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

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. The elastic strain is $\boldsymbol{\varepsilon}_e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p$. The stress, $\boldsymbol{\sigma}$, and plastic forces, $\boldsymbol{\psi}$, are found from

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

For general analysis, begin with an elastic stress increment, $d\boldsymbol{\sigma}$, given by

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}_{tot} \tag{2.3}$$

where $\mathbf{C}$ is the stiffness matrix, $d\boldsymbol{\varepsilon}_{tot} = d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res}$ is total strain increment (using tensorial strains) relative to the residual strain increments. Let $f(\boldsymbol{\sigma}, \boldsymbol{\psi})$ be a plastic potential function that depends on components of stress and plastic forces. The potential function is defined such that $f = 0$ is the yield surface, $f < 0$ is the elastic region, and $f > 0$ is not allowed.

First construct a trial update that assumes elastic deformation only or assumes that $d\boldsymbol{\varepsilon}_e = d\boldsymbol{\varepsilon}_{tot}$, $d\boldsymbol{\varepsilon}_p = 0$, and $d\boldsymbol{\alpha} = 0$ (in other words, no plastic deformation). The trial f is given by

$$f_{trial} = f(\boldsymbol{\sigma} + d\boldsymbol{\sigma}, \boldsymbol{\psi}) = f(\boldsymbol{\sigma} + \mathbf{C} d\boldsymbol{\varepsilon}_{tot}, \boldsymbol{\psi}) \tag{2.4}$$

If $f_{trial} \leq 0$, the deformation is elastic, the trial increment is accepted, and the analysis is done.

If $f_{trial} > 0$, the task is to partition the total strain into elastic and plastic strain, $d\boldsymbol{\varepsilon}_{tot} = d\boldsymbol{\varepsilon}_e + d\boldsymbol{\varepsilon}_p$, such that the final f is zero. In other words, the task is to solve

$$f\big(\boldsymbol{\sigma} + \mathbf{C} d\boldsymbol{\varepsilon}_{tot} - \mathbf{C} d\boldsymbol{\varepsilon}_p, \boldsymbol{\psi}(\alpha + d\alpha)\big) = 0 \tag{2.5}$$

The plastic flow laws are assumed to be

$$d\boldsymbol{\varepsilon}_p = \lambda N(\boldsymbol{\sigma}, \boldsymbol{\psi}) = \lambda \frac{\partial \Psi}{\partial \boldsymbol{\sigma}} \quad \text{and} \quad d\alpha = \lambda H(\boldsymbol{\sigma}, \boldsymbol{\psi}) = -\lambda \frac{\partial \Psi}{\partial \boldsymbol{\psi}} \tag{2.6}$$

where Ψ is a flow potential. A common assumption is to use associative flow rule where $\Psi = f$ leading to

$$N(\boldsymbol{\sigma}, \boldsