2 W}{\partial I_1 \partial J} - \frac{1}{J}\frac{\partial W}{\partial I_1}\right) + 2I_2\left(\frac{\partial^2 W}{\partial I_2 \partial J} - \frac{1}{J}\frac{\partial W}{\partial I_2}\right)\right]$$

$$K = J\frac{\partial^2 W}{\partial J^2}$$

8.4.6 Tangent Stiffness Matrix

Writing out the top-half of the symmetric second Piola Kirchoff stress

$$\mathbf{S} = 2\begin{pmatrix} W_1 + (I_1 - C_{11})W_2 + \frac{J}{2}C_{11}^{-1}W_J & -C_{12}W_2 + \frac{J}{2}C_{12}^{-1}W_J & -C_{13}W_2 + \frac{J}{2}C_{13}^{-1}W_J \\ \cdots & W_1 + (I_1 - C_{22})W_2 + \frac{J}{2}C_{22}^{-1}W_J & -C_{23}W_2 + \frac{J}{2}C_{23}^{-1}W_J \\ \cdots & \cdots & W_1 + (I_1 - C_{33})W_2 + \frac{J}{2}C_{33}^{-1}W_J \end{pmatrix}$$

where

$$W_1 = \frac{\partial W}{\partial I_1} \qquad W_2 = \frac{\partial W}{\partial I_2} \qquad W_J = \frac{\partial W}{\partial J}$$

By symmetry, the 81 elements in $\mathbf{C}$ reduce to 21, which are more than contained in the six matrices found by differentiating $\mathbf{S}$ with respect to C_{ij} (top halves only).

From Zienkiewiscz and Taylor (multiplied by J), the tangent stiffness tensor calculated by above methods for $W(I_1, I_2, J)$ is:

$$c_{ijkl} = 4\boldsymbol{b}_{1,ij}\begin{bmatrix} \frac{\partial^2 W}{\partial I_1^2} & \frac{\partial^2 W}{\partial I_1 \partial I_2} & \frac{\partial^2 W}{\partial I_1 \partial J} \\ \frac{\partial^2 W}{\partial I_2 \partial I_1} & \frac{\partial^2 W}{\partial I_2^2} & \frac{\partial^2 W}{\partial I_2 \partial J} \\ \frac{\partial^2 W}{\partial J \partial I_1} & \frac{\partial^2 W}{\partial J \partial I_2} & \frac{\partial^2 W}{\partial J^2} \end{bmatrix}\boldsymbol{b}_{1,kl}^T + \boldsymbol{b}_2\begin{bmatrix} 4\frac{\partial W}{\partial I_2} \\ \frac{\partial W}{\partial J} \end{bmatrix} \tag{8.31}$$

where

$$\boldsymbol{b}_{1,ij} = \left(B_{ij}, I_1 B_{ij} - \sum_m B_{im}B_{mj}, \frac{J}{2}\delta_{ij}\right)$$

$$\boldsymbol{b}_2 = \left(B_{ij}B_{kl} - \frac{1}{2}\left(B_{ik}B_{jl} + B_{il}B_{jk}\right), J\left[\delta_{ij}\delta_{kl} - \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\right]\right)$$

and $\boldsymbol{b}_{1,kl}$ replaces i and j with k and l. If W does not depend on I_2, this result simplifies to

$$\frac{c_{ijkl}}{J} = \frac{4}{J}B_{ij}B_{kl}\frac{\partial^2 W}{\partial I_1^2} + 2(B_{ij}\delta_{kl} + B_{kl}\delta_{ij})\frac{\partial^2 W}{\partial I_1 \partial J} + \left(J\frac{\partial^2 W}{\partial J^2} + \frac{\partial W}{\partial J}\right)\delta_{ij}\delta_{kl} - \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\frac{\partial W}{\partial J} \tag{8.32}$$

When using modified invariants,or $W(\overline{I_1},\overline{I_2},J)$, along with differentials:

$$\begin{aligned}
\frac{\partial\phi}{\partial I_1} &= \frac{\partial\phi}{\partial\overline{I_1}}\frac{\partial\overline{I_1}}{\partial I_1}=\frac{1}{J^{2/3}}\frac{\partial\phi}{\partial\overline{I_1}}\\
\frac{\partial\phi}{\partial I_2} &= \frac{\partial\phi}{\partial\overline{I_2}}\frac{\partial\overline{I_2}}{\partial I_2}=\frac{1}{J^{4/3}}\frac{\partial\phi}{\partial\overline{I_4}}\\
\frac{\partial\phi}{\partial J} &= \frac{\partial\phi}{\partial\overline{I_1}}\frac{\partial\overline{I_1}}{\partial J}+\frac{\partial\phi}{\partial\overline{I_2}}\frac{\partial\overline{I_2}}{\partial J}+\frac{\partial\phi}{\partial J}=-\frac{2\overline{I_1}}{3J}\frac{\partial\phi}{\partial\overline{I_1}}-\frac{4\overline{I_2}}{3J}\frac{\partial\phi}{\partial\overline{I_2}}+\frac{\partial\phi}{\partial J}
\end{aligned}$$

the needed first derivatives are:

$$\frac{\partial W}{\partial I_1}=\frac{1}{J^{2/3}}\frac{\partial W}{\partial\overline{I_1}}\qquad\frac{\partial W}{\partial I_2}=\frac{1}{J^{4/3}}\frac{\partial W}{\partial\overline{I_2}}\qquad\frac{\partial W}{\partial J}=-\frac{2\overline{I_1}}{3J}\frac{\partial W}{\partial\overline{I_1}}-\frac{4\overline{I_2}}{3J}\frac{\partial W}{\partial\overline{I_2}}+\frac{\partial W}{\partial J}$$

The needed second derivatives are:

$$\frac{\partial^2 W}{\partial I_1^2}=\frac{1}{J^{4/9}}\frac{\partial^2 W}{\partial\overline{I_1}^2}\qquad\frac{\partial^2 W}{\partial I_2^2}=\frac{1}{J^{16/9}}\frac{\partial^2 W}{\partial\overline{I_2}^2}\qquad\frac{\partial^2 W}{\partial I_2\partial I_1}=\frac{1}{J^{8/3}}\frac{\partial^2 W}{\partial\overline{I_2}\,\overline{I_1}}$$

$$\frac{\partial^2 W}{\partial I_1\partial J}=\frac{1}{J^{2/3}}\left(-\frac{2}{3J}\frac{\partial W}{\partial\overline{I_1}}-\frac{2\overline{I_1}}{3J}\frac{\partial^2 W}{\partial\overline{I_1}^2}-\frac{4\overline{I_2}}{3J}\frac{\partial^2 W}{\partial\overline{I_1}\,\overline{I_2}}+\frac{\partial^2 W}{\partial\overline{I_1}\partial J}\right)$$

$$\frac{\partial^2 W}{\partial I_2\partial J}=\frac{1}{J^{4/3}}\left(-\frac{2\overline{I_1}}{3J}\frac{\partial^2 W}{\partial\overline{I_1}\,\overline{I_2}}-\frac{4}{3J}\frac{\partial W}{\partial\overline{I_2}}-\frac{4\overline{I_2}}{3J}\frac{\partial^2 W}{\partial\overline{I_2}^2}+\frac{\partial^2 W}{\partial\overline{I_2}\partial J}\right)$$

$$\begin{aligned}
\frac{\partial^2 W}{\partial J^2} &= \frac{10\overline{I_1}}{9J^2}\frac{\partial W}{\partial\overline{I_1}}+\frac{4\overline{I_1}^2}{9J^2}\frac{\partial^2 W}{\partial\overline{I_1}^2}+\frac{28\overline{I_2}}{9J^2}\frac{\partial W}{\partial\overline{I_2}}+\frac{16\overline{I_2}^2}{9J^2}\frac{\partial^2 W}{\partial\overline{I_2}^2}+\frac{16\overline{I_1}\,\overline{I_2}}{9J^2}\frac{\partial^2 W}{\partial\overline{I_1}\,\overline{I_2}}\\
&\quad -\frac{4\overline{I_1}}{3J}\frac{\partial^2 W}{\partial\overline{I_1}\partial J}-\frac{8\overline{I_2}}{3J}\frac{\partial^2 W}{\partial\overline{I_2}\partial J}+\frac{\partial^2 U}{\partial J^2}
\end{aligned}$$

For a special where $W(\overline{I_1},J)$ and $\partial W/\partial J$ is independent of $\overline{I_1}$, the tangent stiffness tensor becomes:

$$\begin{aligned}
\frac{c_{ijkl}}{J} &= \frac{4}{J}B_{ij}B_{kl}\frac{1}{J^{4/9}}\frac{\partial^2 W}{\partial\overline{I_1}^2}-2(B_{ij}\delta_{kl}+B_{kl}\delta_{ij})\left(\frac{2}{3J^{5/3}}\frac{\partial W}{\partial\overline{I_1}}+\frac{2\overline{I_1}}{3J^{5/3}}\frac{\partial^2 W}{\partial\overline{I_1}^2}\right)\\
&\quad+\left(\frac{4\overline{I_1}}{9J}\frac{\partial W}{\partial\overline{I_1}}+\frac{4\overline{I_1}^2}{9J}\frac{\partial^2 W}{\partial\overline{I_1}^2}+J\frac{\partial^2 U}{\partial J^2}+\frac{\partial U}{\partial J}\right)\delta_{ij}\delta_{kl}-\big(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\big)\left(\frac{\partial U}{\partial J}-\frac{2\overline{I_1}}{3J}\frac{\partial W}{\partial\overline{I_1}}\right)
\end{aligned}$$

Collecting terms and revising some gives

$$\begin{aligned}
\frac{c_{ijkl}}{J} &= \frac{4}{3J}\left(\overline{I_1}\left(\frac{1}{2}\big(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\big)-\frac{1}{3}\delta_{ij}\delta_{kl}\right)-\overline{B}^d_{ij}\delta_{kl}-\overline{B}^d_{kl}\delta_{ij}\right)\frac{\partial W}{\partial\overline{I_1}}\\
&\quad+\frac{4}{J}\overline{B}^d_{ij}\overline{B}^d_{kl}\frac{\partial^2 W}{\partial\overline{I_1}^2}+\left(J\frac{\partial^2 U}{\partial J^2}+\frac{\partial U}{\partial J}\right)\delta_{ij}\delta_{kl}-\big(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\big)\frac{\partial U}{\partial J}
\end{aligned}\tag{8.33}$$

where $\overline{B}^d_{ij}=J^{-2/3}B_{ij}-\overline{I_1}\delta_{ij}/3$ is deviatoric, modified B tensor.

8.4.7 Eigenvector Analysis

The real and symmetric matrices, $\mathbf{U}$ and $\mathbf{V}$ can be diagonalized to

$$\mathbf{U} = \mathsf{N}[\Lambda]\mathsf{N}^T = \sum_i \lambda_i \boldsymbol{N}_i \otimes \boldsymbol{N}_i \quad \text{and} \quad \mathbf{V} = \mathsf{n}[\Lambda]\mathsf{n}^T = \sum_i \lambda_i \boldsymbol{n}_i \otimes \boldsymbol{n}_i$$

where $[\Lambda] = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ is diagonal matrix of eigenvalues (which are the same for $\mathbf{U}$ and $\mathbf{V}$), N is matrix with columns $\boldsymbol{N}_i$ as the i^{th} eigenvector of $\mathbf{U}$, and n is matrix with columns $\boldsymbol{n}_i$ as the i^{th} eigenvector of $\mathbf{V}$. The eigenvectors are normalized and orthogonal such that $\boldsymbol{N}_i \cdot \boldsymbol{N}_j = \delta_{ij}$ and $\boldsymbol{n}_i \cdot \boldsymbol{n}_j = \delta_{ij}$. Through polar decomposition, $\mathbf{F}$ and its inverse can be written as

$$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R} = \mathsf{n}[\Lambda]\mathsf{N}^T = \sum_i \lambda_i \boldsymbol{n}_i \otimes \boldsymbol{N}_i \quad \text{and} \quad \mathbf{F}^{-1} = \mathsf{N}\left[\frac{1}{\Lambda}\right]\mathsf{n}^T = \sum_i \frac{1}{\lambda_i} \boldsymbol{N}_i \otimes \boldsymbol{n}_i$$

which follows by using $\mathsf{n} = \mathbf{R}\mathsf{N}$ and $[1/\Lambda] = \text{diag}(1/\lambda_1, 1/\lambda_2, 1/\lambda_3)$. The right and left Cauchy tensors are:

$$\mathbf{C} = \mathsf{N}[\Lambda^2]\mathsf{N}^T = \sum_i \lambda_i^2 \boldsymbol{N}_i \otimes \boldsymbol{N}_i \quad \text{and} \quad \mathbf{B} = \mathsf{n}[\Lambda^2]\mathsf{n}^T = \sum_i \lambda_i^2 \boldsymbol{n}_i \otimes \boldsymbol{n}_i$$

Because energy for an isotropic material depends only on invariants (*i.e.*, functions of the eigenvalues), the first Piola-Kirchoff stress ($\mathbf{P}$), second Piola-Kirchoff stress ($\mathbf{S}$), Kirchoff stress ($\boldsymbol{\tau}$), and Cauchy stress ($\boldsymbol{\sigma}$) are:

$$\begin{aligned}
\mathbf{P} &= \frac{\partial W}{\partial \mathbf{F}} = \mathsf{n}\,\text{diag}\left[\frac{\partial W}{\partial \lambda_i}\right]\mathsf{N}^T = \sum_i \frac{\partial W}{\partial \lambda_i} \boldsymbol{n}_i \otimes \boldsymbol{N}_i \\
\mathbf{S} = \mathbf{F}^{-1}\mathbf{P} &= \mathsf{N}\,\text{diag}\left[\frac{1}{\lambda_i}\frac{\partial W}{\partial \lambda_i}\right]\mathsf{N}^T = \sum_i \frac{1}{\lambda_i}\frac{\partial W}{\partial \lambda_i} \boldsymbol{N}_i \otimes \boldsymbol{N}_i \\
\boldsymbol{\tau} = \mathbf{P}\mathbf{F}^T &= \mathsf{n}\,\text{diag}\left[\lambda_i \frac{\partial W}{\partial \lambda_i}\right]\mathsf{n}^T = \sum_i \lambda_i \frac{\partial W}{\partial \lambda_i} \boldsymbol{n}_i \otimes \boldsymbol{n}_i \\
\boldsymbol{\sigma} = \frac{\boldsymbol{\tau}}{J} &= \mathsf{n}\,\text{diag}\left[\frac{\lambda_i}{J}\frac{\partial W}{\partial \lambda_i}\right]\mathsf{n}^T = \sum_i \frac{\lambda_i}{J}\frac{\partial W}{\partial \lambda_i} \boldsymbol{n}_i \otimes \boldsymbol{n}_i
\end{aligned}$$

These relations apply only for isotropic materials because for anisotropic materials, the stress will depend on the eigenvectors as well.

8.4.8 Uniaxial Loading

Under uniaxial loading to extension λ, and isotropic material will have equal elogations in the tranverse direction of λ_T. The volume change gives $J = \lambda\lambda_T^2$ or $\lambda_T = \sqrt{J/\lambda}$. This section gives some general results for four types of uniaxial loading — simple tension where transverse stresses are zero, incompressible extension where $J = 1$, constrained tension where $\lambda_T = 1$ or $J = \lambda$, and hydrostatic tension where $J = \lambda^3$.

In uniaxial loading in the x direction, only diagonal elements of $\mathbf{F}$ and $\mathbf{B}$ are nonzero and $\mathbf{F} = \text{diag}(\lambda, \sqrt{J/\lambda}, \sqrt{J/\lambda})$ and $\mathbf{B} = \mathbf{C} = \text{diag}(\lambda^2, J/\lambda, J/\lambda)$. Other terms are

$$I_1 = \lambda^2 + \frac{2J}{\lambda}, \qquad I_2 = 2J\lambda + \frac{J^2}{\lambda^2} \quad I_1\mathbf{B} - \mathbf{B}^2 = \text{diag}\left(2J\lambda, \frac{J(J+\lambda^3)}{\lambda^2}, \frac{J(J+\lambda^3)}{\lambda^2}\right)$$

Using standard invariants, the axial and transverse stresses in general Cauchy stresses are:

$$\sigma_{xx} = \frac{\partial W}{\partial J} + \frac{2\lambda}{J}\left(\lambda\frac{\partial W}{\partial I_1} + 2J\frac{\partial W}{\partial I_2}\right) \qquad \sigma_{yy} = \frac{\partial W}{\partial J} + \frac{2}{\lambda^2}\left(\lambda\frac{\partial W}{\partial I_1} + (J+\lambda^3)\frac{\partial W}{\partial I_2}\right)$$

For simple tension, eliminate $\partial W/\partial J$ using $\sigma_{yy}=0$ and substitute to get

$$\sigma_{xx}=\frac{2(\lambda^3-J)}{J\lambda^2}\left(\lambda\frac{\partial W}{\partial I_1}+J\frac{\partial W}{\partial I_2}\right)\qquad \sigma_{yy}=0$$

For incompressible tension

$$\sigma_{xx}=\frac{\partial W}{\partial J}+2\lambda\left(\lambda\frac{\partial W}{\partial I_1}+2\frac{\partial W}{\partial I_2}\right)\qquad \sigma_{yy}=\frac{\partial W}{\partial J}+\frac{2}{\lambda^2}\left(\lambda\frac{\partial W}{\partial I_1}+(1+\lambda^3)\frac{\partial W}{\partial I_2}\right)$$

For constrained tension

$$\sigma_{xx}=\frac{\partial W}{\partial J}+2\lambda\left(\frac{\partial W}{\partial I_1}+2\frac{\partial W}{\partial I_2}\right)\qquad \sigma_{yy}=\frac{\partial W}{\partial J}+\frac{2}{\lambda}\left(\frac{\partial W}{\partial I_1}+(1+\lambda^2)\frac{\partial W}{\partial I_2}\right)$$

For hydrostatic tension

$$\sigma_{xx}=\sigma_{yy}=\frac{\partial W}{\partial J}+\frac{2}{\lambda}\frac{\partial W}{\partial I_1}+4\lambda\frac{\partial W}{\partial I_2}$$

When using modified invariants, the new terms are

$$\overline{I_1}=\frac{2J+\lambda^3}{J^{2/3}\lambda}\quad \overline{I_2}=\frac{J+2\lambda^3}{J^{1/3}\lambda^2}\quad \mathrm{dev}(\mathbf{B})=\frac{(\lambda^3-J)}{3\lambda}\mathrm{diag}\,(2,-1,-1)$$

$$\mathrm{dev}(I_1\mathbf{B}-\mathbf{B}^2)=\frac{J(\lambda^3-J)}{3\lambda^2}\mathrm{diag}\,(2,-1,-1)$$

The general Cauchy stresses are:

$$\sigma_{xx}=\frac{\partial W}{\partial J}+\frac{4(\lambda^3-J)}{3J^{5/3}\lambda^2}\left(\lambda\frac{\partial W}{\partial \overline{I_1}}+J^{1/3}\frac{\partial W}{\partial \overline{I_2}}\right)\qquad \sigma_{yy}=\frac{\partial W}{\partial J}-\frac{2(\lambda^3-J)}{3J^{5/3}\lambda^2}\left(\lambda\frac{\partial W}{\partial \overline{I_1}}+J^{1/3}\frac{\partial W}{\partial \overline{I_2}}\right)$$

For simple tension, eliminate $\partial W/\partial J$ using $\sigma_{yy}=0$ and substitute to get

$$\sigma_{xx}=\frac{2(\lambda^3-J)}{J^{5/3}\lambda^2}\left(\lambda\frac{\partial W}{\partial \overline{I_1}}+J^{1/3}\frac{\partial W}{\partial \overline{I_2}}\right)\qquad \sigma_{yy}=0$$

For incompressible tension

$$\sigma_{xx}=\frac{\partial W}{\partial J}+\frac{4(\lambda^3-1)}{3\lambda^2}\left(\lambda\frac{\partial W}{\partial \overline{I_1}}+\frac{\partial W}{\partial \overline{I_2}}\right)\qquad \sigma_{yy}=\frac{\partial W}{\partial J}-\frac{2(\lambda^3-1)}{3\lambda^2}\left(\lambda\frac{\partial W}{\partial \overline{I_1}}+\frac{\partial W}{\partial \overline{I_2}}\right)$$

For constrained tension

$$\sigma_{xx}=\frac{\partial W}{\partial J}+\frac{4(\lambda^2-1)}{3\lambda^{7/3}}\left(\lambda^{2/3}\frac{\partial W}{\partial \overline{I_1}}+\frac{\partial W}{\partial \overline{I_2}}\right)\qquad \sigma_{yy}=\frac{\partial W}{\partial J}-\frac{2(\lambda^2-1)}{3\lambda^{7/3}}\left(\lambda^{2/3}\frac{\partial W}{\partial \overline{I_1}}+\frac{\partial W}{\partial \overline{I_2}}\right)$$

For hydrostatic tension

$$\sigma_{xx}=\sigma_{yy}=\frac{\partial W}{\partial J}$$

When using eigenvalues, the eigenvectors are along x, y, and z axes. The general stresses are:

$$\sigma_{xx}=\frac{\lambda}{J}\frac{\partial W}{\partial \lambda_1}\qquad \sigma_{yy}=\frac{1}{\sqrt{J\lambda}}\frac{\partial W}{\partial \lambda_2}$$

When the material is isotropic, $\partial W/\partial \lambda_i$ must be the same function, $f(\lambda_i, J)$, that depends only on λ_i and J. For simple tension, solve $f(\sqrt{J/\lambda}, J) = 0$ for J and substitute into σ_{xx}. Additional results cannot be written down without specifying more details about $f(\lambda_i, J)$. For incompressible tension:

$$\sigma_{xx} = \lambda f(\lambda, 1) \qquad \sigma_{yy} = \frac{f\left(\frac{1}{\sqrt{\lambda}}, 1\right)}{\sqrt{\lambda}}$$

For constrained tension

$$\sigma_{xx} = f(\lambda, \lambda) \qquad \sigma_{yy} = \frac{f(1, \lambda)}{\lambda}$$

For hydrostatic tension

$$\sigma_{xx} = \sigma_{yy} = \frac{f(\lambda, \lambda^3)}{\lambda^2}$$

8.4.9 Linear Shear Loading

In linear shear loading, $F_{ii} = 1$ and $F_{12} = \gamma$ (which is measure of shear strain) and $J = 1$. The $\mathbf{B}$ tensor is

$$\mathbf{B} = \begin{pmatrix} 1+\gamma^2 & \gamma & 0 \\ \gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The eigenvalues and normalize, orthogonal eigenvectors are:

$$\begin{aligned}
\lambda_1^2 &= \frac{1}{2}\left(2+\gamma^2+\gamma\sqrt{4+\gamma^2}\right) \\
\lambda_2^2 &= \frac{1}{2}\left(2+\gamma^2-\gamma\sqrt{4+\gamma^2}\right) \\
\lambda_3^2 &= 1 \\
\boldsymbol{n}_1 &= \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4+\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma+\sqrt{4+\gamma^2}\right), 1, 0\right) \\
\boldsymbol{n}_2 &= \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4-\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma-\sqrt{4+\gamma^2}\right), 1, 0\right) \\
\boldsymbol{n}_3 &= (0, 0, 1)
\end{aligned}$$

The invariants in the extra tensor are

$$I_1 = \overline{I_1} = 3+\gamma^2 \qquad I_2 = \overline{I_2} = 3+\gamma^2$$

$$I_1\mathbf{B} - \mathbf{B}^2 = \begin{pmatrix} 2+\gamma^2 & \gamma & 0 \\ \gamma & 2 & 0 \\ 0 & 0 & 2+\gamma^2 \end{pmatrix}$$

Using standard invariants, the axial and transverse stresses in general Cauchy stresses are: The Kirchoff stresses (which equal Cauchy strresses because $J = 1$) becomes:

$$\boldsymbol{\tau} = 2\left(\begin{pmatrix} 1+\gamma^2 & \gamma & 0 \\ \gamma & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 2+\gamma^2 & \gamma & 0 \\ \gamma & 2 & 0 \\ 0 & 0 & 2+\gamma^2 \end{pmatrix}, \frac{1}{2}\mathbf{I}\right) \cdot \left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right)$$

Explicitly, the non-zero stresses are

$$\begin{aligned}
\tau_{xx} &= 2\left(1+\gamma^2, 2+\gamma^2, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right) \\
\tau_{yy} &= 2\left(1, 2, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right) \\
\tau_{zz} &= 2\left(1, 2+\gamma^2, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right) \\
\tau_{xy} &= 2\gamma\left(\frac{\partial W}{\partial I_1} + \frac{\partial W}{\partial I_2}\right)
\end{aligned}$$

From $W(\overline{I_1}, \overline{I_2}, J)$ the stresses are

$$\boldsymbol{\tau} = 2\left(\begin{pmatrix} \frac{2\gamma^2}{3} & \gamma & 0 \\ \gamma & -\frac{\gamma^2}{3} & 0 \\ 0 & 0 & -\frac{\gamma^2}{3} \end{pmatrix}, \begin{pmatrix} \frac{\gamma^2}{3} & \gamma & 0 \\ \gamma & -\frac{2\gamma^2}{3} & 0 \\ 0 & 0 & \frac{\gamma^2}{3} \end{pmatrix}, \frac{1}{2}\mathbf{I}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right)$$

Explicitly, the non-zero stresses are

$$\begin{aligned}
\tau_{xx} &= 2\left(\frac{2\gamma^2}{3}, \frac{\gamma^2}{3}, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right) \\
\tau_{yy} &= 2\left(-\frac{\gamma^2}{3}, -\frac{2\gamma^2}{3}, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right) \\
\tau_{zz} &= 2\left(-\frac{\gamma^2}{3}, \frac{\gamma^2}{3}, \frac{1}{2}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right) \\
\tau_{xy} &= 2\gamma\left(\frac{\partial W}{\partial \overline{I_1}} + \frac{\partial W}{\partial \overline{I_2}}\right)
\end{aligned}$$

From eigenvalues and eigenvectors, the Kirchoff stresses are

$$\begin{aligned}
\boldsymbol{\tau} &= \left(\sqrt{\frac{1}{2}\left(2+\gamma^2+\gamma\sqrt{4+\gamma^2}\right)}\boldsymbol{n}_1\otimes\boldsymbol{n}_2, \sqrt{\frac{1}{2}\left(2+\gamma^2-\gamma\sqrt{4+\gamma^2}\right)}\boldsymbol{n}_1\otimes\boldsymbol{n}_2, \boldsymbol{n}_3\otimes\boldsymbol{n}_3\right) \\
&\quad \cdot\left(\frac{\partial W}{\partial \lambda_1}, \frac{\partial W}{\partial \lambda_2}, \frac{\partial W}{\partial \lambda_3}\right)
\end{aligned}$$

8.4.10 Dealing with Thermal and Moisture Strains

To handle thermal and moisture strains the deformation can be written as product of increments deformations:

$$\mathbf{F} = \prod_i d\mathbf{F}_i d\mathbf{F}_i^{(res)}$$

where each step has residual stress deformation, $d\mathbf{F}_i^{(res)}$, followed by mechanical deformation, $d\mathbf{F}_i$. For an isotropic materials and by assuming thermal expansion coefficient does not depend on deformation straight, all $d\mathbf{F}_i^{(res)}$ can be written as

$$d\mathbf{F}_i^{(res)} = d\lambda_i^{(res)}\mathbf{I} \qquad \text{where} \qquad d\lambda_i^{(res)} = \exp\left(\alpha dT_i + \beta dc_i\right)$$

where α and β are linear thermal and moisture expansion coefficients for increments in temperature and moisture of dT_i and dc_i. Because $d\mathbf{F}_i^{(res)}$ is diagonal, the total deformation gradient product can be rearranged to:

$$\mathbf{F} = \left(\prod_i d\mathbf{F}_i\right)\left(\prod_i d\mathbf{F}_i^{(res)}\right) = \mathbf{F}^*\mathbf{F}^{(res)}$$

and

$$\mathbf{F}^{(res)} = \lambda_{res}\mathbf{I} \qquad \text{where} \qquad \lambda_{res} = \exp(\alpha\Delta T + \beta\Delta c)$$

where ΔT and Δc are total temperature and moisture changes (or sums of dT_i and dc_i). In other words, a material that is deformation and subjected to change in temperature and moisture content is assumed to reach the final stress regardless of when the temperature and moisture changes are applied. For example, one can change temperature and then deform or deform first and then change temperature. A material to follows above conditions would get the same stress is these two cases.

The stresses (or any other prior results) should be found from $\mathbf{F}^*\mathbf{F}(\mathbf{F}^{(res)})^-1$, which is done by revising any result using

$$\mathbf{F} \to \mathbf{F}* = \frac{\mathbf{F}}{\lambda_{res}}, \quad \mathbf{B} \to \mathbf{B}^* = \frac{\mathbf{B}}{\lambda_{res}^2}, \quad J \to J^* = \frac{J}{\lambda_{res}^3}$$

$$I_1 \to I_1^* = \frac{I_1}{\lambda_{res}^2}, \quad I_2 \to I_2^* = \frac{I_2}{\lambda_{res}^2}, \quad \lambda_i^* = \frac{\lambda_i}{\lambda_{res}}$$

For example the Cauchy stress in vector form changes to

$$\boldsymbol{\sigma} = \frac{2}{J}\left(\mathbf{B}J_{res}^{1/3}, \frac{I_1\mathbf{B}-\mathbf{B}^2}{J_{res}^{1/3}}, \frac{J}{2}\mathbf{I}\right)\cdot\left(\frac{\partial W}{\partial I_1}, \frac{\partial W}{\partial I_2}, \frac{\partial W}{\partial J}\right) \tag{8.34}$$

where $J_{res} = \lambda_{res}^3$ and the derivatives are evaluated at I_I^*, I_2^*, and J^*. Using modified invariants, the results can be written as

$$\boldsymbol{\sigma} = \left(\frac{2J_{res}\text{dev}(\mathbf{B})}{J^{5/3}}, \frac{2J_{res}\text{dev}(I_1\mathbf{B}-\mathbf{B}^2)}{J^{7/3}}, \mathbf{I}\right)\cdot\left(\frac{\partial W}{\partial \overline{I_1}}, \frac{\partial W}{\partial \overline{I_2}}, \frac{\partial W}{\partial J}\right) \tag{8.35}$$

and the derivatives are evaluated at $\overline{I_I}^*$, $\overline{I_2}^*$, and J^*. With eigenvalues, use

$$\boldsymbol{\tau} = \sum_i \frac{\lambda_i}{J_{res}^{1/3}}\frac{\partial W}{\partial \lambda_i}\boldsymbol{n}_i \otimes \boldsymbol{n}_i$$

and derivatives are evaluated at λ_i^*.

When doing incremental deformation, $\mathbf{F}_{k+1} = \mathbf{dF}\cdot\mathbf{F}_k$ and incremental volume ratio is $dJ = |\mathbf{dF}| = V_{k+1}/V_k$, but J^* is V/V_{sf} where V_{sf} is the current stress free volume. For incremental deformation, $J_{k+1} = dJJ_k$, but we really want to increment ${J^*}_{k+1} = d{J^*}{J^*}_k$, which is

$${J^*}_{k+1} = \frac{V_{k+1}}{V_{sf,k+1}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}\frac{V_k}{V_{sf,k}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}J_{eff,k} = d{J^*}{J^*}_k$$

which implies that

$$dJ^* = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}} = dJ/d\lambda_{res}^3 \tag{8.36}$$

where

$$d\lambda_{res} = \exp(\alpha dT + \beta dc) \approx 1 + \alpha dT + \beta dc \tag{8.37}$$

where dT and dc are temperature and concentration changes on the current time step.

8.4.11 Small-Strain Expansion to Guide Neo-Hookean Materials

A neo-Hookean material extends small strain analysis to large deformation material while retain only two material properties. Potential energy functions can be suggested by looking and small-strain theory potential energy and replacing small terms with small-strain limits of large-strain invariants. The small-strain potential energy is:

$$W(\boldsymbol{\varepsilon}) = G\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} + \frac{\lambda}{2}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2$$

The small-strain limits (to second order needed for energy) of large deformation terms (using logarithmic strain) are:

$$\mathbf{F} = \exp(\boldsymbol{\varepsilon}) \implies \mathbf{B} = \mathbf{C} = \exp(2\boldsymbol{\varepsilon}) = \mathbf{I} + 2\boldsymbol{\varepsilon} + 2\boldsymbol{\varepsilon}^2 \text{ and } \mathbf{B}^2 = \mathbf{C}^2 = \exp(4\boldsymbol{\varepsilon}) = \mathbf{I} + 4\boldsymbol{\varepsilon} + 8\boldsymbol{\varepsilon}^2 \tag{8.38}$$

$$J = |\mathbf{F}| = \exp\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big) \implies J = 1 + \mathrm{Tr}(\boldsymbol{\varepsilon}) + \frac{1}{2}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2$$

Expanding in Taylor series to second order, we can recover small strain results in various forms:

$$\begin{aligned}
I_1 - 3 = \mathrm{Tr}(\mathbf{B}) - 3 \quad &\rightarrow \quad 2\mathrm{Tr}(\boldsymbol{\varepsilon}) + 2\mathrm{Tr}(\boldsymbol{\varepsilon}^2) = 2\mathrm{Tr}(\boldsymbol{\varepsilon}) + 2\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \\
\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \quad &= \quad \frac{1}{2}(I_1 - 3) - \mathrm{Tr}(\boldsymbol{\varepsilon}) \\
\overline{I_1} - 3 = \frac{\mathrm{Tr}(\mathbf{B})}{J^{2/3}} - 3 \quad &\rightarrow \quad -\frac{2}{3}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2 + 2\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \\
\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} \quad &= \quad \frac{1}{2}(\overline{I_1} - 3) + \frac{1}{3}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2
\end{aligned}$$

Substituting each version into W gives two neo-Hookean materials

$$\begin{aligned}
W\big(I_1, \mathrm{Tr}(\boldsymbol{\varepsilon})\big) \quad &= \quad \frac{G}{2}\big(I_1 - 3 - \mathrm{Tr}(\boldsymbol{\varepsilon})\big) + \frac{\lambda}{2}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2 \\
W\big(\overline{I_1}, \mathrm{Tr}(\boldsymbol{\varepsilon})\big) \quad &= \quad \frac{G}{2}(\overline{I_1} - 3) + \left(\frac{\lambda}{2} + \frac{G}{3}\right)\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2 = \frac{G}{2}(\overline{I_1} - 3) + \frac{K}{2}\big(\mathrm{Tr}(\boldsymbol{\varepsilon})\big)^2
\end{aligned}$$

where K is bulk modulus. These are implemented in Neohookean and Mooney-Rivlin materials. The specific implementations need to pick $\mathrm{Tr}(\boldsymbol{\varepsilon})$ with one option being $\mathrm{Tr}(\boldsymbol{\varepsilon}) \approx \ln J$.

8.5 Anisotropic, Hyperelastic Materials

Papers by Spencer (1982,1986) derives extra invariants for anistropic materials and used them to derive Cauchy stress. These papers also modified the isotropic material results by using the Cayley-Hamilton theory to expand $\mathbf{B}^3$ as follows

$$\begin{aligned}
\mathbf{B}^2 \quad &= \quad \mathbf{B}^3\mathbf{B}^{-1} = (J^2\mathbf{I} - I_2\mathbf{B} + I_1\mathbf{B}^2)\mathbf{B}^{-1} = J^2\mathbf{B}^{-1} - I_2\mathbf{I} + I_1\mathbf{B} \\
\mathbf{B}^{-1} \quad &= \quad \frac{1}{J^2}\left(I_2\mathbf{I} - I_1\mathbf{B} + \mathbf{B}^2\right) \\
I_1\mathbf{B} - \mathbf{B}^2 \quad &= \quad J^2\mathbf{B}^{-1} - I_2\mathbf{I}
\end{aligned}$$

The Cauchy stress in terms of J or I_3 can be rewritten as:

$$\boldsymbol{\sigma} = \frac{2}{J}\left[\left(\frac{J}{2}\frac{\partial W}{\partial J} - I_2\frac{\partial W}{\partial I_2}\right)\mathbf{I} + \frac{\partial W}{\partial I_1}\mathbf{B} - J^2\frac{\partial W}{\partial I_2}\mathbf{B}^{-1}\right] \tag{8.39}$$

$$= \frac{2}{J}\left[\left(I_3\frac{\partial W}{\partial I_3} - I_2\frac{\partial W}{\partial I_2}\right)\mathbf{I} + \frac{\partial W}{\partial I_1}\mathbf{B} - I_3\frac{\partial W}{\partial I_2}\mathbf{B}^{-1}\right] \tag{8.40}$$

For a transversely isotropic material, we introduce two new invariants (based on symmetry group analysis):

$$I_4 = \boldsymbol{A}\cdot\mathbf{C}\boldsymbol{A} = \lambda_A^2 \quad \text{and} \quad I_5 = \boldsymbol{A}\cdot\mathbf{C}^2\boldsymbol{A}$$

Here $\boldsymbol{A}$ is unit vector in the axial direction of the undeformed configuration and $\lambda_A = |\mathbf{F}\boldsymbol{A}|$ is elongation of the axial direction in the deformed configuration. The Cauchy stress is the isotropic terms plus new terms with the new invariants:

$$\begin{aligned}\boldsymbol{\sigma} &= \frac{2}{J}\left[\left(I_3\frac{\partial W}{\partial I_3} - I_2\frac{\partial W}{\partial I_2}\right)\mathbf{I} + \frac{\partial W}{\partial I_1}\mathbf{B} - I_3\frac{\partial W}{\partial I_2}\mathbf{B}^{-1} + \frac{\partial W}{\partial I_4}\boldsymbol{a}\otimes\boldsymbol{a} + \frac{\partial W}{\partial I_5}(\boldsymbol{a}\otimes\mathbf{B}\boldsymbol{a} + \boldsymbol{a}\mathbf{B}\otimes\boldsymbol{a})\right] \\ &= \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\mathbf{B} + \frac{\partial W}{\partial I_2}(I_1\mathbf{B} - \mathbf{B}^2) + I_3\frac{\partial W}{\partial I_3}\mathbf{I} + \frac{\partial W}{\partial I_4}\boldsymbol{a}\otimes\boldsymbol{a} + \frac{\partial W}{\partial I_5}(\boldsymbol{a}\otimes\mathbf{B}\boldsymbol{a} + \boldsymbol{a}\mathbf{B}\otimes\boldsymbol{a})\right] \end{aligned} \tag{8.41}$$

where $\boldsymbol{a} = \mathbf{F}\boldsymbol{A}$ is the axial unit vector transformed and elongated in the deformed configuration.

8.6 Mooney-Rivlin Material

The Mooney-Rivilin material is an isotropic, elastic, hyperelastic material. It's stresses are based on a strain energy function that is assumed to be

$$W(\overline{I_1}, \overline{I_2}, J) = \frac{G_1}{2}\left(\overline{I_1} - 3\right) + \frac{G_2}{2}\left(\overline{I_2} - 3\right) + U(J)$$

where G_1 and G_2 are material properties and $U(J)$ is dilational energy term that can use various options defined below. For low strains, this material is equivalent for a linear elastic, isotropic material with shear modulus $G_1 + G_2$ and bulk modulus

$$K = \lim_{J\to 1} J\frac{\partial^2 U}{\partial J^2}$$

If $G_2 = 0$, the material is one form or a neo-Hookean material (two other forms are a "Neohookian Material" and a "Modifed Co-Rotational Model"). Some hyperelastic rubber models assume incompressible materials, which corresponds to $K \to \infty$; such models do not work in dynamic code (because wave speed is infinite), although they can be used in membranes.

The Cauchy stress is found by Eq. (8.35):

$$\boldsymbol{\sigma} = \frac{J_{res}G_1}{J^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{J_{res}G_2}{J^{7/3}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right) + \frac{\partial U(J^*)}{\partial J^*}\mathbf{I} \tag{8.42}$$

This result includes residual stresses (see above); in their absence, $J_{res} = 1$ and $J^* = J$. These results reduce to the proper low-strain thermoelastic relation at small strain. In this limit

$$\mathbf{B} \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad I_1 \approx 3 + 2\mathrm{Tr}(\boldsymbol{\varepsilon}), \quad \mathbf{B}^2 \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad J^* = \frac{J}{J_{res}} \approx 1 + \mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T \tag{8.43}$$

Assuming this limit also has $\partial U(J^*)/\partial J^* \approx K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)$ with K as small-strain bulk modulus (which it does for all implemented dilational energy terms), the small strain limit is

$$\boldsymbol{\sigma} = G_1\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + G_2\left(2\boldsymbol{\varepsilon} + \left(I_1\left(1 - \frac{I_1}{3}\right) - 1 + \frac{\mathbf{B}\cdot\mathbf{B}}{3}\right)\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} \tag{8.44}$$

Using $\mathbf{B}\cdot\mathbf{B} \approx 3 + 4\mathrm{Tr}(\boldsymbol{\varepsilon})$ leads to

$$\boldsymbol{\sigma} = (G_1+G_2)\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} \tag{8.45}$$

$$= \left[\left(K - \frac{2}{3}(G_1+G_2)\right)\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3K\alpha\Delta T\right]\mathbf{I} + 2(G_1+G_2)\boldsymbol{\varepsilon} \tag{8.46}$$

which is the expected result where G_1+G_2 is the low-strain shear modulus.

The stress components can be divided into pressure, P, and deviatoric stress, $\mathbf{s} = \boldsymbol{\sigma} + P\mathbf{I}$, which explicitly evaluate to:

$$\begin{aligned}
P &= -\frac{\partial U(J^*)}{\partial J^*} \\
s_{xx} &= J_{res}G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}} + J_{res}G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2-B_{xz}^2+2B_{yz}^2}{3J^{7/3}} \\
s_{yy} &= J_{res}G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}} + J_{res}G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2+2B_{xz}^2-B_{yz}^2}{3J^{7/3}} \\
s_{zz} &= J_{res}G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}} + J_{res}G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2-B_{xz}^2-B_{yz}^2}{3J^{7/3}} \\
s_{xy} &= J_{res}G_1\frac{B_{xy}}{J^{5/3}} + J_{res}G_2\frac{B_{zz}B_{xy}-B_{xz}B_{yz}}{J^{7/3}} \\
s_{xz} &= J_{res}G_1\frac{B_{xz}}{J^{5/3}} + J_{res}G_2\frac{B_{yy}B_{xz}-B_{xy}B_{yz}}{J^{7/3}} \\
s_{yz} &= J_{res}G_1\frac{B_{yz}}{J^{5/3}} + J_{res}G_2\frac{B_{xx}B_{yz}-B_{xy}B_{xz}}{J^{7/3}}
\end{aligned}$$

8.6.1 Plane Strain, Plane Stress, and Axisymmetric Analysis

For 2D analyses, $F_{xz} = F_{yz} = F_{zx} = F_{zy} = 0$, which leads to zero for corresponding terms in $\mathbf{B}$. The resulting stresses are $P = -\partial U(J^*)/\partial J^*$, $s_{xz} = s_{yz} = 0$, and

$$s_{xx} = J_{res}G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}} + J_{res}G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{8.47}$$

$$s_{yy} = J_{res}G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}} + J_{res}G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{8.48}$$

$$s_{zz} = J_{res}G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}} + J_{res}G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2}{3J^{7/3}} \tag{8.49}$$

$$s_{xy} = J_{res}G_1\frac{B_{xy}}{J^{5/3}} + J_{res}G_2\frac{B_{zz}B_{xy}}{J^{7/3}} \tag{8.50}$$

For plane strain analysis $B_{zz} = 1$. For axisymmetric analysis, B_{zz} is provided by the input deformation.

For plane stress analysis, one has to solve numerically for B_{zz} to get $\sigma_{zz} = 0$ or $s_{zz} = P$ and then use that result to find z direction deformation along with the other stresses; $\sigma_{zz} = 0$ is found by solving $f = 0$ where

$$f = -3J_{res}(J^*)^2P(J^*) + G_1J^{1/3}(2B_{zz}-\alpha_1) + \frac{G_2}{J^{1/3}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{8.51}$$

where $P(J^*)$ is the pressure model used, $\alpha_1 = B_{xx} + B_{yy}$, $\alpha_2 = B_{xx}B_{yy} - B_{xy}^2$, and $J^2 = \det(\mathbf{B}) = B_{zz}\alpha_2$. More explicitly in B_{zz}, the function is

$$f = -3J_{res}J^{*2}P(J^*) + G_1 B_{zz}^{1/6}\alpha_2^{1/6}(2B_{zz} - \alpha_1) + \frac{G_2}{B_{zz}^{1/6}\alpha_2^{1/6}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{8.52}$$

For more efficient Newton's method, we need

$$\frac{df}{dB_{zz}} = -3J_{res}\frac{d\left(J^{*2}P(J^*)\right)}{dJ^*}\frac{dJ^*}{dB_{zz}} + \frac{G_1 J^{1/3}(14B_{zz} - \alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1 B_{zz} + 2\alpha_2)}{6B_{zz}J^{1/3}} \tag{8.53}$$

where $J^* = \sqrt{B_{zz}\alpha_2}/J_{res}$ and $B_{zz}(dJ^*/dB_{zz}) = \sqrt{B_{zz}\alpha_2}/(2J_{res})$. The first term simplifies to:

$$\frac{df}{dB_{zz}} = -\frac{3J}{2B_{zz}}\frac{d\left(J^{*2}P(J^*)\right)}{dJ^*} + \frac{G_1 J^{1/3}(14B_{zz} - \alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1 B_{zz} + 2\alpha_2)}{6B_{zz}J^{1/3}} \tag{8.54}$$

8.6.2 Dilational Energy Term Options

Three options are available for the dilational energy term (which determines pressure and bulk modulus but using J^* for J):

$$\begin{aligned}
&\text{Option 0:} \quad U(J) = \frac{K}{2}\left(\frac{1}{2}(J^2-1) - \ln J\right) \quad \Longrightarrow \quad P = -\frac{K}{2}\left(J - \frac{1}{J}\right)\\
&\text{Option 1:} \quad U(J) = \frac{K}{2}(J-1)^2 \quad \Longrightarrow \quad P = -K(J-1)\\
&\text{Option 2:} \quad U(J) = \frac{K}{2}(\ln J)^2 \quad \Longrightarrow \quad P = -K\frac{\ln J}{J}
\end{aligned}$$

Although these three compressibility terms show some significant differences when J deviates significantly from 1, under most problems, J will stay close to one. Two exceptions could be constrained compression or tension. Here, the only one that works well to very small or large J is option 0. This one correctly leads to infinite positive stress as $J \to \infty$ and infinite negative stress as $J \to 0$. Thus `UJOption=0` is the default setting in `NairnMPM`.

The various bulk moduli using Eq. (8.30) are:

$$\begin{aligned}
&\text{Option 0:} \quad K(J) = \frac{K}{2}\left(J + \frac{1}{J}\right)\\
&\text{Option 1:} \quad K(J) = KJ\\
&\text{Option 2:} \quad K(J) = K\frac{1 - \ln J}{J^2}
\end{aligned}$$

If implementing an incremental pressure law, the result is:

$$P_n = P_{n-1} - K(J^*)d\ln J^* = P_{n-1} - K(J^*)\frac{dJ^*}{J^*} \tag{8.55}$$

These three bulk moduli are plotted in Fig. 8.2.

When implementing plane stress, the $d(J^{*2}P(J^*))/dJ*$ terms are

$$\begin{aligned}
&\text{Option 0:} \quad -\frac{K}{2}\frac{d\left(J^{*3} - J^*\right)}{dJ^*} = -\frac{K}{2}(3J^{*2} - 1)\\
&\text{Option 1:} \quad -K\frac{d\left(J^{*3} - J^{*2}\right)}{dJ^*} = -KJ^*(3J^* - 2)\\
&\text{Option 2:} \quad -K\frac{d\left(J^*\ln J^*\right)}{dJ^*} = -K(1 + \ln J^*)
\end{aligned}$$

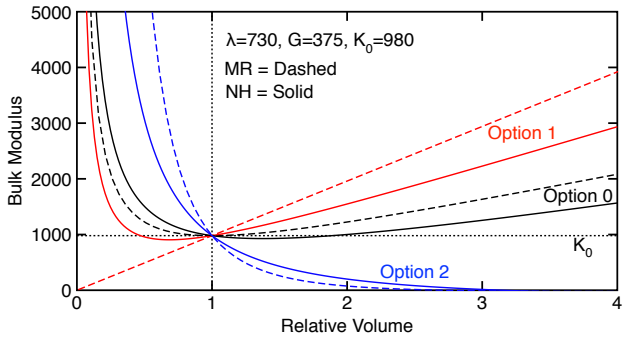

Figure 8.2: Bulk modulus as a function of J for Mooney-Rivlin (dashed lines) and Neohookean (solid lines) materials The curves are for the three dilational energy functions.

8.6.3 Tangent Stiffness Tensor

To use Eq. (8.31), switch to energy in terms of I_1, I_2, and J:

$$W(I_1,I_2,J)=\frac{G_1}{2}\left(\frac{I_1}{J^{2/3}}-3\right)+\frac{G_2}{2}\left(\frac{I_2}{J^{4/3}}-3\right)+U(J)$$

with derivatives

$$\frac{\partial W}{\partial I_1}=\frac{G_1}{2J^{2/3}}\qquad \frac{\partial W}{\partial I_2}=\frac{G_2}{2J^{4/3}}\qquad \frac{\partial W}{\partial J}=-\frac{G_1 I_1}{3J^{5/3}}-\frac{2G_2 I_2}{3J^{7/3}}+\frac{\partial U}{\partial J}$$

which correspond to Cauchy stress in Eq. (8.42). The non-zero second derivatives are:

$$\frac{\partial^2 W}{\partial I_1 \partial J}=-\frac{G_1}{3J^{5/3}}\qquad \frac{\partial^2 W}{\partial I_2 \partial J}=-\frac{2G_2}{3J^{7/3}}\qquad \frac{\partial^2 W}{\partial J^2}=\frac{5G_1 I_1}{9J^{8/3}}+\frac{14G_2 I_2}{9J^{10/3}}+\frac{\partial^2 U}{\partial J^2}$$

The final term for various $U(J)$ options becomes

$$\frac{\partial^2 U}{\partial J^2}=\left\{\text{Option 0}: K\frac{1+J^2}{2J^2},\text{Option 1}: K,\text{Option 2}: K\frac{1-\ln J}{J^2}\right\}$$

The tangent stiffness becomes

$$\begin{aligned}\frac{c_{ijkl}}{J} &= \frac{4}{J}\left(B_{ij},I_1B_{ij}-\sum_m B_{im}B_{mj},\frac{J}{2}\delta_{ij}\right)\cdot\left(-\frac{G_1}{6J^{2/3}}\delta_{kl},-\frac{G_2}{3J^{4/3}}\delta_{kl},\right.\\
&\quad -\frac{G_1}{3J^{5/3}}B_{kl}-\frac{2G_2}{3J^{7/3}}\left(I_1B_{kl}-\sum_m B_{km}B_{ml}\right)+\left(\frac{5G_1I_1}{18J^{5/3}}+\frac{7G_2I_2}{9J^{7/3}}+\frac{K_1}{2}\right)\delta_{kl}\Big)\\
&\quad +\left(B_{ij}B_{kl}-\frac{1}{2}\left(B_{ik}B_{jl}+B_{il}B_{jk}\right)\right)\frac{2G_2}{J^{7/3}}+\left[\delta_{ij}\delta_{kl}-\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\right]\left(K_2-\frac{G_1I_1}{3J^{5/3}}-\frac{2G_2I_2}{3J^{7/3}}\right)\end{aligned}$$

where $K_1=K(1+J^2)/(2J)$, KJ, or $K(1-\ln J)/J$ and $K_2=K(J^2-1)/(2J)$, $K(J-1)$, or $K\ln J/J$ for options 0, 1, and 2, respectively. Collecting terms gives

$$\begin{aligned}\frac{c_{ijkl}}{J} &= \frac{2G_1}{3J^{5/3}}\left[\frac{I_1}{2}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)+\frac{I_1}{3}\delta_{kl}\delta_{ij}-B_{ij}\delta_{kl}-B_{kl}\delta_{ij}\right]\\
&\quad +\frac{G_2}{J^{7/3}}\left[\frac{8I_2}{9}\delta_{kl}\delta_{ij}+\frac{2I_2}{3}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)+2B_{ij}B_{kl}-B_{ik}B_{jl}-B_{il}B_{jk}\right.\\
&\quad \left.-\frac{4}{3}\left(I_1B_{kl}-B_{kl}^2\right)\delta_{ij}-\frac{4}{3}\left(I_1B_{ij}-B_{ij}^2\right)\delta_{kl}\right]+K_3\delta_{ij}\delta_{kl}-K_2\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\end{aligned}$$

where $K_3 = K_1 + K_2 = KJ$, $K(2J-1)$, or K/J for options 0, 1, and 2, respectively. Revising in terms of deviatoric tensors gives:

$$\begin{aligned}\frac{c_{ijkl}}{J} &= \frac{2G_1}{3J}\left[\overline{I_1}\left(\frac{1}{2}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)-\frac{1}{3}\delta_{kl}\delta_{ij}\right)-\overline{B}^d_{ij}\delta_{kl}-\overline{B}^d_{kl}\delta_{ij}\right] \\ &\quad +\frac{4G_2}{3J}\left[\overline{I_2}\left(\frac{1}{2}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)-\frac{2}{3}\delta_{kl}\delta_{ij}\right)+\frac{3}{2}\overline{B}_{ij}\overline{B}_{kl}-\frac{3}{4}\overline{B}_{ik}\overline{B}_{jl}-\frac{3}{4}\overline{B}_{il}\overline{B}_{jk}-D_{kl}\delta_{ij}-D_{ij}\delta_{kl}\right] \\ &\quad +K_3\delta_{ij}\delta_{kl}-K_2\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\end{aligned}$$

where $\overline{B}_{ij} = J^{-2/3}B_{ij}$, $\overline{B}^d_{ij} = \overline{B}_{ij} - \overline{I_1}\delta_{ij}/3$, $\overline{D}^d_{ij} = (\overline{I_1}\overline{B}_{ij} - \overline{B}^2_{ij})^d = \overline{I_1}\overline{B}_{ij} - \overline{B}^2_{ij} - 2\overline{I_2}\delta_{ij}/3$, $\overline{I_1} = J^{-2/3}I_1$, and $\overline{I_2} = J^{-4/3}I_2$.

Voight Stiffness Matrix

The elements of the 6×6 stiffness matrix are all non zero. In other words, a Mooney-Rivlin material becomes anisotropic at large strain and has coupling between tensile and shear strains. The explicit results for the tension-tension quadrant are:

$$\begin{aligned}C_{ii} = c_{iiii} &= K_1 - K_2 + \frac{4}{3J}\left(G_1\left(\frac{2\overline{I_1}}{3}-\overline{B}_{ii}\right)+G_2\left(\frac{5\overline{I_2}}{3}-2\overline{D}_{ii}\right)\right) \quad \text{for } i=1,2,3 \\ C_{12} = c_{1122} &= K_1 + K_2 - \frac{2}{3J}\left(G_1\left(\frac{2\overline{I_1}}{3}-\overline{B}_{33}\right)-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{33}\right)\right) \\ C_{13} = c_{1133} &= K_1 + K_2 - \frac{2}{3J}\left(G_1\left(\frac{2\overline{I_1}}{3}-\overline{B}_{22}\right)-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{22}\right)\right) \\ C_{23} = c_{2233} &= K_1 + K_2 - \frac{2}{3J}\left(G_1\left(\frac{2\overline{I_1}}{3}-\overline{B}_{11}\right)-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{11})\right)\right)\end{aligned}$$

Explicit results for the shear-shear quadrant are:

$$\begin{aligned}C_{44} = c_{2323} &= -K_2 + \frac{1}{J}\left(G_1\frac{\overline{I_1}}{3}-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{11}\right)\right) \\ C_{55} = c_{1313} &= -K_2 + \frac{1}{J}\left(G_1\frac{\overline{I_1}}{3}-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{22}\right)\right) \\ C_{66} = c_{1212} &= -K_2 + \frac{1}{J}\left(G_1\frac{\overline{I_1}}{3}-G_2\left(\frac{\overline{I_2}}{3}-\overline{D}_{33}\right)\right) \\ C_{45} = c_{2313} &= -\frac{G_2}{J}\overline{D}_{12} \qquad C_{46} = c_{2312} = -\frac{G_2}{J}\overline{D}_{13} \qquad C_{56} = c_{1312} = -\frac{G_2}{J}\overline{D}_{23}\end{aligned}$$

These relations used the usual Voight ordering where indices 4, 5, and 6 correspond to $(i,j) \to (2,3)$, $(1,3)$, and $(1,2)$. Note that this block is diagonal if $G_2 = 0$. Explicit results for the tension-shear quadrant are:

$$\begin{aligned}C_{14} = c_{1123} &= -\frac{2}{3J}\left(G_1\overline{B}_{23}-G_2\overline{D}_{23}\right) \qquad C_{24} = C_{34} = c_{2223} = c_{3323} = -\frac{2}{3J}\left(G_1\overline{B}_{23}+2G_2\overline{D}_{23}\right) \\ C_{25} = c_{2213} &= -\frac{2}{3J}\left(G_1\overline{B}_{13}-G_2\overline{D}_{13}\right) \qquad C_{15} = C_{35} = c_{1113} = c_{1113} = -\frac{2}{3J}\left(G_1\overline{B}_{13}+2G_2\overline{D}_{13}\right) \\ C_{36} = c_{3312} &= -\frac{2}{3J}\left(G_1\overline{B}_{12}-G_2\overline{D}_{12}\right) \qquad C_{16} = C_{26} = c_{1112} = c_{2212} = -\frac{2}{3J}\left(G_1\overline{B}_{12}+2G_2\overline{D}_{12}\right)\end{aligned}$$

Note that these relations used the non-deviatoric, but renormalized matrices $\overline{\mathbf{B}}$ and $\overline{\mathbf{D}}$. Setting $J = 1$, $\overline{I_1} = \overline{I_2} = 3$, $\overline{B}_{ij} = 4\delta_{ij}$, $\overline{D}_{ij} = 2\delta_{ik}$ $K_1 = K$, and $K_2 = 0$, these results reduce to stiffness matrix of a small-strain, linear elastic material with shear modulus $G = G_1 + G_2$.

8.6.4 Uniaxial Loading

The general Cauchy stresses, now including residual stresses, are:

$$\sigma_{xx} = \frac{2J_{res}(\lambda^3 - J)}{3J^{5/3}\lambda^2}\left(\lambda G_1 + J^{1/3}G_2\right) - P(J^*) \quad \sigma_{yy} = -\frac{J_{res}(\lambda^3 - J)}{3J^{5/3}\lambda^2}\left(\lambda G_1 + J^{1/3}G_2\right) - P(J^*)$$

For simple tension, solve $\sigma_{yy} = 0$ for $P(J^*)$ and substitute to get:

$$\sigma_{xx} = \frac{J_{res}(\lambda^3 - J)}{J^{5/3}\lambda^2}\left(\lambda G_1 + J^{1/3}G_2\right) \qquad \sigma_{yy} = 0$$

To express in terms of λ alone, solve $\sigma_{yy} = 0$ for J and substitute into this equation. For incompressible tension (but possible thermal expansion or $J = J_{res}$ and $J^* = 1$):

$$\sigma_{xx} = \frac{2(\lambda^3 - J_{res})}{3J_{res}^{2/3}\lambda^2}\left(\lambda G_1 + J_{res}^{1/3}G_2\right) \quad \sigma_{yy} = -\frac{(\lambda^3 - J)}{3J^{2/3}\lambda^2}\left(\lambda G_1 + J_{res}^{1/3}G_2\right)$$

For constrained tension ($J = \lambda$ and $J^* = \lambda/J_{res}$):

$$\sigma_{xx} = \frac{2J_{res}(\lambda^2 - 1)}{3\lambda^{5/3}}\left(G_1 + \frac{G_2}{\lambda^{2/3}}\right) - P\left(\frac{\lambda}{J_{res}}\right) + \quad \sigma_{yy} = -\frac{J_{res}(\lambda^2 - 1)}{3\lambda^{5/3}}\left(G_1 + \frac{G_2}{\lambda^{2/3}}\right) - P\left(\frac{\lambda}{J_{res}}\right)$$

For hydrostatic tension ($J = \lambda^3$):

$$\sigma_{xx} = \sigma_{yy} = -P(J^*)$$

The three pressure options are are given above.

8.6.5 Linear Shear Loading

From the Linear Shear section (and noting that $\partial W/\partial J \to 0$ for $J = 1$), the Kirchoff stresses (which equal the Cauchy stresses when $J = 1$) including residual stress effect are:

$$\tau_{xx} = \frac{J_{res}\gamma^2}{3}(2G_1 + G_2) \qquad \tau_{yy} = -\frac{J_{res}\gamma^2}{3}(G_1 + 2G_2)$$

$$\tau_{zz} = \frac{J_{res}\gamma^2}{3}(-G_1 + G_2) \qquad \tau_{xy} = J_{res}\gamma(G_1 + G_2)$$

8.7 Neo-Hookean Material

Although using $G_2 = 0$ as a special case of a Mooney-Rivlin material is a neo-Hookean material, some literature results define a different neo-Hookean material using the strain energy function:

$$W(I_1, I_2, J) = \frac{G}{2}(I_1 - 3 - 2\ln J) + U(J) \tag{8.56}$$

where G is shear modulus $U(J)$ is a dilational term that uses Lamé modulus, λ, in place of bulk modulus, K. The Cauchy stress using Eq. (8.34) is:

$$\boldsymbol{\sigma} = \frac{\partial U(J^*)}{dJ^*}\mathbf{I} + \frac{G}{J^*}\left(\frac{\mathbf{B}}{J_{res}^{2/3}} - \mathbf{I}\right) \tag{8.57}$$

In the low strain limit, $J = 1+\mathrm{Tr}(\boldsymbol{\varepsilon})$, $J_{res} = 1+3\alpha\Delta T$, $\mathbf{B} = \mathbf{I}+2\boldsymbol{\varepsilon}$, and $\partial U(J^*)/\partial J^* \approx \lambda(\mathrm{Tr}(\boldsymbol{\varepsilon})-3\alpha\Delta T)$. The stress simplifies to

$$\boldsymbol{\sigma} = \big(\lambda\mathrm{Tr}(\boldsymbol{\varepsilon}) - (3\lambda+2G)\alpha\Delta T\big)\mathbf{I} + 2G\boldsymbol{\varepsilon} \qquad \text{low strain} \tag{8.58}$$

which is the expected result using low-strain shear and Lamé properties and accounting for residual thermal stresses (note that $3\lambda+2G = 3K$ where K is the low strain bulk modulus).

The stress components can be divided into pressure, P and deviatoric stress, $\boldsymbol{s} = \boldsymbol{\sigma} + P\mathbf{I}$, which explicitly evaluate to:

$$P = P(J^*) - \frac{G}{J^*}\left(\frac{B_{xx}+B_{yy}+B_{zz}}{3J_{res}^{2/3}} - 1\right) \tag{8.59}$$

$$s_{xx} = \frac{J_{res}^{1/3}G}{3J}\big(2B_{xx} - B_{yy} - B_{zz}\big) \tag{8.60}$$

$$s_{yy} = \frac{J_{res}^{1/3}G}{3J}\big(2B_{yy} - B_{xx} - B_{zz}\big) \tag{8.61}$$

$$s_{zz} = \frac{J_{res}^{1/3}G}{3J}\big(2B_{zz} - B_{xx} - B_{zz}\big) \tag{8.62}$$

$$s_{ij} = \frac{J_{res}^{1/3}G}{J}B_{ij} \qquad \text{for } i \neq j \tag{8.63}$$

where $P(J^*)$ uses any pressure above except that K is replaced by λ. The Cauchy stresses are:

$$\begin{aligned}
\sigma_{xx} &= \frac{J_{res}^{1/3}G}{J}\big(B_{xx} - J_{res}^{2/3}\big) - P(J^*)\\
\sigma_{yy} &= \frac{J_{res}^{1/3}G}{J}\big(B_{yy} - J_{res}^{2/3}\big) - P(J^*)\\
\sigma_{zz} &= \frac{J_{res}^{1/3}G}{J}\big(B_{zz} - J_{res}^{2/3}\big) - P(J^*)\\
\sigma_{ij} &= \frac{J_{res}^{1/3}G}{J}B_{ij} \qquad \text{for } i \neq j
\end{aligned}$$

When doing plane stress calculations, one task is to solve for $\sigma_{zz} = 0$, which is equivalent to solving numerically for $f = 0$ given

$$f = -J_{res}^{2/3}J^*P(J^*) + G\left(B_{zz} - J_{res}^{2/3}\right) \tag{8.64}$$

$$\frac{df}{dB_{zz}} = G - \frac{J_{res}^{2/3}J^*}{2B_{zz}}\frac{d(J^*P(J^*))}{dJ^*} \tag{8.65}$$

which used $J^* = \sqrt{B_{zz}\alpha_2}/J_{res}$ with $\alpha_2 = B_{xx}B_{yy} - B_{xy}^2$ leading to $(dJ^*/dB_{zz}) = J^*/(2B_{zz})$. This equation can be solved analytically for two pressure models, but requires numerical solution for the third. The two analytical solutions are:

$$B_{zz} = J_{res}^2\frac{\lambda+2G}{\lambda\alpha_2 + 2GJ_{res}^{4/3}} \tag{8.66}$$

when $J^*P(J^*) = -(\lambda/2)\left(J^{*2}-1\right)$ (or `UJOption=0`) and

$$\sqrt{B_{zz}} = J_{res}\frac{\lambda\sqrt{\alpha_2}+\sqrt{\lambda^2\alpha_2+4G\left(\lambda\alpha_2+GJ_{res}^{4/3}\right)}}{2\left(\lambda\alpha_2+GJ_{res}^{4/3}\right)} \tag{8.67}$$

when $J^*P(J^*) = -\lambda\left(J^{*2}-J^*\right)$ (or `UJOption=1`). The third pressure law has $J^*P(J^*) = -\lambda\ln J^*$ (or `UJOption=2`) leading to

$$f = G\left(B_{zz}-J_{res}^{2/3}\right)+\lambda J_{res}^{2/3}\ln J^* \tag{8.68}$$

$$\frac{df}{dB_{zz}} = G+\frac{\lambda J_{res}^{2/3}}{2B_{zz}} \tag{8.69}$$

This option has to be solved numerically.

8.7.1 Tangent Modulus

This material has $\partial W/\partial I_2 = \partial^2 W/\partial I_1^2 = \partial^2 W/\partial I_1\partial J = 0$. From Eq. (8.32), the tangent modulus is

$$c_{ijkl} = J\left(J\frac{\partial^2 W}{\partial J^2}+\frac{\partial W}{\partial J}\right)\delta_{ij}\delta_{kl}-J\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right)\frac{\partial W}{\partial J}$$

These can be assembled into a 6×6 Voight-notation matrix that matches non-zero elements for an isotropic elastic material, but the nonlinear elements are

$$\begin{aligned} C_{11}=C_{22}=C_{33} &= J^2\frac{\partial^2 W}{\partial J^2}-J\frac{\partial W}{\partial J} \\ C_{12}=C_{13}=C_{23} &= J^2\frac{\partial^2 W}{\partial J^2}+J\frac{\partial W}{\partial J} \\ C_{44}=C_{55}=C_{66} &= -J\frac{\partial W}{\partial J} \end{aligned}$$

and remaining elements are zero. For the various options (`UJOption`=0, 1, 2 in order), these evaluate to:

$$\begin{aligned} &\text{Option 0}: && C_{11}=\lambda+2G, \quad C_{12}=\lambda J^2, \quad C_{44}=\frac{2G+\lambda(1-J^2)}{2} \\ &\text{Option 1}: && C_{11}=\lambda J+2G, \quad C_{12}=\lambda J(2J-1), \quad C_{44}=G+\lambda J(1-J) \\ &\text{Option 2}: && C_{11}=\lambda(1-2\ln J)+2G, \quad C_{12}=\lambda, \quad C_{44}=G-\lambda\ln J \end{aligned}$$

Notice that the material remains incremental isotropic for any amount of deformation, but that behavior may not be very realistic. For example, imagine large tensile deformation on a polymer that stiffens as the molecules align in the loading direction. If the deformed material is then pulled in the transverse direction, the molecular alignment perpendicular to that direction suggests the stiffness would be reduced. This material model, however, predicts it stiffens in all directions by alignment in one direction.

8.7.2 Tangent Bulk Modulus

To support adiabatic heating (or state dependent wave speeds), we need K as a function of deformation. Imagine and current stress state and then apply incremental volumetric change such that the displacement gradient and effective bulk modulus are

$$\nabla u = \text{diag}(1,1,1)\frac{\Delta J}{3J} \qquad \text{and} \qquad \Delta P = -K(J)\frac{\Delta J}{J}$$

Using Eq. (8.18) gives pressure increment of:

$$\Delta P = -\frac{1}{3}\left(\frac{C_{11}+2C_{12}}{J}+P\right)\frac{\Delta J}{J} \quad \text{or} \quad K(J) = \frac{1}{3}\left(\frac{C_{11}+2C_{12}}{J}+P(J)-\frac{G}{J}(I_1-3)\right)$$

The three options give

$$\begin{aligned}
\text{Option 0}: &\qquad K = \frac{\lambda(J^2+1)}{2J}+\frac{G(9-I_1)}{9J}\\
\text{Option 1}: &\qquad K = \lambda J+\frac{G(9-I_1)}{9J}\\
\text{Option 2}: &\qquad K = \frac{\lambda(1-\ln J)}{J}+\frac{G(9-I_1)}{9J}
\end{aligned}$$

These all reduce to $K=\lambda+2G/3$ for low strain (when $J\to 1$ and $I_1\to 3$). For hydrostatic compression $I_1 = 3J^{2/3}$ and the shear term becomes

$$\frac{G\left(3-J^{2/3}\right)}{3J} \tag{8.70}$$

Another approach is direct differentiation of pressure or $K=-J^*dP/dJ^*$. The method gives

$$\begin{aligned}
\text{Option 0}: &\qquad K = \frac{\lambda(1+J^2)}{2J}+\frac{G\left(3-I_1+J\frac{dI_1}{dJ}\right)}{3J}\\
\text{Option 1}: &\qquad K = \lambda J+\frac{G\left(3-I_1+J\frac{dI_1}{dJ}\right)}{3J})\\
\text{Option 2}: &\qquad K = \frac{\lambda(1-\ln J)}{J}+\frac{G\left(3-I_1+J\frac{dI_1}{dJ}\right)}{3J}
\end{aligned}$$

For hydrostatic compression in all models, K_0 is found by substituting $I_1 = 3J^{2/3}$ and then $J=1$ to get the result of $K_0=\lambda+2G/3$. For $J\neq 1$, the shear term becomes

$$\frac{G\left(3-J^{2/3}\right)}{3J} \tag{8.71}$$

These two approaches are identical during hydrostatic loading and that bulk modulus is plotted in Fig. 8.2. When current bulk modulus is needed in calculations (for isoentropic heating or wave speed calculations), the first form is used because it does not need to evaluate derivative of $\partial I_1/\partial J$.

8.7.3 Uniaxial Tension

In uniaxial tension to extension λ_1 in the x direction, the general result from above (with addition now of residual stresses) are

$$\sigma_{xx} = \frac{\partial W(J^*)}{\partial J}+\frac{J_{res}^{1/3}\lambda_1}{J} = \frac{GJ_{res}^{1/3}\left(\lambda_1^2-J_{res}^{2/3}\right)}{J}-P(J^*)$$

$$\sigma_{yy} = \frac{\partial W(J^*)}{\partial J}+\frac{J_{res}^{1/3}G}{\lambda_1} = \frac{GJ_{res}^{1/3}(J-J_{res}^{2/3}\lambda_1)}{J\lambda_1}-P(J^*)$$

For simple tension, solve $\sigma_{yy}=0$ for $P(J^*)$ and substitute to get:

$$\sigma_{xx} = \frac{GJ_{res}^{1/3}\left(\lambda_1^3-J\right)}{J\lambda_1} \qquad \sigma_{yy}=0$$

To express in terms of λ_1 alone, solve $\sigma_{yy} = 0$ for J and substitute into this equation. For incompressible tension (but possible thermal expansion or $J = J_{res}$ and $J^* = 1$):

$$\sigma_{xx} = G\left(\frac{\lambda_1^2}{J_{res}^{2/3}} - 1\right) \qquad \sigma_{yy} = G\left(\frac{J_{res}^{1/3}}{\lambda_1} - 1\right)$$

For constrained tension ($J = \lambda$ and $J^* = \lambda_1/J_{res}$)

$$\sigma_{xx} = GJ_{res}^{2/3}\left(\frac{\lambda_1}{J_{res}^{1/3}} - \frac{J_{res}^{1/3}}{\lambda_1}\right) - P\left(\frac{\lambda_1}{J_{res}}\right) \qquad \sigma_{yy} = \frac{GJ_{res}^{1/3}(1 - J_{res}^{2/3})}{\lambda_1} - P\left(\frac{\lambda_1}{J_{res}}\right)$$

For hydrostatic tension ($\lambda^3 = J$):

$$\sigma_{xx} = \sigma_{yy} = \frac{GJ_{res}^{1/3}\left(J^{2/3} - J_{res}^{2/3}\right)}{J} - P(J^*)$$

Note that bulk modulus found using this stress and $K = J(d\sigma_{xx}/dJ)$ agrees with bulk modulus above. The three pressure options are above using λ in place of K.

8.7.4 Linear Shear Loading

From the Linear Shear section, the Kirchoff stresses (which equal the Cauchy stresses when $J = 1$) including residual stress effects are:

$$\tau_{xx} = GJ_{res}\gamma^2 \qquad \tau_{yy} = \tau_{zz} = 0 \qquad \tau_{xx} = GJ_{res}\gamma$$

8.8 Co-rotated Neo-Hookean Material and Disney Snow Model

According to a paper on Disney snow animation, MPM was used to model snow in the movie *Frozen*. The constitutive model for snow was based on a hyperelastic-plastic model. The strain energy function is

$$W = G(J_P)||\mathbf{F}_E - \mathsf{R}_E||_F^2 + \frac{\lambda(J_p)}{2}(J_E - 1)^2 \tag{8.72}$$

where $G(J_P)$ and $\lambda(J_p)$ are shear and Lamé moduli and J_P is the plastic dilation, The mechanical properties undergo hardening according to

$$G(J_P) = G_0 e^{\xi(1-J_P)} \qquad \text{and} \qquad \lambda(\mathrm{J_P}) = \lambda_0 \mathrm{e}^{\xi(1-\mathrm{J_P})} \tag{8.73}$$

where ξ is a hardening parameter and μ_0 and λ_0 are the initial Lamé coefficients. Note the plastic stretch ($J_P > 1$) causes softening that leads to contitutitive law-based fracture. The $\mathbf{F}_E$, R_E, and J_E in strain energy are for the elastic part of the loading. The first term, which is Frobenius norm squared of a matrix, can be written as

$$\begin{aligned} ||\mathbf{F} - \mathsf{R}||_F^2 &= \mathrm{Tr}\big((\mathbf{F} - \mathsf{R})^T(\mathbf{F} - \mathsf{R})\big) = \mathrm{Tr}\big((\mathsf{U} - \mathbf{I})^T R^T R(\mathsf{U} - \mathbf{I})\big) = ||\mathsf{U} - \mathbf{I}||_F^2 & (8.74)\\ &= ||\mathsf{n}(\Lambda - \mathbf{I})\mathsf{n}^T||_F^2 = ||\Lambda - \mathbf{I}||_F^2 = (\lambda_1 - 1)^2 + (\lambda_2 - 1)^2 + (\lambda_3 - 1)^2 & (8.75)\end{aligned}$$

The energy function is more practically written as

$$\begin{aligned} W(\lambda_1, \lambda_2, \lambda_3, J_p) &= G(J_P)\sum_i (\lambda_i - 1)^2 + \frac{\lambda(J_p)}{2}(\lambda_1\lambda_2\lambda_3 - 1)^2 \\ &= G(J_P)(I_1 - 3 - 2(\lambda_1 + \lambda_2 + \lambda_3 - 3)) + \frac{\lambda(J_p)}{2}(\lambda_1\lambda_2\lambda_3 - 1)^2 \end{aligned}$$

where λ_i are the stretches of the elastic part of the deformation. Note that Ogden (1972) (who used variants of this style) points out this material does not work well for compressible materials. To handle high compression, both the $G(J_p)$ and $\lambda(J_P)$ likely need to change. One options, a done in the neo-Hookean material is replace the second part of the $G(J_p)$ term with

$$\lambda_1+\lambda_2+\lambda_3-3 \rightarrow \ln(\lambda_1\lambda_2\lambda_3)$$

These two are similar for small compression, but diverge for high compression. An option in `NairnMPM` lets this material switch to model that works better at high compression and to use different $\lambda(J_p)$ terms as well.

This law corresponds to a modified co-rotated, neo-Hookean material (where the modification changed the pressure term from prior co-rotated, neo-Hookean models). The Cauchy stress and pressure are

$$\boldsymbol{\sigma} = \sum_k \left(\frac{2G(J_P)}{J_E}\lambda_k(\lambda_k-1)+\lambda(J_p)(J_E-1)\right)\boldsymbol{n}_k\otimes\boldsymbol{n}_k \tag{8.76}$$

$$P = -\lambda(J_p)(J_E-1)-\frac{2G(J_P)}{3J_E}\left(\lambda_1^2+\lambda_2^2+\lambda_3^2-\lambda_1-\lambda_2-\lambda_3\right) \tag{8.77}$$

where $\boldsymbol{n}_k$ are eigenvectors of elastic $\mathbf{B}$ tensor (and the $\mathbf{V}$ tensor). To account for residual stress, replace J_E by J_E/J_{res} and λ_k by λ_k/λ_{res}.

To be elastic/plastic, the snow material clamps the elongations to a range of $[1-\theta_c, 1+\theta_s]$ where θ_c and θ_s are critical strains in compression and tension, respectively. The material is implemented as follows:

1. Track total $\mathbf{F}$ and elastic $\mathbf{B}$ on the particles and track J and J_P as two history variables. On each time step, update $\mathbf{F}$ and J and find a trial elastic $\mathbf{B}$:

$$\mathbf{F}_{n+1} = d\mathbf{F}\,\mathbf{F}_n, \qquad J_{n+1} = |d\mathbf{F}|J_n, \qquad \text{and} \qquad \mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{8.78}$$

2. Find eigenvalues and eigenvectors of $\mathbf{B}_{n+1}^{trial}$ as $(\lambda^2_{1,trial},\lambda^2_{2,trial},\lambda_{2,trial})$ and the matrix n with eigenvectors on the columns.

3. If all $\lambda^2_{i,trial}$ are within the range $[(1-\theta_c)^2,(1+\theta_s)^2]$, then $\mathbf{B}_{n+1}=\mathbf{B}_{n+1}^{trial}$, J_P is unchanged, and updated $J_{n+1}=J_{E,n+1}J_P$ or $J_{E,n+1}=J_{n+1}/J_P$.

4. If any $\lambda^2_{i,trial}$ exceeds the range, clamp them to that range and find $\mathbf{B}_{n+1}=\mathsf{n}\Lambda\mathsf{n}^T$ where Λ is diagonal matrix with the clamped values of λ_i on the diagonal, $J_{E,n+1}=\lambda_1\lambda_2\lambda_3$, and update J_P to:

$$J_{P,n+1} = \frac{J_{n+1}}{J_{E,n+1}} = \frac{\lambda_{1,trial}\lambda_{2,trial}\lambda_{2,trial}}{\lambda_1\lambda_2\lambda_3}$$

   Note that deformation within the clamped region may cause J_P to increase or decrease for clamping in tension or compression. Because a decrease in J_P corresponds to an increase in energy, the material is a non-physical implementation of plasticity or damage methods.

5. Calculate new mechanical properties $\lambda(J_p)$ and $G(J_p)$.

6. Find the Kirchoff stress from $\boldsymbol{\tau}=J\boldsymbol{\sigma}(\mathbf{B}_{n+1})$. Here J is total J and the stress depends only on elastic $\mathbf{B}_{n+1}$ (and its determinant, eigenvalues, and eigenvectors).

8.8.1 Uniaxial Tension

In uniaxial loading to extension λ is the x direction (now including residual stresses), we need the function

$$\frac{\partial W}{\partial \lambda_i} = f(\lambda_i^*, J^*) = 2G(J_p)(\lambda_i^* - 1) + \lambda(J_p)\frac{J^*(J^*-1)}{\lambda_i^*}$$

For incompressible tension ($J^* = 1$ and $J = J_{res}$):

$$\sigma_{xx} = \lambda^* f(\lambda^*, 1) = \frac{2G(J_p)}{J_{res}^{2/3}}\lambda(\lambda - J_{res}^{1/3}) \qquad \sigma_{yy} = \frac{f\left(\frac{1}{\sqrt{\lambda^*}}, 1\right)}{\sqrt{\lambda^*}} = 2G(J_p)\left(\frac{J_{res}^{1/3}}{\lambda} - \sqrt{\frac{J_{res}^{1/3}}{\lambda}}\right)$$

For constrained tension

$$\sigma_{xx} = f(\lambda^*, \lambda^*) = \frac{\lambda(J_p) + 2G(J_p)}{J_{res}^{1/3}}\left(\lambda - J_{res}^{1/3}\right) \qquad \sigma_{yy} = \frac{f(1, \lambda^*)}{\lambda^*} = \frac{\lambda(J_p)}{J_{res}^{1/3}}\left(\lambda - J_{res}^{1/3}\right)$$

Note that these results are linear and directly gives small strain results when $\lambda = 1 + \varepsilon + \varepsilon_{res}$. For hydrostatic tension (which also has $\lambda_i^* = J^{*1/3}$):

$$\begin{aligned}\sigma_{xx} = \sigma_{yy} &= \frac{f(\lambda^*, \lambda^{*3})}{\lambda^{*2}} = \frac{2G(J_p)J_{res}^{1/3}}{J^{2/3}}\left(J^{1/3} - J_{res}^{1/3}\right) + \frac{\lambda(J_p)}{J_{res}}(J - J_{res}) \\ &= \frac{2G(J_P)}{J^{2/3}}(J^{1/3} - 1) + \lambda(J_p)(J-1)\end{aligned}$$

The second form is without residual stresses. This hydrostatic state means pressure $P = -\sigma_{xx}$ and therefore bulk modulus of:

$$K = J\frac{d\sigma_{xx}}{dJ} = \lambda(J_p)J + \frac{2G(J_P)(2 - J^{1/3})}{3J^{2/3}} \tag{8.79}$$

This result has the correct small-strain limit of:

$$\lim_{J\to 1} K = \lambda(J_p) + \frac{2G(J_P)}{3} \tag{8.80}$$

For unconstrained, uniaxial, plane strain tension ($\lambda_x = \lambda$, $\lambda_z = 1$, $\lambda_y = J_E/\lambda_x$, and eigenvectors = $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$):

$$\sigma_{xx} = \frac{2G(J_P)}{\lambda\lambda_y}\lambda(\lambda - 1) + \lambda(J_p)(\lambda\lambda_y - 1) \tag{8.81}$$

$$\sigma_{yy} = \frac{2G(J_P)}{\lambda}(\lambda_y - 1) + \lambda(J_p)(\lambda\lambda_y - 1) \tag{8.82}$$

Solving for zero stress in the y direction gives

$$\lambda_y = \frac{2G(J_P) + \lambda\lambda(J_p)}{2G(J_P) + \lambda^2\lambda(J_p)} \tag{8.83}$$

Substituting into axial stress gives

$$\sigma_{xx} = \frac{2G(J_P)(\lambda - 1)}{1 + \lambda^2\frac{\lambda(J_p)}{2G(J_P)}}\left(\frac{\lambda(J_p)}{2G(J_P)} + \frac{\left(1 + \lambda^2\frac{\lambda(J_p)}{2G(J_P)}\right)^2}{1 + \lambda\frac{\lambda(J_p)}{2G(J_P)}}\right) \tag{8.84}$$

8.8.2 Linear Shear Loading

The Cauchy stress reduces to

$$\boldsymbol{\sigma} = 2G(J_P)\left(\lambda_1(\lambda_1-1)\boldsymbol{n}_1\otimes\boldsymbol{n}_1 + \lambda_2(\lambda_2-1)\boldsymbol{n}_2\otimes\boldsymbol{n}_2\right) \tag{8.85}$$

where eigenvalues and eigenvectors are given in above. The algebra is messy. With the help of Mathematica, the stress terms reduce too

$$\sigma_{xx} = G(J_P)\left(2(1+\gamma^2) + \frac{k_1(\gamma-\sqrt{4+\gamma^2}) - k_2(\gamma+\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{8.86}$$

$$\sigma_{yy} = G(J_P)\left(2 - \frac{k_1(\gamma+\sqrt{4+\gamma^2}) - k_2(\gamma-\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{8.87}$$

$$\tau_{xy} = 2G(J_P)\left(\gamma + \frac{k_1-k_2}{\sqrt{8+2\gamma^2}}\right) \tag{8.88}$$

$$\sigma_{zz} = 0 \tag{8.89}$$

where

$$k_1 = \sqrt{2+\gamma^2-\gamma\sqrt{4+\gamma^2}} \qquad \text{and} \qquad k_2 = \sqrt{2+\gamma^2+\gamma\sqrt{4+\gamma^2}} \tag{8.90}$$

Expanding in γ and keeping only linear terms reduces to small strain result of $\tau_{xy} = G\gamma$ with all other stresses zero.

8.9 Transversely Isotropic Neo-Hookean Material

8.9.1 Linear Elastic

First, rewrite the transversely-isotropic stiffness matrix when axial direction is along the x axis as sum of isotropic stiffness matrix and changes caused by aniostropy:

$$\mathbf{C} = \begin{bmatrix} \lambda+2G+\gamma & \lambda+\beta & \lambda+\beta & 0 & 0 & 0 \\ \lambda+\beta & \lambda+2G & \lambda & 0 & 0 & 0 \\ \lambda+\beta & \lambda & \lambda+2G & 0 & 0 & 0 \\ 0 & 0 & 0 & G & 0 & 0 \\ 0 & 0 & 0 & 0 & G+\alpha & 0 \\ 0 & 0 & 0 & 0 & 0 & G+\alpha \end{bmatrix}$$

where

$$\lambda = K_T - G_T \quad G = G_T \quad \alpha = G_A - G_T \quad \gamma = E_A - G_T - K_T(1-4\nu_A^2) \quad \beta = G_T - K_T(1-2\nu_A)$$

The symmetric stress is

$$\boldsymbol{\sigma} = \begin{pmatrix} (2G+\gamma)\varepsilon_{xx} + \lambda\mathrm{Tr}(\boldsymbol{\varepsilon}) + \beta(\varepsilon_{yy}+\varepsilon_{zz}) & 2(G+\alpha)\varepsilon_{xy} & 2(G+\alpha)\varepsilon_{xz} \\ 2(G+\alpha)\varepsilon_{xy} & \beta\varepsilon_{xx} + 2G\varepsilon_{yy} + \lambda\mathrm{Tr}(\boldsymbol{\varepsilon}) & 2G\varepsilon_{yz} \\ 2(G+\alpha)\varepsilon_{xz} & 2G\varepsilon_{yz} & \beta\varepsilon_{xx} + 2G\varepsilon_{yy} + \lambda\mathrm{Tr}(\boldsymbol{\varepsilon}) \end{pmatrix}$$

The strain energy can be written as

$$W = G\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon} + \frac{\lambda}{2}\mathrm{Tr}(\boldsymbol{\varepsilon})^2 + 2\alpha(\varepsilon_{xx}^2+\varepsilon_{xy}^2+\varepsilon_{xz}^2) + \beta\varepsilon_{xx}(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}) + \left(\frac{\gamma}{2}-2\alpha-\beta\right)\varepsilon_{xx}^2$$

To map to a hyperelastic energy, we add I_4 and I_5 terms, which are pseudo invariants that depend on the axial direction in the material. If axial direction in the initial configuration is along unit vector $\boldsymbol{A}$, the pseudo-invariants are:

$$I_4 = \boldsymbol{A}\cdot\mathbf{C}\boldsymbol{A} \qquad \text{and} \qquad \boldsymbol{A}\cdot\mathbf{C}^2\boldsymbol{A}$$

For example, if $\boldsymbol{A}$ is along the x axis, then $I_4 = C_{11}$ and $I_5 = (\mathbf{C}^2)_{11} = C_{11}^2 + C_{12}^2 + C_{13}^3$, which are exactly the terms shown by Ogden needed to specify energy of a transversely isotropic material. Expanding these invariants for second-order, small strain expansions (see Eq. (8.38) gives the mappings:

$$\begin{aligned}
I_4 - 1 = C_{11} &\rightarrow 2\varepsilon_{xx} + 2(\varepsilon_{xx}^2 + \varepsilon_{xy}^2 + \varepsilon_{xz}^2)\\
I_5 - 1 = (\mathbf{C}^2)_{11} &\rightarrow 4\varepsilon_{xx} + 8(\varepsilon_{xx}^2 + \varepsilon_{xy}^2 + \varepsilon_{xz}^2)\\
\frac{1}{2}(I_5-1) - (I_4-1) &\rightarrow 2(\varepsilon_{xx}^2 + \varepsilon_{xy}^2 + \varepsilon_{xz}^2)\\
\frac{1}{4}(I_4-1)^2 &= \varepsilon_{xx}^2
\end{aligned}$$

The isotropic parts could use any isotropic, neo-Hookian material while the anisotropic parts of W could map from

$$W = \alpha\left(\frac{1}{2}(I_5-1) - (I_4-1)\right) + \frac{\beta}{2}(I_4-1)\ln J + \frac{\gamma - 2\alpha - \beta}{4}(I_4-1)^2$$

This anisotropic energy matches the energy used by Bonet and Burton (1998):

$$W(I_1, J, I_4, I_5) = \frac{G}{2}(I_1 - 3 - 2\ln J) + \lambda U(J) + \alpha^*\left(I_4 - 1 - \frac{1}{2}(I_5-1)\right) + 2\beta^*(I_4-1)\ln J + \gamma^*(I_4-1)^2$$

by redefining their constants (starred here) with the ones derived here using:

$$\alpha^* = -\alpha \qquad \beta^* = \frac{\beta}{4} \qquad \gamma^* = \frac{\gamma - 2\alpha - \beta}{4} \qquad U(J) = \frac{1}{2}(\ln J)^2 \tag{8.91}$$

8.9.2 Hyperelastic Stresses

Switching from previous section terms to terms defined in Bonet and Burton (1998), the potential energy is rewritten as:

$$W(I_1, J, I_4, I_5) = \frac{G}{2}(I_1 - 3 - 2\ln J) + \lambda U(J) + \alpha\left(I_4 - 1 - \frac{1}{2}(I_5-1)\right) + 2\beta(I_4-1)\ln J + \gamma(I_4-1)^2$$

where $2U(J)$ is $(1/2)(J^2-1) - \ln J$, $(J-1)^2$, or $(\ln J)^2$ for options 0, 1, or 2, respectively. Note that the first two terms are usual terms for an isotropic, neo-Hookean material. The remaining terms are changes due to anisotropy. Other models could be derived by using different isotropic or anisotropic functions. Here the anisotropic terms are recast to:

$$W_{aniso}(I_4, I_5, J) = \big(\alpha + 2\beta\ln J + \gamma(I_4-1)\big)(I_4-1) - \frac{\alpha}{2}(I_5-1)$$

Note that Bonet and Burton (1998) energy expression has β instead of 2β, but their stress calculations are based on using 2β.

The derivatives from above and two new derivatives are:

$$\mathbf{S} = 2\frac{\partial W}{\partial \mathbf{C}}, \quad \frac{\partial I_1}{\partial \mathbf{C}} = \mathbf{I}, \quad \frac{\partial J}{\partial \mathbf{C}} = \frac{J}{2}\mathbf{C}^{-1}, \quad \frac{\partial I_4}{\partial \mathbf{C}} = \boldsymbol{A}\otimes\boldsymbol{A}, \quad \text{and} \quad \frac{\partial I_5}{\partial \mathbf{C}} = \boldsymbol{A}\otimes\mathbf{C}\boldsymbol{A} + \mathbf{C}\boldsymbol{A}\otimes\boldsymbol{A}$$

The second Poila-Kirchoff stress (for option 1) becomes:

$$\begin{aligned}\mathbf{S} &= G\left(\mathbf{I}-\mathbf{C}^{-1}\right)+\left(\lambda J(J-1)+2\beta(I_4-1)\right)\mathbf{C}^{-1} \\ &\quad +2\left(\alpha+2\beta\ln J+2\gamma(I_4-1)\right)\boldsymbol{A}\otimes\boldsymbol{A}-\alpha\left(\boldsymbol{A}\otimes\mathbf{C}\boldsymbol{A}+\mathbf{C}\boldsymbol{A}\otimes\boldsymbol{A}\right)\end{aligned}$$

In the low strain limit, $J=1+\mathrm{Tr}(\boldsymbol{\varepsilon})$, $\mathbf{C}=\mathbf{I}+2\boldsymbol{\varepsilon}$, $\mathbf{C}^{-1}=\mathbf{I}-2\boldsymbol{\varepsilon}$, $I_4=2\boldsymbol{A}\cdot\boldsymbol{\varepsilon}\boldsymbol{A}$ and the stress reduces to:

$$\mathbf{S}=2G\boldsymbol{\varepsilon}+(\lambda\mathrm{Tr}(\boldsymbol{\varepsilon})+4\beta\boldsymbol{A}\cdot\boldsymbol{\varepsilon}\boldsymbol{A})\mathbf{I}+2\left(2\beta\mathrm{Tr}(\boldsymbol{\varepsilon})+4\gamma\boldsymbol{A}\cdot\boldsymbol{\varepsilon}\boldsymbol{A}\right)\boldsymbol{A}\otimes\boldsymbol{A}-2\alpha\left(\boldsymbol{A}\otimes\boldsymbol{\varepsilon}\boldsymbol{A}+\boldsymbol{\varepsilon}\boldsymbol{A}\otimes\boldsymbol{A}\right)$$

For a material with axial direction along the x axis or $\boldsymbol{A}=(1,0,0)$, the small-strain limit terms become

$$\boldsymbol{A}\cdot\boldsymbol{\varepsilon}\boldsymbol{A}=\varepsilon_{xx},\qquad \boldsymbol{A}\otimes\boldsymbol{A}=\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix},\qquad \boldsymbol{A}\otimes\boldsymbol{\varepsilon}\boldsymbol{A}+\boldsymbol{\varepsilon}\boldsymbol{A}\otimes\boldsymbol{A}=\begin{pmatrix}2\varepsilon_{xx}&\varepsilon_{xy}&\varepsilon_{xz}\\\varepsilon_{xy}&0&0\\\varepsilon_{xz}&0&0\end{pmatrix}$$

The stress components are:

$$\begin{aligned}S_{xx} &= (2G+\lambda+8\beta+8\gamma-4\alpha)\varepsilon_{xx}+(\lambda+4\beta)(\varepsilon_{yy}+\varepsilon_{zz}) \\ S_{yy} &= (\lambda+4\beta)\varepsilon_{xx}+(2G+\lambda)\varepsilon_{yy}+\lambda\varepsilon_{zz} \\ S_{zz} &= (\lambda+4\beta)\varepsilon_{xx}+\lambda\varepsilon_{yy}+(2G+\lambda)\varepsilon_{zz} \\ S_{yz} &= 2G\varepsilon_{yz} \\ S_{xz} &= (2G-2\alpha)\varepsilon_{xz} \\ S_{xy} &= (2G-2\alpha)\varepsilon_{xy}\end{aligned}$$

Comparing to stiffness tensor of a small-strain, transversely isotropic material:

$$G=G_T\qquad \alpha=G_T-G_A\qquad \lambda=K_T-G_T$$

$$\beta=\frac{1}{4}\left(G_T-K_T(1-2\nu_A)\right)\qquad \gamma=\frac{1}{8}\left(E_A-4G_A+G_T+K_T(1-2\nu_A)^2\right)$$

These derived constants match the mapping in Eq. (8.91) or the constants can be defined without need to compare to the low strain limit. If the material is isotropic, $G\to G$, $\lambda\to\lambda$, $\alpha\to 0$, $\beta\to 0$, and $\gamma\to 0$. Compared to low strain stiffness matrix, we can write

$$G=C_{44}\qquad \alpha=C_{44}-C_{55}\qquad \lambda=C_{23}\qquad \beta=\frac{C_{12}-C_{23}}{4}\qquad \lambda+4\beta=C_{12}$$

$$\lambda+2G+4(2\gamma-\alpha+2\beta)=C_{11}$$

Note the Bonet and Burton (1998) found constants based on assuming that $\nu_A=\nu_T E_T/E_A$, which is not correct for transversely isotropic materials. This assumption reduces to only four material properties instead of the required five independent properties. The above relations correct that error.

8.9.3 Kirchoff and Cauchy Stresses

The Kirchoff stress is found from $\boldsymbol{\tau}=J\boldsymbol{\sigma}=\mathbf{F}\mathbf{S}\mathbf{F}^T$ (or from Eq. (8.41)). The calculations give:

$$\boldsymbol{\tau}=G\left(\mathbf{B}-\mathbf{I}\right)+\left(\lambda dU+2\beta(\lambda_A^2-1)\right)\mathbf{I}+2\left(\alpha+2\beta\ln J+2\gamma(\lambda_A^2-1)\right)\boldsymbol{a}\otimes\boldsymbol{a}-\alpha\left(\boldsymbol{a}\otimes\mathbf{B}\boldsymbol{a}+\mathbf{B}\boldsymbol{a}\otimes\boldsymbol{a}\right)$$

where $dU=(J^2-1)/2$, $J(J-1)$ or $\ln J$ for options 0, 1, and 2, respectively, and $\boldsymbol{a}=\mathbf{F}\boldsymbol{A}$ is deformed fiber direction in the current configuration. The I_4 term simplifies to

$$I_4=\sum_i\sum_j\sum_k A_iA_jF_{ki}F_{kj}=\sum_k a_ka_k=\boldsymbol{a}\cdot\boldsymbol{a}\quad\text{and}\quad I_4-1=\boldsymbol{a}\cdot\boldsymbol{a}-1=\lambda_A^2-1$$

Here λ_A is the elongation of fiber direction in current configuration relative to initial configuration.

8.9.4 Dealing with Thermal and Moisture Strains

To handle thermal and moisture strains the deformation is divided into two steps. The first is free expansion to the new stress free volume and then deformation to the final volume. The total deformation will be

$$\mathbf{F} = \mathbf{F}^{*}\mathbf{F}^{res}$$

where

$$\mathbf{F}^{res} = \exp\left(\varepsilon_T^{res}\mathbf{I} + \left(\varepsilon_A^{res} - \varepsilon_T^{res}\right)\boldsymbol{A}\otimes\boldsymbol{A}\right)$$

where $\varepsilon_T^{res} = \alpha_T\Delta T + \beta_T\Delta c$ and $\varepsilon_A^{res} = \alpha_A\Delta T + \beta_A\Delta c$ are residual strains dues to thermal and moisture expansion. The matrix being exponentiated has eigenvalues ε_A, ε_T, and ε_T. If $A_1 \neq 0$, the orthogonal and normalized eigenvectors are:

$$\boldsymbol{e}_1 = \boldsymbol{A}, \quad \boldsymbol{e}_2 = \frac{1}{\sqrt{A_1^2 + A_3^2}}(-A_3, 0, A_1), \quad \boldsymbol{e}_2 = \frac{1}{\sqrt{A_1^2 + A_2^2}}(-A_2, A_1, 0)$$

If $A_1 = 0$, the orthogonal and normalized eigenvectors are:

$$\boldsymbol{e}_1 = \boldsymbol{A}, \quad \boldsymbol{e}_2 = \frac{1}{\sqrt{A_2^2 + A_3^2}}(0, -A_2, A_3), \quad \boldsymbol{e}_2 = (1, 0, 0)$$

Then

$$\begin{aligned}
\mathbf{F}^{res} &= \lambda_A^{res}\boldsymbol{A}\otimes\boldsymbol{A} + \lambda_T^{res}\left(\boldsymbol{e}_2\otimes\boldsymbol{e}_2 + \boldsymbol{e}_3\otimes\boldsymbol{e}_3\right) = \lambda_T^{res}\mathbf{I} + \left(\lambda_A^{res} - \lambda_A^{res}\right)\boldsymbol{A}\otimes\boldsymbol{A} \\
(\mathbf{F}^{res})^{-1} &= \frac{1}{\lambda_A^{res}}\boldsymbol{A}\otimes\boldsymbol{A} + \frac{1}{\lambda_T^{res}}\left(\boldsymbol{e}_2\otimes\boldsymbol{e}_2 + \boldsymbol{e}_3\otimes\boldsymbol{e}_3\right) = \frac{1}{\lambda_T^{res}}\mathbf{I} + \frac{1}{\lambda_A^{res} - \lambda_A^{res}}\boldsymbol{A}\otimes\boldsymbol{A}
\end{aligned}$$

and its determinant is

$$|\mathbf{F}^{res}| = \lambda_A^{res}(\lambda_T^{res})^2$$

where

$$\lambda_A^{res} = \exp(\varepsilon_A^{res}) \qquad \text{and} \qquad \lambda_T^{res} = \exp(\varepsilon_T^{res})$$

8.9.5 Constrained Axial Tension

For constrained loading in the axial direction (taken here as the x axis), $F_{11} = \lambda_A$, $F_{22} = F_{33} = 1$, rest are zero, $B_{ii} = F_{ii}^2$, $J = \lambda_A$, and $\boldsymbol{a} = (\lambda_A, 0, 0)$. The Kirchoff stress (for option 0 with $dU = (\lambda_A^2 - 1)/2$) is:

$$\begin{aligned}
\tau_{xx} &= \frac{\lambda + 2(G + 2\beta + 2(2\gamma - \alpha)\lambda_A^2)}{2}(\lambda_A^2 - 1) + 4\beta\lambda_A^2\ln\lambda_A \\
&= \left(K_T\nu_A + G_T + 2(2\gamma - \alpha)\lambda_A^2\right)(\lambda_A^2 - 1) + 4\beta\lambda_A^2\ln\lambda_A \\
\tau_{yy} = \tau_{zz} &= \frac{\lambda + 4\beta}{2}(\lambda_A^2 - 1) = K_T\nu_A(\lambda_A^2 - 1) \\
\tau_{ij} &= 0 \ (i \neq j)
\end{aligned}$$

For small strain, $\lambda_A = 1 + \varepsilon_{xx}$ and this result reduces to $\tau_{xx} = (E_A + 4K_T\nu_A^2)\varepsilon_{xx}$ and $\tau_{yy} = \tau_{zz} = 2K_T\nu_A\varepsilon_{xx}$, which matches small-strain elasticity.

For constrained loading in the transverse direction (taken here as the y axis), $F_{22} = \lambda_T$, $F_{11} = F_{33} = 1$, rest are zero, $B_{ii} = F_{ii}^2$, $J = \lambda_T$, and $\boldsymbol{a} = (1,0,0)$. The Kirchoff stress (for option 0 with $dU = (\lambda_T^2 - 1)/2$) is:

$$\begin{aligned}
\tau_{xx} &= \frac{\lambda}{2}(\lambda_T^2 - 1) + 4\beta \ln \lambda_T = \frac{K_T - G_T}{2}(\lambda_T^2 - 1) + 4\beta \ln \lambda_T \\
\tau_{yy} &= \frac{\lambda + 2G}{2}(\lambda_T^2 - 1) = \frac{K_T + G_T}{2}(\lambda_T^2 - 1) \\
\tau_{zz} &= \frac{\lambda}{2}(\lambda_T^2 - 1) = \frac{K_T - G_T}{2}(\lambda_T^2 - 1) \\
\tau_{ij} &= 0 \ (i \neq j)
\end{aligned}$$

For small strain, $\lambda_T = 1 + \varepsilon_{yy}$ and this result reduces to $\tau_{xx} = 2K_T \nu_A \varepsilon_{yy}$, $\tau_{yy} = (K_T + G_T)\varepsilon_{yy}$, and $\tau_{zz} = (K_T - G_T)\varepsilon_{yy}$, which matches small-strain elasticity.

For simple tension in the axial direction (taken here as the x axis), $F_{11} = \lambda_A$, $F_{22} = F_{33} = \lambda_T$, rest are zero, $B_{ii} = F_{ii}^2$, $J = \lambda_A \lambda_T^2$, and $\boldsymbol{a} = (\lambda_A, 0, 0)$. The Kirchoff stress (for option 0 with $dU = (\lambda_A^2 - 1)/2$) for transverse stress is:

$$\tau_{yy} = \tau_{zz} = G(\lambda_T^2 - 1) + \frac{\lambda}{2}(\lambda_A^2 \lambda_T^4 - 1) + 2\beta(\lambda_A^2 - 1)$$

Setting this stress to zero and substituting into axial stress gives

$$\tau_{xx} = G\frac{\lambda_A^3 - J}{\lambda_A} + 2\big((2\gamma - \alpha)(\lambda_A^2 - 1) + 2\beta \ln J\big)\lambda_A^2$$

where J is found by solving for λ_T^2 needed for zero transverse stress, which is:

$$J = \lambda_A \lambda_T^2 = \frac{-G + \sqrt{(\lambda\lambda_A^2 + G)^2 - \lambda(\lambda + 4\beta)(\lambda_A^2 - 1)\lambda_A^2}}{\lambda\lambda_A}$$

For small strain, $\lambda_A = 1 + \varepsilon_{xx}$ and $\lambda_T = 1 + \varepsilon_T$ (where $\varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_T$) and transverse stress reduces to the expected result:

$$\tau_{yy} = \tau_{zz} = 2K_T \nu_A \varepsilon_{xx} + 2K_T \varepsilon_T \implies \varepsilon_T = -\nu_A \varepsilon_{xx}$$

Solving for zero transverse stress (or expansion of J above) both lead to:

$$J = 1 + \varepsilon_{xx} + 2\varepsilon_T = 1 + \varepsilon_{xx}(1 - 2\nu_A)$$

and finally (all with checks in Mathematica) of

$$\tau_{xx} = E_A \varepsilon_{xx}$$

8.10 Mie-Grüniesen Equation of State

The Mie-Grüniesen Equation of State defines the pressure only and the Cauchy pressure is

$$P = \frac{\rho_0 C_0^2 \eta \left(1 - \frac{1}{2}\gamma_0 \eta\right)}{(1 - S_1\eta - S_2\eta^2 - S_3\eta^3)^2} + \rho_0 \gamma_0 U \tag{8.92}$$

where η is fraction compression and defined from density by

$$\eta = 1 - \frac{\rho_0}{\rho} = 1 - \frac{V}{V_0} = 1 - J \tag{8.93}$$

C_0 is the material's waves speed, γ_0 and S_i are dimensionless material properties, and U is total internal energy (per unit mass). Note that initial bulk modulus is $K_0 = \rho_0 C_0^2$. The above equation applies only in compression ($\eta > 0$). In tension, the pressure uses one of the Mooney-Rivlin pressure laws:

$$P = -\rho_0 C_0^2 (J^* - 1) = -K_0 (J^* - 1) \tag{8.94}$$

The Kirchhoff pressure needed by MPM is

$$\frac{\tau}{\rho_0} = \frac{JP}{\rho_0} \tag{8.95}$$

This material model also causes a temperature change. Using general Eq. (4.10), the temperature change is:

$$\frac{dT_{dS=0}}{T} = -\frac{K\alpha_V}{\rho C_v}\frac{\Delta V}{V} = -\gamma\frac{\Delta V}{V} = -\gamma_0\frac{\Delta V}{V_0} \tag{8.96}$$

where γ is the Grüniesen (not to be confused with $\gamma = C_p/C_v$ in an ideal gas). The last form is approximation asserted in Mie-Grüniesen theory that $\gamma/V \approx \gamma_0/V_0$. The temperature rise here then becomes:

$$dT_{dq=0} = -JT\gamma_0\frac{\Delta V}{V} \qquad vs. \qquad dT_{dq=0} = -JT\frac{K}{K_0}\gamma_0\frac{\Delta V}{V} \tag{8.97}$$

from above (see Eq. (4.10)). The result here differs by a factor (K/K_0). The first result is one used in literature for compression and is the one implemented in code. In tension, however, the code uses the thermodynamics results with $(K/K_0) = J^*$. See Eq. (8.166) for comparable results in an ideal gas. Note that assumption $\gamma/V \approx \gamma_0/V_0$ for a material with constant C_V implies:

$$\frac{K}{K_0} = \frac{\alpha_{V0}}{\alpha_V} \tag{8.98}$$

where α_{V0} is initial volumetric thermal expansion coefficient.

Using $d\eta = -JdV/V$ (and $dV = -Vd\eta/J = -V_0 d\eta$), differential equations for isoentropic temperature heating are:

$$\frac{dT_{dq=0}}{d\eta} - \gamma_0 T = 0 \qquad and \qquad \frac{dT_{dq=0}}{d\eta} - \frac{K}{K_0}\gamma_0 T = 0 \tag{8.99}$$

for compression and tension, respectively. These equation can be integrated to find total temperature change. For adibatic compression, the result is

$$T = T_0 \exp(\gamma_0 \eta) \tag{8.100}$$

Thus the total small-strain temperature rise (assuming C_v is constant) is

$$dT = T_0\big(\exp(\gamma_0\eta) - 1\big) + \frac{\Phi}{C_v} \tag{8.101}$$

where Φ is the cumulative dissipated energy due to plasticity.

Rather then calculate temperature changes, which are needed for internal energy, `NairnMPM/OSParticulas` tracks total work, w, and heat, q, to find internal energy as $U = w + q$. The details are given above in the section on "Thermodynamics of Deformation."

8.10.1 Rapid Adiabatic Loading

For rapid load such that all heating remains on the particles, the internal energy per unit mass is solely $-PdV/(\rho V)$, which leads to:

$$\rho_0\gamma_0 U = -\gamma_0\int_{V_0}^{V}\frac{\rho_0 P}{\rho V}dV = \gamma_0\int_0^{\eta}\frac{\rho_0 V_0 P}{\rho V}d\eta = \gamma_0\int_0^{\eta} P\,d\eta \tag{8.102}$$

Substituting into Eq. 8.92 gives an integral equation for pressure. Differentiating that equation gives a differential equation for pressure:

$$\frac{dP}{d\eta}-\gamma_0 P = \frac{K_h}{1-\eta} \quad \text{where} \quad K_h = -V\frac{dP_h}{dV} = (1-\eta)\frac{dP_h}{d\eta} \tag{8.103}$$

where P_h is first term in Eq. 8.92. In other words, K_h is bulk modulus that would be found by ignoring the internal energy term. Explicitly, it is:

$$K_h = K_0\frac{(1-\eta)(1-\gamma_0\eta(1+\eta^2(S_2+2S_3\eta))+\eta(S_1+\eta(3S_2+5S_3\eta)))}{(1-\eta(S_1+\eta(S_2+S_3\eta)))^3} \tag{8.104}$$

The differential equation can be solved for P (using Mathematical and answer in terms of exponential integral functions) and then used to find $K=(1-\eta)dP/d\eta$. In sample calculations, it appears that $K\approx K_h$. Alternatively, substituting K definition into Eq. 8.103 leads to adiabatic bulk modulus of

$$K_{ad} = K_h + \gamma_0(1-\eta)P \tag{8.105}$$

8.10.2 Slow Isothermal Loading

For slow, isothermal loading, it is assumed that the isoentropic temperature increment is expelled to the exterior causing a change in heat energy of

$$dQ = C_v J T_0\gamma_0\frac{dV}{V} \tag{8.106}$$

where C_v is heat capacity (per unit mass) and T_0 is the isothermal temperature. This heat energy adds to the internal energy term as:

$$\rho_0\gamma_0 Q = \rho_0 C_v T_0\gamma_0^2\int_{V_0}^{V} J\frac{dV}{V} = -\rho_0 C_v T_0\gamma_0^2\int_0^{\eta} d\eta = -\rho_0 C_v T_0\gamma_0^2\eta \tag{8.107}$$

which assumes C_v is independent of pressure. The differential equation becomes:

$$\frac{dP}{d\eta}-\gamma_0 P+\rho_0 C_v T_0\gamma_0^2 = \frac{K_h}{1-\eta} \tag{8.108}$$

and the isothermal bulk modulus becomes:

$$K = K_h + \gamma_0(1-\eta)(P-\rho_0\gamma_0 C_v T_0) \tag{8.109}$$

or slightly lower than the adiabatic bulk modulus (but second term is normally small) or

$$K_{ad} = K + J\gamma_0^2\rho_0 C_v T_0 \tag{8.110}$$

From thermodynamics, $K_{ad}/K = C_p/C_v$. From isothermal K and adiabatic K_{ad}, the result becomes

$$\frac{C_p}{C_v} = 1+\frac{J\gamma_0^2\rho_0 C_v T}{K} = 1+\frac{K_0}{K}\frac{K_0\alpha_{V0}^2 T}{\rho C_v} \tag{8.111}$$

For small strain ($K\to K_0$), this reduces to standard thermodynamics result for solids. The K_0/K term in this equation may by a consequence of the above assumption that $\gamma/V\approx\gamma_0/V_0$.

8.10.3 K_{max} Option

In compression, J is physically limited to be between 0 and 1, which means η is also between 0 and 1. But for most materials that have been fit to the Mie-Grüneisen equation of state, the denominator in pressure might becomes zero before η reaches 1 (and corresponds to a limiting compression in shock loading). For example, Tungsten has $S_1 = 1.24$ and $S_2 = S_3 = 0$. The denominator becomes zero when

$$\eta = 1/1.24 = 0.806 \tag{8.112}$$

If the time step is too large in dynamic code, the compression could potentially pass this value. If that happens for any particle, the results will likely be poor. By default, `NairnMPM/OSParticulas` does not check for exceeding this limit (and it really happens in normal simulations). You can optionally set a material parameter called `Kmax` that will limit K_h to $K_{max}K_0$ (*i.e.*, `Kmax` is relative increase allowed in K_h). A warning is printed the first time the compression reaches the limiting value.

8.10.4 Residual Stresses

This equation of state has no thermal expansion coefficient, but thermal expansion occurs naturally with proper tracking of heat flow and temperature. The volumetric thermal expansion coefficient from input properties is:

$$3\alpha = \frac{\rho_0\gamma_0 C_v}{K_0} \qquad \text{or} \qquad \gamma_0 = \frac{3K_0\alpha}{\rho_0 C_v} \tag{8.113}$$

which is same as defined above in Eq. (4.11).

Under free thermal expansion, $U = C_v\Delta T$ (which comes from the temperature boundary condition required to heat up the material). In small strain compression

$$P = -K_0\frac{\Delta V}{V_0} + 3K_0\alpha\Delta T \tag{8.114}$$

and for free thermal expansion, $P = 0$ which leads to

$$\frac{\Delta V}{V_0} = 3\alpha\Delta T \tag{8.115}$$

This volume change is the expected volume change for free thermal expansion.

8.11 Isotropic Hyperelastic-Plastic Material

The `HEIsotropic` material is an anisotropic material with plasticity. The elastic part of this material uses the Mooney-Rivlin material but restricts it to $G_2 = 0$ (*i.e.*, a neo-Hookean material). For 3D (with plane strain and axisymmetry as easy special cases, but plane stress not handled), the Kirchhoff stress update, including residual stresses is is

$$P = JP(J^*) \tag{8.116}$$

$$s_{xx}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{xx}^{trial} - B_{yy}^{trial} - B_{zz}^{trial}\right) \tag{8.117}$$

$$s_{yy}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{yy}^{trial} - B_{xx}^{trial} - B_{zz}^{trial}\right) \tag{8.118}$$

$$s_{zz}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{zz}^{trial} - B_{xx}^{trial} - B_{yy}^{trial}\right) \tag{8.119}$$

$$s_{ij}^{trial} = \frac{J_{res}G_1}{J^{2/3}}B_{ij}^{trial} \qquad \text{for } i \neq j \tag{8.120}$$

where $P(J^*)$ is any hyperelaastic pressure model, J is relative volume change, J_{res} is the volume change related to residual stresses, and $J^* = J/J_{res}$. Here the deviatoric Kirchoff stresses are trial stresses based on trial, elastic, left Cauchy-Green strain in $\mathbf{B}^{trial}$. This material tracks the elastic $\mathbf{B}$. At the start of the update, $\mathbf{B}^{trial}$ is found from:

$$\mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{8.121}$$

where $\mathbf{dF}$ is the incremental deformation gradient for this time step and $\mathbf{B}_n$ is the elastic $\mathbf{B}$ from previous step. Notice that the deviatoric Kirchoff stresses can be rewritten more concisely as

$$\mathbf{s} = J_{res}G_1 \mathrm{dev}\,\overline{\mathbf{B}} \tag{8.122}$$

where $\overline{\mathbf{B}} = \mathbf{B}/J^{2/3}$.

The yielding criterion is handled by methods nearly identical to J_2 plasticity for isotropic materials (and can use any available hardening law). The first step is to find

$$f_{trial} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}K(\alpha) \tag{8.123}$$

if $\mathbf{f}_{trial}$ is less than zero, the trial stresses and $\mathbf{B}_{n+1}^{trial}$ are copied to the particle and the update is done. If yielding is occurring, the task is to solve for λ such that $f = 0$ and thereby determine the amount of yielding. The key equations for final results are:

$$\mathbf{B} = \mathbf{B}^{trial} - \frac{2}{3}\lambda\overline{I_1}\mathbf{n} \tag{8.124}$$

$$\mathbf{s} = \mathbf{s}^{trial} - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right)\mathbf{n} \tag{8.125}$$

$$\|\mathbf{s}\| = \|\mathbf{s}^{trial}\| - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right) \tag{8.126}$$

where $\mathbf{n}$ is normal defined from deviatoric stress tensor and

$$\overline{I_1} = \frac{B_{xx} + B_{yy} + B_{zz}}{J^{2/3}} \tag{8.127}$$

Notice that the updates for the deviatoric stress and its magnitude are identical to low-strain J_2 plasticity theory provided we replace shear modulus G in that theory with $\overline{\mu}$ defined by

$$\overline{\mu} = \frac{J_{res}G\overline{I_1}}{3} \tag{8.128}$$

After this substitution, any hardening law available in the code can solve for plasticity in this hyperelastic material as well (this mapping relies on constitutive law in Eq. (8.122) and therefore is specific to this material model). This modification works for plane strain, axisymmetric, and 3D, but not for plane stress, because J_2 plane stress analysis makes use of low-strain constitutive laws. For this reason, the `HEIsotropic` material cannot do plane stress calculations. Once the hardening law finds λ, the above equations are used to update $\mathbf{s}$ and $\mathbf{B}$ on the particle.

8.12 Ideal Gas

The ideal gas material implements ideal gas law as a large deformation, hyperelastic material. It seems to work well for gas confined within a solid or constrained by rigid particles. It does not handle gas

dynamics such as irreversible free expansion, but does handle reversible processes including coupled conversion of energy into heat (*i.e.*, cooling on expansion and heating on compression).

The ideal gas law is

$$PV = nRT \tag{8.129}$$

The ideal gas properties are defined by picking any reference pressure, P_0, reference temperature, T_0, and reference density, ρ_0. If M is the molecular weight of the gas molecules, the reference density can be found from:

$$\rho_0 = \frac{P_0}{T_0}\frac{M}{R} \tag{8.130}$$

We can now eliminate n and R to derive

$$P = P_0\frac{V_0}{V}\frac{T}{T_0} = P_0\frac{T}{T_0}\frac{1}{J} \tag{8.131}$$

where $J = \det \mathbf{F} = V/V_0$ is relative volume relative to reference conditions.

The Cauchy stress due to this pressure is $-P\mathbf{I}$, which implies hyperelastic energy function determined from:

$$\boldsymbol{\sigma} = -P_0\frac{T}{T_0}\frac{1}{J}\mathbf{I} = \frac{dU(J)}{dJ}\mathbf{I} \qquad \text{or} \qquad U(J) = -P_i \ln J \tag{8.132}$$

where $P_i = P_0 T/T_0$. This energy is equal to the energy per unit reference volume for isothermal compression or expansion of an ideal gas:

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\, dV = -\frac{P_0 T}{T_0}\int_{V_0}^{V}\frac{1}{V}\, dV = -P_i \ln\frac{V}{V_0} = -P_i \ln J \tag{8.133}$$

For MPM calculations, the code needs a specific Kirchoff stress normalized to ρ_0:

$$\boldsymbol{\tau}^{(s)} = \frac{\boldsymbol{\tau}}{\rho_0} = -\frac{PJ}{\rho_0}\mathbf{I} = -\frac{P_0}{\rho_0}\frac{T}{T_0}\mathbf{I} \tag{8.134}$$

In coding, an incremental approach is possible (but seems slightly less stable). If $\tau_n^{(s)}$ is any diagonal element of the specific Kirchoff stress tensor for time step n, then

$$\tau_{n+1}^{(s)} = -\frac{P_0}{\rho_0}\frac{T_{n+1}}{T_0} = -\frac{P_0}{\rho_0}\frac{T_n}{T_0}\frac{T_{n+1}}{T_n} = \tau_n^{(s)}\frac{T_{n+1}}{T_n} \tag{8.135}$$

Note that the Kirchoff stress normalized to ρ_0 remains constant for isothermal expansion and compression.

When gas particles are present, they have to be initialized to pressure corresponding to initial volume and temperature. If initial particle temperature is T_{init} (*i.e.* the simulation starting temperature and need not equal T_0) and initial particle volume remains at V_0 (or $J_{init} = 1$), we have to set

$$J_{init} = 1 = \frac{MP_{init}}{\rho_0 R T_{init}} \qquad \text{or} \qquad P_{init} = P_0\frac{T_{init}}{T_0} \tag{8.136}$$

The energy increment associated with this stress change is $dU = -P\, dV$ work. The energy per unit mass using midpoint rule between initial and final pressure is therefore

$$\frac{dU}{\rho_0 V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1} - V_n}{V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1}}{V_0}\left(1 - \frac{V_n}{V_{n+1}}\right) \tag{8.137}$$

Let deformation gradient for step $n+1$ be

$$\mathbf{F}_{n+1} = \mathbf{f} \cdot \mathbf{F}_n \quad \text{where} \quad \mathbf{f} = \exp(\Delta t \nabla \boldsymbol{v}) \quad \text{and} \quad J_{n+1} = \det \mathbf{f} J_n \tag{8.138}$$

which leads to

$$\frac{dU}{\rho_0 V_0} = -\frac{J_{n+1}}{2}\frac{P_n + P_{n+1}}{\rho_0}\left(1 - \frac{1}{\det f}\right) = -\frac{1}{2}\left(\frac{P_n}{\rho_n}\det f + \frac{P_{n+1}}{\rho_{n+1}}\right)\left(1 - \frac{1}{\det f}\right) \tag{8.139}$$

But, P/ρ is $-\tau^{(s)}$ leading to

$$\frac{dU}{\rho_0 V_0} = \frac{1}{2}\left(\tau_n^{(s)}\det f + \tau_{n+1}^{(s)}\right)\left(1 - \frac{1}{\det f}\right) \tag{8.140}$$

This material always needs heat capacity and needs thermal conductivity when doing conduction. Heat capacity per unit mass is calculated using ideal gas law theory ($C_v = (3/2)nR/(\rho_0 V_0)$ for monotonic gas and $C_v = (5/2)nR/(\rho_0 V_0)$ for diatomic gas in J/(kg-K)). To find heat capacity from input parameters, substitute $nR = P_0 V_0/T_0$ at reference conditions to get

$$C_v = \frac{3}{2}\frac{P_0}{\rho_0 T_0} \tag{8.141}$$

for monatomic gas (or replace 3/2 with 5/2 for diatomic gas). For conduction, the current code assumes conductivity is a temperature-independent property (as entered), although conductivity of a gas does vary with temperature. If simulations with large temperature changes of the gas are important, this material will need to be improved to allow temperature-dependent thermal conductivity.

The adiabatic bulk modulus is a derivative from thermodynamics tables as:

$$\frac{1}{K} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_S = \frac{C_v \beta}{C_p} \quad \text{where} \quad \beta = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T \tag{8.142}$$

is isothermal compressibility. For an ideal gas, $\beta = -(1/V)(-nRT/P^2) = 1/P$ leading to

$$K = \gamma P = \frac{\gamma \rho R T}{M} \tag{8.143}$$

In terms of defined material properties, the wave speed reduces to

$$C = \sqrt{\frac{K}{\rho}} = \sqrt{\frac{\gamma \rho_0 P_0 T}{T_0}} \tag{8.144}$$

where T is particle temperature.

8.12.1 Verification Examples

A simple gas problem is to confine all sides by rigid particles and move one wall for compression or expansion. If the movable wall is in the x direction, the volume will be $V = V_0(1+\varepsilon_{xx})$. For isothermal compression and expansion:

$$P = \frac{P_i}{1+\varepsilon_{xx}} \tag{8.145}$$

$$U = 0 \tag{8.146}$$

$$w = -P_i V_0 \ln(1+\varepsilon_{xx}) \tag{8.147}$$

$$q = -w \tag{8.148}$$

$$S = nR\ln(1+\varepsilon_{xx}) = \frac{P_0 V_0}{T_0}\ln(1+\varepsilon_{xx}) \tag{8.149}$$

For adiabatic compression and expansion

$$P = \frac{P_i}{(1+\varepsilon_{xx})^\gamma} \tag{8.150}$$

$$T = \frac{T_i}{(1+\varepsilon_{xx})^{\gamma-1}} \tag{8.151}$$

$$U = C_v(T-T_i) = \frac{3P_0V_0}{2T_0}T_i\left(\frac{1}{(1+\varepsilon_{xx})^{\gamma-1}}-1\right) \tag{8.152}$$

$$w = U \tag{8.153}$$

$$q = 0 \tag{8.154}$$

$$S = -(\gamma-1)C_v\ln(1+\varepsilon_{xx}) + \frac{P_0V_0}{T_0}\ln(1+\varepsilon_{xx}) = 0 \tag{8.155}$$

where $\gamma = C_P/C_v = 5/3$ for monotonic gas or $\gamma = 7/5$ for diatomic. An undocumented custom task in `NairnMPM` can subject an ideal gas to a Carnot cycle and recover an efficiency close to the theoretical maximum of:

$$\eta = 1 - \frac{T_2}{T_1} \tag{8.156}$$

where T_1 is the hot reservoir and T_2 is the cold one.

8.12.2 Isothermal *vs.* Adiabatic *vs.* General Constitutive Law

Equation (8.131) can be rewritten as an increment in pressure from initial pressure P_0 at temperature T_0:

$$P - P_0 = \kappa_0\left[\left(\frac{J_{res}}{J}\right)-1\right] \tag{8.157}$$

where κ_0 is the bulk modulus at P_0:

$$\frac{1}{\kappa_0} = -\frac{1}{V_0}\left(\frac{\partial V_0}{\partial P}\right)_T = \frac{1}{P_0} \tag{8.158}$$

and

$$J = \frac{V(P,T)}{V(P_0,T_0)} = \frac{V}{V_0} \qquad \text{and} \qquad J_{res} = \frac{V(P_0,T)}{V(P_0.T_0)} = \frac{T}{T_0} \tag{8.159}$$

Here J_{res} is the volume ratio for free thermal expansion at reference pressure P_0. For an isothermal process $J_{res} = 1$. For a (reversible) adiabatic compression or expansion, the temperature change is:

$$T = \frac{T_0}{J^{\gamma-1}} \qquad \text{and} \qquad J_{res} = \frac{1}{J^{\gamma-1}} \tag{8.160}$$

Two special cases of the general law, therefore, are:

$$P - P_0 = \kappa_0\left[\left(\frac{1}{J}\right)-1\right] \qquad \text{isothermal} \tag{8.161}$$

$$P - P_0 = \kappa_0\left[\left(\frac{1}{J}\right)^\gamma-1\right] \qquad \text{adiabatic} \tag{8.162}$$

But if code implements either of these laws, it will be restricted to either isothermal or adiabatic conditions only.

The preferred approach is to implement the general law because it includes both these limits as special cases and can be used for nonisothermal, nonadiabatic simulations as well. When using a general law, however, each material point must correctly change its temperature according to how much energy should be converted into heat for a given increment in deformation. The isoentropic temperature changes (needed in constitutive laws) in general is:

$$\left(\frac{\partial T}{\partial V}\right)_S = -\frac{\alpha_V T}{\rho V C_v \beta} \tag{8.163}$$

For an ideal gas, $\beta = 1/P$ and $\alpha_V = (1/V)(nR/P) = 1/T$ leading to

$$dT_{q=0} = -\frac{P}{\rho V C_v} dV = -\frac{nRT}{\rho V C_v}\frac{dV}{V} = -T(\gamma-1)\frac{dV}{V} \tag{8.164}$$

or

$$\frac{dT_{q=0}}{T} = -(\gamma-1)\frac{dV}{V} = -\frac{(\gamma-1)}{J}\frac{dV}{V_{ref}} \tag{8.165}$$

Here $C_v = nR/((\gamma-1)\rho V)$ is heat capacity per unit mass for an ideal gas. Notice that this equation implies that all PdV work is converted into temperature increase or that $\rho V C_v dT_{q=0} = -PdV$. Defining $\eta = 1 - \frac{V}{V_{ref}} = 1 - J$ which leads to $d\eta = -dV/V_{ref} = -JdV/V$, this result can be written as

$$\frac{dT}{T} = \frac{(\gamma-1)}{J} d\eta \tag{8.166}$$

See similar equations derived for general thermodyanamics (Eq. (4.10)) and for a Mie-Grüniesen material (Eq. (8.97)). This result is identical to general thermodynamics by noting that

$$\frac{K\alpha_V}{\rho C_v} = \frac{C_p - C_v}{C_v \alpha_V T} = \frac{\gamma-1}{\alpha_V T} = \gamma - 1 \tag{8.167}$$

The first three results are general and last is for ideal gas only. For comparison, an ideal gas has

$$\frac{(\gamma-1)}{J} = \frac{K\alpha_V}{\rho C_v}\frac{\rho}{\rho_{ref}}\frac{K_{ref}}{K_{ref}} = \frac{K}{K_{ref}}\gamma_0 \tag{8.168}$$

where γ_0 is defined for reference conditions.

8.12.3 Van der Waals Gas Law

The van der Wasls gas material implements a non-ideal gas law as a large deformation, hyperelastic material. It seems to work well for gas confined within a solid or constrained by rigid particles. It does not handle gas dynamics such as irreversible free expansion, but does handle reversible processes including coupled conversion of energy into heat (*i.e.*, cooling on expansion and heating on compression).

The van der Waals gas law is

$$\left(P - \frac{an^2}{V^2}\right)\left(\frac{V}{n} - b\right) = RT \tag{8.169}$$

The nonideal gas properties are defined by picking any reference pressure, P_0, reference temperature, T_0, and reference density, ρ_0, along with a and b. The law can then be transformed to pressure of

$$P = \left(P_0 - a'\right)\left(\frac{1-b'}{J-b'}\right)\frac{T}{T_0} + \frac{a'}{J^2} \tag{8.170}$$

where $J = V/V_0$, V_0 is initial particle volume, $a' = an^2/V_0^2$, and $b' = nbV_0$. Writing $P = -dU(J)/dJ$ implies a hyperelastic energy function of

$$U(J) = -\left[\left(P_i - a'\right)\left(1 - b'\right)\ln(J - b') - \frac{a'}{J}\right] \tag{8.171}$$

where P_i is the initial particle pressure (when $J = 1$) of

$$P_i = \left(P_0 - a'\right)\frac{T}{T_0} + a' \tag{8.172}$$

This energy is equal to the energy per unit initial volume for isothermal compression or expansion of a van der Waals gas:

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\,dV = -\int_1^J \left(\left(P_i - a'\right)\left(\frac{1 - b'}{J - b'}\right) + \frac{a'}{J^2}\right) dJ \tag{8.173}$$

In `NairnMPM`, the cumulative work is tracked in the particle's plastic energy (which is $= PdV$ work and can tracked the same as for an ideal gas). The particle's strain energy tracks total internal energy in the gas per unit mass, which for a van der Waals gas is

$$U = C_v(T - T_0) - \frac{a'}{\rho_0 J} \tag{8.174}$$

In hyperelastic code, an incremental form is

$$dU = C_v dT + \frac{a'}{\rho_0 J^2} dJ \tag{8.175}$$

For a van der Waals gas, the heat capacity is same as for ideal gas, $C_v = (3/2)nR/(\rho_0 V_0)$ for monatomic (or $5/2$ for diatomic gas), but the n is found differently from reference conditions. It can be found as root to

$$\frac{ab}{V_0^2}n^3 - \frac{a}{V_0}n^2 - (P_0 b + RT_0)n + P_0 V_0 = 0 \tag{8.176}$$

This n is needed to find a', b' and C_v.

8.13 Tait Liquid

The Tait liquid uses the Tait equation for the pressure response and assumes the shear term follows Newtonian viscosity. The Tait equation for volume of a liquid at any temperature and pressure is:

$$V(P,T) = V(0,T)\left[1 - C\ln\left(1 + \frac{P}{B(T)}\right)\right] \tag{8.177}$$

where $C = 0.0894$ is the universal Tait constant. The volume is expressed in terms of the zero pressure volume, which can be fit (for a given liquid) to various equations. Two common approaches are

$$V(0,T) = A_0 + A_1 T + A_2 T^2 + \cdots \tag{8.178}$$

$$V(0,T) = V(0,T_0)e^{\beta(T - T_0)} \tag{8.179}$$

The first is simply a polynomial fit to volume data with fitting parameters A_i. The second assumes constant volumetric thermal expansion coefficient (β) around some reference temperature T_0. `NairnMPM`

uses the second fit where $V(0,T_0)$ is found from input density, T_0 is from stress free temperature, and $\beta = 3\alpha$.

A common fit for $B(T)$ is

$$B(T) = B_0 e^{-B_1 T} \tag{8.180}$$

Note that bulk modulus from the Tait equation is

$$\frac{1}{K(P,T)} = -\frac{1}{V}\left(\frac{dV}{dP}\right)_T = \frac{C}{P+B(T)}\frac{1}{\left[1-C\ln\left(1+\frac{P}{B(T)}\right)\right]} = \frac{C}{P+B(T)}\frac{V(P,T)}{V(0,T)} \tag{8.181}$$

which shows that $B(T)$ is proportional to the temperature dependence of the zero-pressure bulk modulus:

$$B(T) = CK(0,T) \tag{8.182}$$

`NairnMPM` currently assumes temperature independent bulk modulus or assumes $B_1 = 0$. The pressure dependence to the thermal expansion coefficient is

$$\beta(P,T) = \frac{1}{V}\left(\frac{dV}{dT}\right)_P = \beta(0,T) - \frac{PB_1}{K(P,T)} \tag{8.183}$$

When bulk modulus is independent of temperature ($B_1 = 0$), the thermal expansion coefficient is independent of pressure.

For implementation as a hyperelastic material, we define

$$J = \frac{V(P,T)}{V(0,T_0)} \qquad \text{and} \qquad J_{res} = \frac{V(0,T)}{V(0,T_0)} = e^{\beta_0(T-T_0)} \tag{8.184}$$

as relative volumes. In other words, J is set to one for initial particle volume at zero pressure and at the stress-free temperature and J_{res} is volume change under zero pressure between stress free temperature T_0 and current temperature T. The J_{dP} due to change in pressure at T is $J_{dP} = J/J_{res}$ (*i.e.*, total $J = J_{dP}J_{res}$ or product of J due to pressure and temperature changes. The constitutive law is rewritten as

$$\frac{J}{J_{res}} = 1 - C\ln\left(1+\frac{P}{CK_0}\right) \tag{8.185}$$

where K_0 is the zero-pressure bulk modulus. This equation can be solved for pressure:

$$P = CK_0\left[\exp\left(\frac{1-J^*}{C}\right)-1\right] \tag{8.186}$$

where $J^* = J/J_{res}$. The tracked Kirchoff stress normalized to initial density is

$$\boldsymbol{\tau}^{(s)} = -JC\frac{K_0}{\rho_0}\left[\exp\left(\frac{1-J^*}{C}\right)-1\right]\mathbf{I} \tag{8.187}$$

This material is equivalent to a hyperelastic material with volumetric strain energy function of

$$U(J^*) = CK_0\left[C\exp\left(\frac{1-J^*}{C}\right)+J^*\right] \tag{8.188}$$

This energy function equals the energy per unit initial volume for isothermal compression or expansion of a Tait liquid.

Imagine a simulation where particle starts at T_{init} and P_{init}. Ignoring residual stresses (they will appear dynamically in the simulation if $T_{init} \neq T_0$), the initial J_{dP}, which is equated to initial J, is

$$\frac{V(P_{init}, T_{init})}{V(0, T_{init})} = \frac{V_p}{V_0} = J_{init} = 1 - C \ln\left(1 + \frac{P_{init}}{CK_0}\right) \tag{8.189}$$

When the particle is created, its mass is set to $m_{p0} = \rho_0 V_p$ where V_p is now $V(P_{init}, T_{init})$. We need to correct this mass to be:

$$m_p = \rho V_p = \frac{\rho \rho_0 V_p}{\rho_0} = \frac{\rho_0 V_p V_0}{V_p} = \frac{m_{p0}}{J_{init}} \tag{8.190}$$

Note that particle temperatures are set to T_{init} but the previous temperature is set to T_0. The first time step will get $dT = T_{init} - T_0$ which will cause J_{res} and a change in stresses. If this temperature change is large, it could cause dynamic effects. It is better to start with $T_{init} = T_0$ and if needed, ramp temperatures slowly to a desired temperature causing residual stresses.

For shear stress calculations, this material is assumed to be a Newtonian fluid, which means that the shear stress is proportional to deviatoric, symmetrized velocity gradient:

$$\tau = \eta\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T - \frac{2}{3}\mathrm{Tr}(\nabla\mathbf{v})\mathbf{I}\right) = 2\eta\left(\frac{1}{2}(\nabla\mathbf{v} + \nabla\mathbf{v}^T) - \frac{1}{3}\mathrm{Tr}(\nabla\mathbf{v})\mathbf{I}\right) = 2\eta\,\mathrm{dev}(\mathsf{D}) \tag{8.191}$$

where $\nabla\mathbf{v}$ is the velocity gradient,η is the viscosity, and $\mathsf{D} = (1/2)(\nabla\mathbf{v} + \nabla\mathbf{v}^T)$ is the symmetic, rate of deformation tensor (and $\nabla\mathbf{v} = \nabla\mathbf{u}/\Delta t$ in code implementation). The total stress is given by $\sigma = -P\mathbf{I} + \tau$ and the tracked, normalized Kirchoff stress is:

$$\boldsymbol{\tau}^{(s)} = -JC\frac{K_0}{\rho_0}\left[\exp\left(\frac{1-J^*}{C}\right) - 1\right]\mathbf{I} + 2J\frac{\eta}{\rho_0}\mathrm{dev}(\mathsf{D}) \tag{8.192}$$

For viscosity to depend on shear rate, the effective shear rate is from $2|\mathrm{dev}(\mathsf{D})|$ where 2 converts to engineering shear strain rate.

When the low-pressure bulk modulus is independent of temperature, the pressure dependent bulk modulus is

$$K(P,T) = \frac{P + CK_0}{C}J^* = K_0 \exp\left(\frac{1-J^*}{C}\right)J^* \tag{8.193}$$

This result can be used to adjust time step as a function of current pressure.

An incremental pressure law can be derived from dP/dJ^* to get

$$dP = -K_0 \exp\left(\frac{1-J^*}{C}\right)dJ^* = -K(P,T)d\ln J^* = -K(P,T)\ln dJ^* \tag{8.194}$$

Another option might to find finite dP and expand in a series:

$$\Delta P = CK_0\left[\exp\left(\frac{1-dJ^*J^*}{C}\right) - \exp\left(\frac{1-J^*}{C}\right)\right] \tag{8.195}$$

where $dJ^* = dJ/dJ_{res}$ is change in volume and residual stress term. Expanding in a series (using Mathematica):

$$\Delta P = -K_0 \exp\left(\frac{1-J^*}{C}\right)\left(\Delta J^* - \frac{(\Delta J^*)^2}{2C} + \frac{(\Delta J^*)^3}{6C^2} - \frac{(\Delta J^*)^4}{24C^3} + \cdots\right) \tag{8.196}$$

$$= -K_0 \exp\left(\frac{1-J^*}{C}\right)\left(\Delta J^* - \frac{\Delta J^*}{2C}\left(\Delta J^* - \frac{\Delta J^*}{3C}\left(\Delta J^* - \frac{(\Delta J^*)^2}{4C} + \cdots\right)\right)\right) \tag{8.197}$$

where

$$\Delta J^* = \left(\frac{dJ}{dJ_{res}} - 1\right)J^* \tag{8.198}$$

is the increment in J^* in the time step.

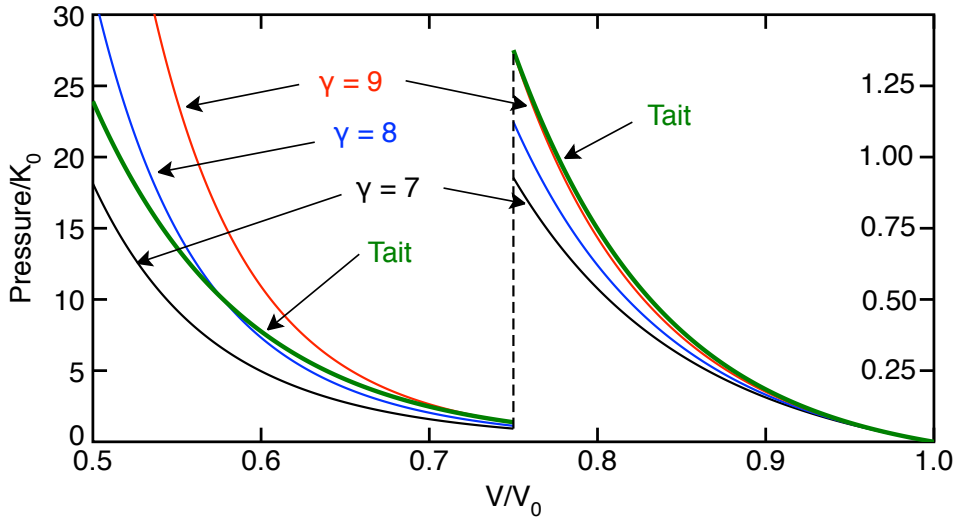

Figure 8.3: Liquid pressure calculated using the Tait equation or an empirical model from the SPH literature for three different values of its parameter γ. Note that pressures for $V/V_0 = 0.75$ are multiplied by 20 for clarity (see scale on the right).

8.13.1 SPH Liquid Model

A popular model used in many SPH codes has a different pressure law. Compared to Tait pressure, the two laws are:

$$\frac{P}{K_0} = \begin{cases} C\left[\exp\left(\frac{1-J^*}{C}\right)-1\right] & \text{Tait Equation} \\ \frac{1}{\gamma}\left[\left(\frac{1}{J^*}\right)^{\gamma}-1\right] & \text{SPH Modeling} \end{cases} \tag{8.199}$$

Figure 8.3 compares Tait equation to SPH modeling for three different values of γ. For $J^* > 0.7$, an SPH model with $\gamma = 9$ is close to Tait equation, but they different significantly for $J < 0.7$.

Chapter 9

Viscoelastic Materials

9.1 Introduction

The stress-strain relation for an isotropic viscoelastic material in which bulk modulus is independent of time, but shear modulus depends on time and the analysis is 3D (or plane strain by setting $\varepsilon_{zz} = 0$ and ignoring τ_{xz} and τ_{yz} or axisymmetric by ignoring τ_{xz} and τ_{yz}) can be written as

$$P = -K(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} - 3\varepsilon^{(res)}) \tag{9.1}$$

$$s_{ij} = \int_0^t 2G(t-\tau)\frac{de_{ij}}{d\tau}d\tau \tag{9.2}$$

where P is pressure, $s_{ij} = \sigma_{ij} + \delta_{ij}P$ and $e_{ij} = \varepsilon_{ij} - (\delta_{ij}/3)\mathrm{Tr}(\boldsymbol{\varepsilon})$ are elements of the deviatoric stress and strain tensors, and $\varepsilon^{(res)} = \alpha\Delta T + \beta\Delta c$. The pressure is straightforward, but the deviatoric stress terms require more work. The only form of $G(t)$ the permits efficient evaluation of all strain history effects is when it is a sum of exponentials or

$$G(t) = G_0 + \sum_{k=1}^{n} G_k e^{-t/\tau_k} \tag{9.3}$$

Each element of deviatoric stress (with $e(0) = 0$) becomes:

$$s = 2G_0 e(t) + \sum_{k=1}^{n} 2G_k \int_0^t e^{-(t-\tau)/\tau_k}\frac{de(\tau)}{d\tau}d\tau \tag{9.4}$$

where subscripts ij on s and e have been dropped for simplicity,

9.2 Small Strain, Internal Variables Analysis

Following Simo and Hughes, we introduce the internal variables, α_k (with implied subscript ij for each component of deviatoric stress), that satisfy

$$\frac{d\alpha_k}{dt} + \frac{\alpha_k}{\tau_k} = \frac{e(t)}{\tau_k} \tag{9.5}$$

This first order differential equations (with $\alpha_k(0) = 0$) can be solved and integrated by parts to get

$$\alpha_k = \int_0^t e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau = e(t) - \int_0^t e^{-(t-\tau)/\tau_k} \frac{de(\tau)}{d\tau} d\tau \tag{9.6}$$

$$= \int_0^t \left(1 - e^{-(t-\tau)/\tau_k}\right) \frac{de(\tau)}{d\tau} d\tau \tag{9.7}$$

Substitution into stress give

$$\frac{s(t)}{2} = G_0 e(t) + \sum_{k=1}^{n} G_k (e(t) - \alpha_k) = G_e e(t) - \sum_{k=1}^{n} G_k \alpha_k \tag{9.8}$$

where

$$G_e = \sum_{k=0}^{n} G_k \tag{9.9}$$

is the modulus at $t = 0$. In numerical implementation, the internal variable increment, $d\alpha_k = \alpha_k(t + \Delta t) - \alpha_k(t)$, can be found from

$$d\alpha_k = e^{-\Delta t/\tau_k} \int_0^{t+\Delta t} e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau - \int_0^t e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau \tag{9.10}$$

$$= \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + e^{-\Delta t/\tau_k} \int_t^{t+\Delta t} e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau \tag{9.11}$$

Evaluating the second term by midpoint rule gives

$$d\alpha_k = \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + \frac{\Delta t}{2\tau_k} \left(e(t + \Delta t) + e^{-\Delta t/\tau_k} e(t)\right) \tag{9.12}$$

$$= \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + \frac{\Delta t}{2\tau_k} \left(\left(e^{-\Delta t/\tau_k} + 1\right) e(t) + de\right) \tag{9.13}$$

where de is the increment in deviatoric strain in the time step. Note that α_k can be updated on each time step without needing a sum of strain history, thereby avoiding the need to store strain history. This ability to track strain history without storing strain history is only possible because of properties of exponentials used in $G(t)$. In the limit of small step size, this increment reduces to:

$$\alpha_k \approx \frac{\Delta t}{\tau_k} \left(\frac{1}{2} de + e(t) - \alpha_k\right) \tag{9.14}$$

An different form found in Abaqus theory manual writes

$$\alpha_k = \int_0^t \left(1 - e^{-(t-\tau)/\tau_k}\right) \frac{de(\tau)}{d\tau} d\tau \tag{9.15}$$

leading to

$$d\alpha_k = \int_0^{t+\Delta t} \left(1-e^{-(t+\Delta t-\tau)/\tau_k}\right)\frac{de(\tau)}{d\tau}d\tau - \int_0^{t} \left(1-e^{-(t-\tau)/\tau_k}\right)\frac{de(\tau)}{d\tau}d\tau \tag{9.16}$$

$$= \int_0^{t+\Delta t} \left(1-e^{-\Delta t/\tau_k}+e^{-\Delta t/\tau_k}\left(1-e^{-(t-\tau)/\tau_k}\right)\right)\frac{de(\tau)}{d\tau}d\tau - \int_0^{t} e^{-\Delta t/\tau_k}\left(1-e^{-(t-\tau)/\tau_k}\right)\frac{de(\tau)}{d\tau}d\tau - \left(1-e^{-\Delta t/\tau_k}\right)\alpha_k \tag{9.17}$$

$$= e^{-\Delta t/\tau_k}\int_t^{t+\Delta t} \left(1-e^{-(t-\tau)/\tau_k}\right)\frac{de(\tau)}{d\tau}d\tau + \left(1-e^{-\Delta t/\tau_k}\right)[e(t)+de-\alpha_k] \tag{9.18}$$

Now we set $de(\tau)/d\tau = de/\Delta t$ (linear variation) in the integral from t to $t+\Delta t$:

$$d\alpha_k = e^{-\Delta t/\tau_k}\frac{de}{\Delta t}\left[\Delta t+\tau_k\left(1-e^{\Delta t/\tau_k}\right)\right] + \left(1-e^{-\Delta t/\tau_k}\right)[e(t)+de-\alpha_k] \tag{9.19}$$

$$= \left[e^{-\Delta t/\tau_k}+\frac{\tau_k}{\Delta t}\left(e^{-\Delta t/\tau_k}-1\right)\right]de + \left(1-e^{-\Delta t/\tau_k}\right)[e(t)+de-\alpha_k] \tag{9.20}$$

$$= \left[1+\frac{\tau_k}{\Delta t}\left(e^{-\Delta t/\tau_k}-1\right)\right]de + \left(1-e^{-\Delta t/\tau_k}\right)[e(t)-\alpha_k] \tag{9.21}$$

This result agrees with Abaqus manual. Note that in limit of small Δt, this result is identical to one derived above using midpoint rule. Furthermore, the difference is

$$d\alpha_k(\text{difference}) = \frac{(\Delta \text{t})^2 \text{de}}{6\tau_{\text{k}}^2} + \text{O}[(\Delta \text{t})^3] \tag{9.22}$$

which is third order in differential terms.

9.3 Final, Small Strain, Incremental Results

The pressure change is

$$dP = -K(d\varepsilon_{xx}+d\varepsilon_{yy}+d\varepsilon_{zz}-3d\varepsilon^{(res)}) \tag{9.23}$$

The deviatoric stress updates using

$$ds_{ij} = 2\left(G_e de_{ij} - \sum_{k=1}^{n} G_k d\alpha_{ij,k}\right) \tag{9.24}$$

where $d\alpha_{ij,k}$ is the ij^{th} element of $d\alpha_k$ found using Eq. (9.13) or (9.21). The dissipated energy is

$$\Phi = \sum_{ij}\sum_{k=1}^{n} 2G_k(e_{ij}(t+\Delta t)-\alpha_{ij,k})d\alpha_{ij,k} \tag{9.25}$$

where $\alpha_{ij,k}$ is $\alpha_k(t+\Delta t)$ for the ij^{th} element of deviatoric strain at the end of the time step.

9.4 Axisymmetric, Plane Strain, and Plane Stress

Axisymmetric and plane strain analysis can use the above 3D analysis without any modifications. The special case of axisymmetric will have $d\varepsilon_{xz} = d\varepsilon_{yz} = 0$ and $d\varepsilon_{zz}$ for the hoop strain. The special case of plane strain will have $d\varepsilon_{zz} = d\varepsilon_{xz} = d\varepsilon_{yz} = 0$.

In plane stress, however, the final $d\sigma_{zz} = ds_{zz} - dP = 0$, which is achieved by solving for $d\varepsilon_{zz} \neq 0$ to satisfy plane stress conditions. But on input to the constitutive law, $d\varepsilon_{zz}$ is not known. The calculations will need to find it as part of the calculations. This section looks at plane stress analysis and how it needs to modify the standard coding for 3D analysis. The inputs to constitutive law calculations are displacement gradient, $\nabla \boldsymbol{u}^0$, and residual strain terms (*e.g.*, dT and dc). Here superscript 0 means the displacement gradient as input for 2D plane stress or plane strain and that input always has $\nabla u^0_{zz} = 0$. The following steps look at how that input affects each step and the constitutive law calculations.

1. Get previous particle deformation gradient $\mathsf{F}^{(n-1)}$. In plane stress, $F^{(n-1)}_{zz}$ will be tracked zz deformation (and approximately equal to $(1+\varepsilon_{zz})$in small-strain analysis).

2. Get incremental deformation from input displacement gradient using $d\mathsf{F}^0 = \exp(\nabla \boldsymbol{u}^0)$. In this calculation, $d\mathsf{F}^0_{zz} = 1$, but in plane stress, it needs to be

$$dF_{zz} = \exp(d\varepsilon_{zz}) = dF^0_{zz} + d\varepsilon_{zz} + \frac{d\varepsilon^2_{zz}}{2} + \cdots$$

   where the expansion depends on number of deformation gradient terms in the simulation.

3. Update the particle deformation gradient. Using input terms, $\mathsf{F}^{(n0)} = d\mathsf{F}^0\mathsf{F}^{(n-1)}$. This updated deformation gradient will not change F_{zz}. Once $d\varepsilon_{zz}$ and final dF_{zz} are found, the plane stress update should include

$$F^{(n)}_{zz} = dF_{zz}F^{(n-1)}_{zz} = dF_{zz}F^{(n0)}_{zz} \approx (1+d\varepsilon_{zz})F^{(n0)}_{zz}$$

4. Use standard methods to find current strain and strain increment in current configuration. From input values, $\boldsymbol{\varepsilon}^{(n0)} = \mathsf{V}_0 - \mathsf{I}$ (where V_0 is left stretch tensor decomposed from F^0) and $d\boldsymbol{\varepsilon}^0$ is found from $d\mathsf{F}^0 - d\mathsf{R}$ (which has zz component zero because $d\mathsf{F}^0_{zz} = dR_{zz} = 1$). In plane stress, the zz compnents change to $\varepsilon_{zz} = \varepsilon^{(n0)}_{zz} + d\varepsilon_{zz}$ and $d\varepsilon_{zz} = d\varepsilon^0_{zz} + d\varepsilon_{zz} = d\varepsilon_{zz}$. Note that $\varepsilon^{(n0)}_{zz}$ is form prior particle deformation and will not be zero in plane stress, but $d\varepsilon^0_{zz}$ found from input displacement gradient will be zero.

5. For residual stresses, find linear $d\varepsilon_{res}$, which is same in plane stress and plane strain and in all normal directions (due to isotropy).

6. The incremental volume change accounting for residual strains is $dV = \mathrm{Tr}(d\boldsymbol{\varepsilon}) - 3d\varepsilon_{res}$. From input values, $dV^0 = d\varepsilon_{xx} + d\varepsilon_{yy} - 3d\varepsilon_{res}$. For plane stress $dV = dV^0 + d\varepsilon_{zz}$.

7. Let $\boldsymbol{e}$ and $d\boldsymbol{e}$ be current deviatoric strain and deviatoric strain increment. The deviatoric strain is $\boldsymbol{e} = \boldsymbol{\varepsilon} - \frac{1}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})$. After finding $\boldsymbol{e}$ using $\boldsymbol{\varepsilon}^{(n0)}$, the plane stress, deviatoric strain is:

$$e_{xx} = e^0_{xx} - \frac{d\varepsilon_{zz}}{3}, \quad e_{yy} = e^0_{yy} - \frac{d\varepsilon_{zz}}{3}, \quad e_{zz} = e^0_{zz} + \frac{2d\varepsilon_{zz}}{3}, \quad e_{xy} = e^0_{xy}$$

   Note that this adjusted the "input" result only by the increment because when running in plane stress, $\boldsymbol{e}_0$ will include non-zero $e^{(n0)}_{zz}$ from tracked particle deformation. The deviatoric strain increment in plane stress also add the zz component:

$$de_{xx} = de^0_{xx} - \frac{d\varepsilon_{zz}}{3}, \quad de_{yy} = de^0_{yy} - \frac{d\varepsilon_{zz}}{3}, \quad de_{zz} = de^0_{zz} + \frac{2d\varepsilon_{zz}}{3}, \quad de_{xy} = de^0_{xy}$$

8. The next task is to update the internal variables

$$\begin{aligned}
d\boldsymbol{\alpha}_k &= \left(e^{-\Delta t/\tau_k}-1\right)\boldsymbol{\alpha}_k^{(n-1)} + \frac{\Delta t}{2\tau_k}\left(\left(e^{-\Delta t/\tau_k}+1\right)\boldsymbol{e}+d\boldsymbol{e}\right)\\
d\alpha_{xx,k} &= \left(e^{-\Delta t/\tau_k}-1\right)\alpha_{k,xx}^{(n-1)} + \frac{\Delta t}{2\tau_k}\left(\left(e^{-\Delta t/\tau_k}+1\right)\left(e_{xx}^0-\frac{d\varepsilon_{zz}}{3}\right)+de_{xx}^0-\frac{d\varepsilon_{zz}}{3}\right)\\
&= d\alpha_{xx,k}^0 - \frac{\Delta t}{2\tau_k}\left(e^{-\Delta t/\tau_k}+2\right)\frac{d\varepsilon_{zz}}{3} = d\alpha_{xx,k}^0 - \phi_k\frac{d\varepsilon_{zz}}{3}\\
d\alpha_{yy,k} &= d\alpha_{yy,k}^0 - \phi_k\frac{d\varepsilon_{zz}}{3} \qquad d\alpha_{zz,k} = d\alpha_{zz,k}^0 + 2\phi_k\frac{d\varepsilon_{zz}}{3} \qquad d\alpha_{xy,k} = d\alpha_{xy,k}^0
\end{aligned}$$

where

$$\phi_k = \frac{\Delta t}{2\tau_k}\left(e^{-\Delta t/\tau_k}+2\right)$$

9. The deviatoric stress update in plane stress is:

$$\begin{aligned}
ds_{xx} &= 2\left(G_e\left(de_{xx}^0-\frac{d\varepsilon_{zz}}{3}\right)-\sum_{k=1}^{n}G_k\left(d\alpha_{xx,k}^0-\phi_k\frac{d\varepsilon_{zz}}{3}\right)\right)\\
&= ds_{xx}^0 - \frac{2d\varepsilon_{zz}}{3}\left(G_e-\sum_{k=1}^{n}G_k\phi_k\right) = ds_{xx}^0 - \frac{2\phi\, d\varepsilon_{zz}}{3}\\
ds_{yy} &= ds_{yy}^0 - \frac{2\phi\, d\varepsilon_{zz}}{3} \qquad ds_{zz} = ds_{zz}^0 + \frac{4\phi\, d\varepsilon_{zz}}{3} \qquad ds_{xy} = ds_{xy}^0
\end{aligned}$$

where

$$\phi = G_e - \sum_{k=1}^{n}G_k\phi_k$$

The pressure update for small-strain linear elasticity is:

$$dP = -KdV = -K(dV^0 + d\varepsilon_{zz})$$

10. To keep $\sigma_{zz}=0$, we need $d\sigma_{zz} = ds_{zz} - dP = 0$ or

$$d\varepsilon_{zz} = -\frac{KdV^0 + ds_{zz}^0}{K+\frac{4\phi}{3}}$$

If elastic ($G_0 = G$ and $G_{k>0} = 0$), then $ds_{zz}^0 = -2G(d\varepsilon_{xx}+d\varepsilon_{yy})/3$, $dV^0 = d\varepsilon_{xx}+d\varepsilon_{yy}$, and $\phi = G$ leading to

$$d\varepsilon_{zz} = -\frac{K-\frac{2G}{3}}{K+\frac{4G}{3}}(d\varepsilon_{xx}+d\varepsilon_{yy}) = -\frac{\lambda}{\lambda+2G}(d\varepsilon_{xx}+d\varepsilon_{yy})$$

This result matches the linear elastic result.

11. Once $d\varepsilon_{zz}$ is found, the remaining plane stress tasks are:

- Find $d\boldsymbol{s}$ using $d\varepsilon_{zz}$ for stress update.
- Find $\boldsymbol{e}$ and $d\boldsymbol{e}$ using $d\varepsilon_{zz}$ for history update and dissipated energy calculations.
- Find $dV = dV^0 + d\varepsilon_{zz}$ and for particle pressure update

- Set $d\varepsilon_{zz}$ in tensor to calculated $d\varepsilon_{zz}$ for use in elastic energy calculations.
- Set $F_{zz}^{(n)} = (1 + d\varepsilon_{zz})F_{zz}^{(n0)}$ and store new deformation gradient on the particle.
- Update history variables and add dissipation energy.

The above method requires small-strain viscoelasticity and no artificial viscosity. Using a non-linear pressure law or artificial viscosity would likely require numerical solutions for $d\varepsilon_{zz}$, although some nonlinear laws might have analytical solutions.

9.5 Nonlinear Pressure Law

A pseudo large-deformation model might implement non-linear, elastic law for pressure but return small-strain theory for deviatoric stresses. When this is down, this material tracks Kirchoff stress instead of generic small strain stress (where Kirchoff and Cauchy stress are the same). The only difference in code are:

1. The material point tracks J and J_{res}. These are updated with $J^{(n)} = |d\mathsf{F}|J^{(n-1)}$ and $J_{res}^{(n)} = e^{3d\varepsilon_{res}}J_{res}^{(n-1)}$ and used to update the particle Kirchoff pressure. That pressure will be function of $J^{(n)}$ and $J_{res}^{(n)}$.

2. After finding small-strain deviatoric stress increment, convert to Kirchoff deviatoric stress increment using
$$\boldsymbol{s}^{(n)} = |d\mathsf{F}|\boldsymbol{s}^{(n-1)} + J^{(n)}d\boldsymbol{s}$$

3. For plane stress modeling, the section above can be revised to final equation to solve for $d\varepsilon_{zz}$ of
$$\frac{P\left((1 + d\varepsilon_{zz})|d\mathsf{F}^0|J^{(n-1)}, e^{3d\varepsilon_{res}}J_{res}^{(n-1)}\right)}{(1 + d\varepsilon_{zz})|d\mathsf{F}^0|J^{(n-1)}} - \frac{P\left(J^{(n-1)}, J_{res}^{(n-1)}\right)}{J^{(n-1)}} = ds_{zz}^0 + \frac{4\phi d\varepsilon_{zz}}{3}$$
where P is tracked Kirchoff pressure. In other words, the Cauchy pressure increment is equated to the small strain deviatoric stress increment to find $d\varepsilon_{zz}$. To be general, write Cauchy pressure as $P(J^*)$ where $J^* = J/J_{res}$ and use Taylor expansion to write
$$P\left(\frac{(1 + d\varepsilon_{zz})|d\mathsf{F}^0|}{e^{3d\varepsilon_{res}}}J^{*(n-1)}\right) = P\left(J^{*(n-1)}\right) + \left(\frac{(1 + d\varepsilon_{zz})|d\mathsf{F}^0|}{e^{3d\varepsilon_{res}}} - 1\right)J^{*(n-1)}\frac{dP}{dJ^*}$$
We can equate to deviatoric stress increment and solve for $d\varepsilon_{zz}$ to get
$$d\varepsilon_{zz} = -\frac{K(J^{*(n-1)})\left(\frac{|d\mathsf{F}^0|}{e^{3d\varepsilon_{res}}} - 1\right) + ds_{zz}^0}{K(J^{*(n-1)})\frac{|d\mathsf{F}^0|}{e^{3d\varepsilon_{res}}} + \frac{4\phi}{3}}$$
where $K(J^{*(n-1)}) = -J^{*(n-1)}(dP/dJ^*)$ is the tangent bulk modulus evaluated at $J^{*(n-1)}$ or the beginning of the time step. This reduces to small strain result in small strain. For any pressure law, the implemention only needs to find the tangent bulk modulus.

9.6 Alternate Internal Variables and Hyperelastic Methods

Physically, the sum of exponential relaxation elements corresponds to a collection of Maxwell elements (springs with stiffness $2G_k$ and dashpot with viscosity $\eta_k = 2\tau_k G_k$ in series) in parallel. The G_0 term corresponds to a single elastic element (spring with stiffness $2G_0$). An alternate set of internal variables is to track an internal force in each Maxwell element, q_k (with implied subscript ij for each component of deviatoric stress), defined such that total deviatoric stress is:

$$s(t) = 2G_e e(t) - \sum_{k=1}^{n} q_k = \frac{dW_S(t)}{de} - \sum_{k=1}^{n} q_k \tag{9.26}$$

where W_s is initial (time zero or elastic) shear energy density and this form is intended to extend to nonlinear materials such as hyperelastic materials. For a small-strain material elastic material, $W_s = G_e||e||^2$. Simo asserts large deformation is done by using shear energy for a hyperelastic material instead. This deviatoric stress is initial (time zero) elastic result minus sum of internal forces. Comparing to Eq. (9.8), the q_k stress variables are related to α_k (as strain variables) by:

$$q_k = 2G_k\alpha_k = 2\gamma_k G_e \alpha_k \tag{9.27}$$

where $\gamma_k = G_k/G_e$ is a normalized stiffness term. This approach is described first by Simo (1987) and in book by Simo and Hughes (1998).

The evolution equation for internal variables become:

$$\frac{dq_k}{dt} + \frac{q_k}{\tau_k} = \frac{2G_k}{\tau_k} e(t) = \frac{\gamma_k}{\tau_k} 2G_e e(t) = \frac{\gamma_k}{\tau_k}\frac{dW_S(t)}{de} \tag{9.28}$$

This first order differential equations (with $q_k(0) = 0$) can be solved and integrated by parts to get

$$q_k = \frac{\gamma_k}{\tau_k}\int_0^t e^{-(t-\tau)/\tau_k}\frac{dW_S}{de}d\tau \tag{9.29}$$

$$= \gamma_k \frac{dW_S(t)}{de} - \gamma_k \int_0^t e^{-(t-\tau)/\tau_k}\frac{d}{d\tau}\left(\frac{dW_S}{de}\right)d\tau \tag{9.30}$$

Substituting into Eq. (9.26) gives for n elements

$$s(t) = \left(1 - \sum_{k=1}^{n}\gamma_k\right)\frac{dW_S(t)}{de} + \sum_{k=1}^{n}\gamma_k \int_0^t e^{-(t-\tau)/\tau_k}\frac{d}{d\tau}\left(\frac{dW_S}{de}\right)d\tau \tag{9.31}$$

Using:

$$1 = \gamma_0 + \sum_{k=1}^{n}\gamma_k \qquad \text{and} \qquad \frac{dW_S(t)}{de} = \int_0^t \frac{d}{d\tau}\left(\frac{dW_S}{de}\right)d\tau \tag{9.32}$$

the deviatoric stress simplifies to:

$$s(t) = \int_0^t \left(\gamma_0 + \sum_{k=1}^{n}\gamma_k e^{-(t-\tau)/\tau_k}\right)\frac{d}{d\tau}\left(\frac{dW_S}{de}\right)d\tau \tag{9.33}$$

$$= \int_0^t g(t-\tau)\frac{d}{d\tau}\left(\frac{dW_S}{de}\right)d\tau \tag{9.34}$$

where the normalized relaxation function is

$$g(t) = \gamma_0 + \sum_{k=1}^{n}\gamma_k e^{-t/\tau_k} \tag{9.35}$$

9.6.1 Implementation

We define:

$$\boldsymbol{s}_n^0 = \frac{dW_S(t_n)}{de} \tag{9.36}$$

$$\boldsymbol{h}_n^k = \int_0^t e^{-(t-\tau)/\tau_k} \frac{d\boldsymbol{s}^0}{d\tau} d\tau \tag{9.37}$$

The deviatoric stress update become:

$$s(t_{n+1}) = \gamma_0 \boldsymbol{s}_{n+1}^0 + \sum_{k=1}^{n} \gamma_k \boldsymbol{h}_{n+1}^{(k)} \tag{9.38}$$

where $\boldsymbol{s}_{n+1}^0$ is updated initial time shear stress (may need to track it or recalculate each time from initial deformation gradient), and updated $\boldsymbol{h}_n^k$ is found using methods from above:

$$h_{n+1}^{(k)} = e^{-\Delta t/\tau_k} h_n^{(k)} + \int_{t_n}^{t_{n+1}} e^{-(t_{n+1}-\tau)/\tau_k} \frac{d\boldsymbol{s}^0}{d\tau} d\tau \tag{9.39}$$

$$= e^{-\Delta t/\tau_k} h_n^{(k)} + e^{-\Delta t/(2\tau_k)} \left(\boldsymbol{s}_{n+1}^0 - \boldsymbol{s}_n^0\right) \tag{9.40}$$

The midpoint rule here multiplied integrand at the midpoint by $\Delta t/2$ rather than adding the two endpoints. The results differ, but are essentially the same for small Δt.

9.7 Alternate Internal Stresses

Yet another approach (based on Zerelli and Armstrong and the one used in Unintah MPM code) is to use stresses in each maxwell element (and s_0 in the spring element):

$$s(t) = s_0 + \sum_{k=1}^{n} s_k \tag{9.41}$$

Comparing to Eq. (9.8), the s_k stress variables are equivalent to α_k (as strain variables) and they are related by:

$$s_0 = 2G_0 e(t), \qquad s_k = 2G_k(e(t) - \alpha_k), \qquad \text{and} \qquad \alpha_k = e(t) - \frac{s_k}{2G_k} \tag{9.42}$$

The evolution equation for Maxwell stresses is the standard differential equation for a single Maxwell element:

$$\frac{1}{2G_k}\frac{ds_k}{dt} + \frac{s_k}{\eta_k} = \frac{de(t)}{dt} \tag{9.43}$$

Substitution of α_k correctly reduces to the evolution equations for α_k variables. The resulting stress update is

$$ds = 2G_0 de(t) + \sum_{k=1}^{n} ds_k \tag{9.44}$$

Using $ds_k = 2G_k de(t) - s_k/\tau_k$, this result reduces to

$$ds = 2G_e de(t) - \sum_{k=1}^{n} \frac{s_k}{\tau_k} \tag{9.45}$$

Replacing α_k in the energy dissipation equation leads to

$$\Phi = \sum_{k=1}^{n} 2G_k(e(t) - \alpha_k)d\alpha_k = \sum_{k=1}^{n} s_k d\alpha_k = \sum_{k=1}^{n} \frac{s_k^2}{2G_k\tau_k} \tag{9.46}$$

Chapter 10

Manufactured Solutions

10.1 Introduction

Brannon (and several coworkers) have proposed manufactured solutions as a method to validate material modeling. In brief, a deformation gradient is imposed on a material and substituted into constitutive law and equilibrium equations. The exact stresses in the material are determined along with boundary conditions and body forces required to create the solution. This chapter has some particular manufactured solutions used in testing `NairnMPM` and easily adapted to testing new material models.

10.2 Constrained Uniaxial Tension

If an object is deformed on one direction at a constant rate while being constrained to no motion in the other two directions, the deformation gradient will be

$$\mathbf{F} = \begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} J & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{where} \qquad \dot{\varepsilon} = \frac{\Lambda - 1}{t_f} \tag{10.1}$$

is axial strain rate. Here Λ is the final extension, which is reached at time $t = t_f$. Because F is independent of position, the stress in the object will be independent of position and determined by the material model being used. The left Cauchy tensor is

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} (1+\dot{\varepsilon}t)^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} J^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.2}$$

and the relative volume change is

$$J = |\mathbf{F}| = 1 + \dot{\varepsilon}t \tag{10.3}$$

To test residual stress (here only thermal), we can also apply linear expansion using $\lambda_{res} = 1 + \dot{\varepsilon}_{res} t = e^{\alpha \Delta T}$, which corresponds to a temperature change ramp of

$$\Delta T = \frac{1}{\alpha} \ln(1 + \dot{\varepsilon}_{res} t) \quad \text{where} \quad \dot{\varepsilon}_{res} = \frac{\Lambda_{res} - 1}{t_f} \tag{10.4}$$

is linear thermal strain rate with Λ_{res} as final thermal elongation at time $t = t_f$.

The large deformation mapping (axial only) and its inverse are

$$\chi(X,t) = x = X + v(X)t = X(1+\dot{\varepsilon}t) \quad \text{and} \quad \chi^{-1}(x,t) = X = \frac{x}{1+\dot{\varepsilon}t} \tag{10.5}$$

The x-components of material and spatial descriptions of velocity are

$$V(X,t) = \frac{d\chi(X,t)}{dt} = \dot{\varepsilon}X \qquad \text{and} \qquad v(x,t) = V(\chi^{-1}(x,t),t) = \frac{\dot{\varepsilon}x}{1+\dot{\varepsilon}t} \tag{10.6}$$

The material velocity is constant on each particle (as specified by X) and the later would be velocities on the nodes during deformation). The material acceleration comes from

$$A(X,t) = \frac{dV(X,t)}{dt} = \frac{d^2\chi(X,t)}{dt^2} = 0 \tag{10.7}$$

To get this same result from spatial velocity requires the material derivative

$$\frac{Dv(x,t)}{Dt} = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} + \frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} = 0 \tag{10.8}$$

The material velocity gradient is

$$\dot{\mathsf{F}} = \frac{dV(X,t)}{dX} \qquad \text{giving} \qquad \dot{F}_{11} = \dot{\varepsilon} \tag{10.9}$$

The spatial velocity gradient comes from

$$\nabla \boldsymbol{v} = \frac{d\mathbf{F}}{dt}\mathbf{F}^{-1} = \begin{pmatrix} \dot{\varepsilon} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{1+\dot{\varepsilon}t} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{giving} \quad l_{11} = \frac{\dot{\varepsilon}}{1+\dot{\varepsilon}t} \tag{10.10}$$

Note that in MPM, the velocity on the grid is extrapolated to the particles using gradients from the mesh, which should result in giving the spatial gradient on the particles. If this gradient is $\boldsymbol{\ell}$, then the incremental particle deformation gradient should be $d\mathsf{F} = \exp(\boldsymbol{\ell}\Delta t) \approx \mathsf{F}(t+\Delta t)\mathsf{F}^{-1}(t)$ (see section 8.2). In this example:

$$\mathsf{F}(t+\Delta t)\mathsf{F}^{-1}(t) = \frac{1+\dot{\varepsilon}(t+\Delta t)}{1+\dot{\varepsilon}t} = 1 + \frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t} \tag{10.11}$$

$$\exp\left(\frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t}\right) \approx 1 + \frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t} \tag{10.12}$$

which is correct for small Δt, but also easily expanded to more terms.

10.2.1 Material Models

Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F}) - 3\big)\mathbf{I} + G(\mathbf{F} + \mathbf{F}^T - 2\mathbf{I}) \tag{10.13}$$

where $\lambda = \nu E/((1+\nu)(1-2\nu))$ is the Lamé constant for the material. For constrained uniaxial tension, the stress is

$$\sigma_{ij} = (\lambda + 2G\delta_{i1})\dot{\varepsilon}t\,\delta_{ij} \tag{10.14}$$

although this stress is based on initial area and not the Cauchy stress. This solution can be imposed by applying traction or velocity boundary conditions. On the $\pm x$ surfaces, the traction condition should be:

$$T_x = \pm(\lambda + 2G)\dot{\varepsilon}t \tag{10.15}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda\dot{\varepsilon}t \qquad \text{or} \qquad v_y = v_z = 0 \tag{10.16}$$

Neo-Hookean, Mooney-Rivlin Material

For a neo-Hookean version of a Mooney-Rivlin material (with $G_2 = 0$) with default pressure term the stress are:

$$\sigma_{xx} = \frac{K}{2}\left(\frac{\lambda}{J_{res}} - \frac{J_{res}}{\lambda}\right) + \frac{2G_1 J_{res}}{3\lambda^{2/3}}\left(\lambda - \frac{1}{\lambda}\right) \quad \sigma_{yy} = \frac{K}{2}\left(\frac{\lambda}{J_{res}} - \frac{J_{res}}{\lambda}\right) - \frac{G_1 J_{res}}{3\lambda^{2/3}}\left(\lambda - \frac{1}{\lambda}\right)$$

This solution can be imposed by applying traction and/or velocity boundary conditions. On the $\pm x$ surface, the traction condition should be $T_x = \pm\sigma_{xx}$. On the $\pm y$ and $\pm z$ surfaces, the conditions should be $T_y = \pm\sigma_{yy}$ and $T_z = \pm\sigma_{yy}$.

Neo-Hookean Material

For an alternate neo-Hookean material using stress above with default pressure term (`UJOption=0`), the constrained tension stress are

$$\sigma_{xx} = GJ_{res}^{2/3}\left(\frac{\lambda_1}{J_{res}^{1/3}} - \frac{J_{res}^{1/3}}{\lambda_1}\right) + \frac{\lambda}{2}\left(\frac{\lambda_1}{J_{res}} - \frac{J_{res}}{\lambda_1}\right) \quad \sigma_{yy} = \frac{GJ_{res}^{1/3}(1 - J_{res}^{2/3})}{\lambda_1} + \frac{\lambda}{2}\left(\frac{\lambda_1}{J_{res}} - \frac{J_{res}}{\lambda_1}\right)$$

where $\lambda_1 = 1 + \dot{\varepsilon}t$ and $J_{res}^{1/3} = 1 + \dot{\varepsilon}_{res}t$. Without residual expansion ($\dot{\varepsilon}_{res} = 0$), the stresses become:

$$\sigma_{xx} = \frac{\lambda + 2G}{2}\left(\lambda_1 - \frac{1}{\lambda_1}\right) = \frac{\lambda + 2G}{2(1 + \dot{\varepsilon}t)}(2 + \dot{\varepsilon}t)\,\dot{\varepsilon}t \tag{10.17}$$

$$\sigma_{zz} = \sigma_{yy} = \frac{\lambda}{2}\left(\lambda_1 - \frac{1}{\lambda_1}\right) = \frac{\lambda}{2(1 + \dot{\varepsilon}t)}(2 + \dot{\varepsilon}t)\,\dot{\varepsilon}t \tag{10.18}$$

This solution can be imposed by applying traction and/or velocity boundary conditions. On the $\pm x$ surface, the traction condition should be $T_x = \pm\sigma_{xx}$. On the $\pm y$ and $\pm z$ surfaces, the conditions should be $T_y = \pm\sigma_{yy}$ and $T_z = \pm\sigma_{yy}$.

Clamped Neohookean

For the neo-Hookean material in the elastic part of the Disney snow model (a modified, co-rotated neo-Hookean material), The stresses from above are:

$$\sigma_{xx} = \frac{\lambda(J_p) + 2G(J_p)}{J_{res}^{1/3}}(\dot{\varepsilon}t - \dot{\varepsilon}_{res}t) \qquad \sigma_{yy} = \sigma_{zz} = \frac{\lambda(J_p)}{J_{res}^{1/3}}(\dot{\varepsilon}t - \dot{\varepsilon}_{res}t)$$

10.3 Linear Shear

If an object is sheared on one direction at a constant rate while being constrained to no motion in the other two directions, the deformation gradient is given in above, but now define $\gamma = \Gamma t/t_f$. Here $\tan\Theta = \Gamma$ is the final shear angle of the deformation, which is reached at $t = t_f$. The initial particle velocities are $\boldsymbol{v} = \left(\Gamma Y/t_f, 0, 0\right)$. The accelerations are always zero. This deformation can be applied in 2D plane strain or in 3D calculations; it might work in plane stress as well. Because F is independent of position, the stress in the object will be independent of position and determined by the material model being used. As a result, the divergence of the stress is zero and the manufactured solution can be derived with zero body force. The remaining task is finding boundary conditions for various material models.

Traction boundary conditions are found from $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}$. On the $\pm y$ and $\pm z$ surfaces, the normal stays constant during deformation, leading to:

$$\begin{aligned} \boldsymbol{T} &= \left(\tau_{xy}, \sigma_{yy}, 0\right) \qquad \text{on } \pm y && (10.19)\\ \boldsymbol{T} &= (0, 0, \sigma_{zz}) \qquad \text{on } \pm z && (10.20)\\ & && (10.21) \end{aligned}$$

On the initially $\pm x$ surface, the normal rotates to be

$$\hat{\boldsymbol{n}} = \left(\frac{1}{\sqrt{1+\gamma^2}}, \frac{-\gamma}{\sqrt{1+\gamma^2}}, 0\right) \tag{10.22}$$

But since $\gamma = \tan\theta$, where θ is the current shear angle, this normal vector is also

$$\hat{\boldsymbol{n}} = (\cos\theta, -\sin\theta, 0) \tag{10.23}$$

For general stress state (but with $\sigma_{xz} = \sigma_{yz} = 0$), the traction will be

$$\boldsymbol{T} = \left(\sigma_{xx}\cos\theta - \sigma_{xy}\sin\theta, \sigma_{xy}\cos\theta - \sigma_{yy}\sin\theta, 0\right) \tag{10.24}$$

This traction can be divided into traction normal and tangential to the current surface:

$$\begin{aligned} T_n = \boldsymbol{T}\cdot\hat{\boldsymbol{n}} &= \sigma_{xx}\cos^2\theta - 2\sigma_{xy}\cos\theta\sin\theta + \sigma_{yy}\sin^2\theta = \frac{\sigma_{xx} - 2\gamma\sigma_{xx} + \gamma^2\sigma_{yy}}{1+\gamma^2} && (10.25)\\ T_t = \boldsymbol{T}\cdot\hat{\boldsymbol{t}} &= (\sigma_{xx} - \sigma_{yy})\cos\theta\sin\theta + \sigma_{xy}(\cos^2\theta - \sin^2\theta) && (10.26)\\ &= \frac{\gamma(\sigma_{xx} - \sigma_{yy}) + \sigma_{xy}(1-\gamma^2)}{1+\gamma^2} && (10.27) \end{aligned}$$

which used $\hat{\boldsymbol{t}} = (\sin\theta, \cos\theta, 0)$. Note that traction boundary conditions in `NairnMPM` have the option of being applied normal and tangential to the current surface orientation. This approach, however, is less stable because an error is surface orientation amplifies and inaccuracies in the solution. Using tractions along analysis axes works better

For velocity conditions, all surfaces should impose

$$\boldsymbol{v} = \left(\Gamma\frac{Y}{t_f}, 0, 0\right) \tag{10.28}$$

Because particles have zero velocity in the y direction Y will equal y for all particles and can be implemented as a function of current position.

10.3.1 Material Models

Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material for shear sliding can be written as

$$\boldsymbol{\sigma} = G(\mathbf{F} + \mathbf{F}^T - 2\mathbf{I})$$

The only non-zero stress is the shear stress:

$$\sigma_{xy} = G\gamma = G\Gamma\frac{t}{t_f}$$

Neo-Hookean, Mooney-Rivlin Material

For a Mooney-Rivlin material linear shear stresses are given above. Unlike for small-strain materials, a Hyperelastic material develops normal stresses during linear shear.

Neo-Hookean Material

For an alternate Neo-Hookean material linear shear stresses are given above The $\pm x$ can account for rotations or can be done instead with normal and tangential tractions:

$$T_n = -\frac{GJ_{res}\gamma^2}{1+\gamma^2} \qquad T_t = \frac{GJ_{res}\gamma}{1+\gamma^2}$$

But T_x and T_y or T_n and T_t tractions work, but T_x and T_y tractions are more stable.

Disney Snow Model

For the neo-Hookean material in the elastic part of the Clamped Neohookean, the stresses are given above.

10.4 Linear Acceleration

If an object is stretched in uniaxial tension, using an acceleration that is linear in x while being constrained to no motion in the other two directions, the deformation gradient will be

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\frac{t^2}{t_f^2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.29}$$

Here Λ is the final extension ratio, which is reached at $t = t_f$. The particle velocities are $\boldsymbol{v} = 2(\Lambda - 1)Xt/t_f^2$; hence the initial velocities are all zero. The particle accelerations are $\boldsymbol{a} = 2(\Lambda-1)X/t_f^2$, which is linear in X. Because the deformation gradient is independent of position, the stresses will be uniform and therefore have zero divergence. To manufacture a solution, the non-zero accelerations have to be balanced by body force on the nodes (in spatial coordinates) or:

$$\boldsymbol{n} = \left(\frac{2(\Lambda-1)\frac{x}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{10.30}$$

To apply velocity boundary conditions, the applied velocity (in spatial nodal coordinates) should be

$$\boldsymbol{v} = \left(\frac{2(\Lambda-1)\frac{xt}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{10.31}$$

10.4.1 Material Models

Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F})-3\big)\mathbf{I} + G(\mathbf{F}+\mathbf{F}^T-2\mathbf{I}) \tag{10.32}$$

where $\lambda = \nu E/((1+\nu)(1-2\nu))$ is the Lamé constant for the material. For constrained uniaxial tension with linear extension, the stress is

$$\sigma_{ij} = (\lambda + 2G\delta_{i1})(\Lambda-1)\frac{t^2}{t_f^2}\delta_{ij} \tag{10.33}$$

although this stress is based on initial area and not the Cauchy stress. This solution can be imposed by applying traction or velocity boundary conditions. On the $\pm x$ surfaces, the traction condition should be:

$$T_x = \pm(\lambda+2G)(\Lambda-1)\frac{t^2}{t_f^2} \tag{10.34}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda(\Lambda-1)\frac{t^2}{t_f^2} \qquad \text{or} \qquad v_y = v_z = 0 \tag{10.35}$$

Neo-Hookean Material

For an alternate neo-Hookean material under constrained uniaxial deformation:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{\lambda+2G}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{10.36}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{10.37}$$

$$\sigma_{zz} = \sigma_{yy} \tag{10.38}$$

This solution can be imposed by applying traction and/or velocity boundary conditions. On the $\pm x$ surface, the traction condition should be $T_x = \pm\sigma_{xx}$. On the $\pm y$ and $\pm z$ surfaces, the conditions should be $T_y = \pm\sigma_{yy}$ and $T_z = \pm\sigma_{yy}$.

10.5 Sinusoidal Acceleration

If an object is stretched in uniaxial tension by sinusoidal function while be constrained in other two directions, the deformation gradient is:

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\sin\omega t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.39}$$

Here Λ is the maximum extension ratio which is reached periodically at $\omega t = (2n-1)\pi/2$ for $n = 1, 2.\ldots$. The large deformation mapping and its inverse are

$$\chi(X,t) = x = X + v(X)t = X\left(1+(\Lambda-1)\sin\omega t\right) \quad \text{and} \quad \chi^{-1}(x,t) = X = \frac{x}{1+(\Lambda-1)\sin\omega t} \tag{10.40}$$

The x-components of material and spatial descriptions of velocity are

$$V(X,t) = \frac{d\chi(X,t)}{dt} = (\Lambda-1)X\omega\cos\omega t \quad \text{and} \quad v(x,t) = V(\chi^{-1}(x,t),t) = \frac{(\Lambda-1)x\omega\cos\omega t}{1+(\Lambda-1)\sin\omega t} \tag{10.41}$$

The material acceleration comes from

$$A(X,t) = \frac{d^2\chi(X,t)}{dt^2} = -(\Lambda-1)X\omega^2\sin\omega t \tag{10.42}$$

To get this same result for spatial velocity requires the material derivative

$$\frac{Dv(x,t)}{Dt} = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{(\Lambda-1)x\omega^2\sin\omega t}{1+(\Lambda-1)\sin\omega t} \tag{10.43}$$

The particle velocities are $\boldsymbol{a} = (\Lambda-1)X\omega\cos\omega t$; hence initial velocities are $(\Lambda-1)X\omega$ linear in position. The particle accelerations are $\boldsymbol{a} = -(\Lambda-1)X\omega^2\sin\omega t$, which start at zero, but then vary in position and time. Because the deformation gradient is independent of position, the stresses will be uniform and therefore have zero divergence. To manufacture a solution, the non-zero accelerations have to be balanced by body force on the nodes (in spatial coordinates) or:

$$\boldsymbol{n} = \left(-\frac{(\Lambda-1)x\omega^2\sin\omega t}{1+(\Lambda-1)\sin\omega t}, 0, 0\right) \tag{10.44}$$

To apply velocity boundary conditions, the applied velocity (in spatial nodal coordinates) should be

$$\boldsymbol{v} = \left(\frac{(\Lambda-1)x\omega\cos\omega t}{1+(\Lambda-1)\sin\omega t}, 0, 0\right) \tag{10.45}$$

10.5.1 Material Models

Neo-Hookean Material

For an alternate neo-Hookean material under constrained uniaxial deformation:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{(\lambda+2G)(\Lambda-1)\sin\omega t}{2\left(1+(\Lambda-1)\sin\omega t\right)}\left(2+(\Lambda-1)\sin\omega t\right) \tag{10.46}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda(\Lambda-1)\sin\omega t}{2\left(1+(\Lambda-1)\sin\omega t\right)}\left(2+(\Lambda-1)\sin\omega t\right) \tag{10.47}$$

$$\sigma_{zz} = \sigma_{yy} \tag{10.48}$$

This solution can be imposed by applying traction and/or velocity boundary conditions. On the $\pm x$ surface, the traction condition should be $T_x = \pm\sigma_{xx}$. On the $\pm y$ and $\pm z$ surfaces, the conditions should be $T_y = \pm\sigma_{yy}$ and $T_z = \pm\sigma_{yy}$.

10.6 Unconstrained Uniaxial Tension

If an object is deformed in two directions at proportional rates while being constrained to no motion in the third direction, the deformation gradient will be

$$\mathbf{F} = \begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & 1+c\dot{\varepsilon}t & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.49}$$

Here Λ is the final extension, which is reached at $t = t_f$ and c will be choosen to make stress in the y direction equal to zero (if possible and it may depend on time). This deformation can be applied in 2D plane strain or in 3D calculations. Because F is independent of position, the stress in the object will be independent of position and determined by the material model being used. The left-Cauchy tensor is

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} (1+\dot{\varepsilon}t)^2 & 0 & 0 \\ 0 & (1+c\dot{\varepsilon}t)^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.50}$$

with volume change

$$J = |\mathbf{F}| = (1+\dot{\varepsilon}t)(1+c\dot{\varepsilon}t) \tag{10.51}$$

The large deformation mapping and its inverse are

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} X(1+\dot{\varepsilon}t) \\ Y(1+c\dot{\varepsilon}t) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \frac{x}{1+\dot{\varepsilon}t} \\ \frac{y}{1+c\dot{\varepsilon}t} \end{pmatrix} \tag{10.52}$$

The x and y components of material and spatial descriptions of velocity are

$$\begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \dot{\varepsilon}X \\ (c+c't)\dot{\varepsilon}Y \end{pmatrix} \tag{10.53}$$

and

$$\begin{pmatrix} v_x(x,t) \\ v_y(y,t) \end{pmatrix} = \begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \begin{pmatrix} \frac{\dot{\varepsilon}x}{1+\dot{\varepsilon}t} \\ \frac{(c+c't)\dot{\varepsilon}y}{1+c\dot{\varepsilon}t} \end{pmatrix} \tag{10.54}$$

The material velocity gradient is

$$\dot{\mathsf{F}} = \begin{pmatrix} \frac{dV_x(X,t)}{dX} & 0 \\ 0 & \frac{dV_y(X,t)}{dY} \end{pmatrix} = \begin{pmatrix} \dot{\varepsilon} & 0 \\ 0 & (c+c't)\dot{\varepsilon} \end{pmatrix} \tag{10.55}$$

The material acceleration comes from

$$\begin{pmatrix} A_x(\boldsymbol{X},t) \\ A_y(\boldsymbol{X},t) \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \begin{pmatrix} 0 \\ (2c'+c''t)\dot{\varepsilon}Y \end{pmatrix} \tag{10.56}$$

To get this same result for spatial velocity requires (and with $v_z = 0$) the material derivative

$$\frac{Dv_x}{Dt} = \frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} = -\frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} + \frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} = 0 \tag{10.57}$$

$$\begin{aligned} \frac{Dv_y}{Dt} &= \frac{\partial v_y}{\partial t} + v_y\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} = \frac{(2c'+c''t)\dot{\varepsilon}y(1+\dot{\varepsilon}t) - (c+c't)\dot{\varepsilon}^2 y}{(1+\dot{\varepsilon}t)^2} + \frac{(c+c't)\dot{\varepsilon}^2 y}{(1+\dot{\varepsilon}t)^2} \\ &= \frac{(2c'+c''t)\dot{\varepsilon}y}{(1+\dot{\varepsilon}t)} = (2c'+c''t)\dot{\varepsilon}Y \end{aligned} \tag{10.58}$$

10.6.1 Neo-Hookean Material

For an alternate neo-Hookean material using `UJOption=0` and no residual stresses ($J_{res}=1$):

$$-P(J^*)=\frac{\lambda}{2J}\left(J^2-1\right)=\frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) \tag{10.59}$$

and the Cauchy stresses are:

$$\begin{aligned}
\sigma_{xx} &= \frac{G}{J}\left((1+\dot{\varepsilon}t)^2-1\right)+\frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) && (10.60)\\
\sigma_{yy} &= \frac{G}{J}\left((1+c\dot{\varepsilon}t)^2-1\right)+\frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) && (10.61)\\
\sigma_{zz} &= \frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) && (10.62)\\
\sigma_{ij} &= 0 \qquad \text{for } i\neq j && (10.63)
\end{aligned}$$

We want zero stress in the y direction, which reduces to:

$$(1+c\dot{\varepsilon}t)^2=\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G} \quad \text{or} \quad c=-\frac{1-\sqrt{\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}}}{\dot{\varepsilon}t} \tag{10.64}$$

Note that for small strain (t close to zero), this result reduces to

$$c=-\frac{\lambda}{\lambda+2G}=-\frac{\nu}{1-\nu} \tag{10.65}$$

which recovers Poisson's contraction in 2D small-strain, plane-strain analysis. For finite strain, c depends on time causing this problem to have accelerations that need to be handled?

Substituting c, the deformation matrix is now

$$\mathbf{F}=\begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0\\ 0 & \sqrt{\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}} & 0\\ 0 & 0 & 1\end{pmatrix} \tag{10.66}$$

The particle Y velocities are now:

$$V_y(Y,t)=(c+c't)\dot{\varepsilon}t=-\lambda(1+\dot{\varepsilon}t)\,\dot{\varepsilon}Y\sqrt{\frac{\lambda+2G}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^3}} \tag{10.67}$$

The acceleration to provide as a body force is:

$$A_y(Y,t)=2\lambda\left(\lambda(1+\dot{\varepsilon}t)^2-G\right)\dot{\varepsilon}^2Y\sqrt{\frac{\lambda+2G}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^5}} \tag{10.68}$$

Now substitute for Y to get

$$A_y(y,t)=\frac{2\lambda\left(\lambda(1+\dot{\varepsilon}t)^2-G\right)\dot{\varepsilon}^2y}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^2} \tag{10.69}$$

For expected stresses and needed tractions, the pressure reduces to:

$$
\begin{aligned}
-P(J^*) &= \frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2\,\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}-1\right) && (10.70)\\
&= \frac{\lambda}{2J}\left(\frac{(1+\dot{\varepsilon}t)^2(\lambda+2G)-\lambda(1+\dot{\varepsilon}t)^2-2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) && (10.71)\\
&= \frac{G}{J}\left(\frac{\lambda\big((1+\dot{\varepsilon}t)^2-1\big)}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) && (10.72)\\
& && (10.73)
\end{aligned}
$$

and the Cauchy stresses become

$$
\begin{aligned}
\sigma_{xx} &= \frac{G}{J}\big((1+\dot{\varepsilon}t)^2-1\big)\left(\frac{\lambda}{\lambda(1+\dot{\varepsilon}t)^2+2G}+1\right) && (10.74)\\
\sigma_{yy} &= 0 && (10.75)\\
\sigma_{zz} &= \frac{\lambda G}{J}\left(\frac{(1+\dot{\varepsilon}t)^2-1}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) && (10.76)\\
\sigma_{ij} &= 0 \qquad \text{for } i\neq j && (10.77)
\end{aligned}
$$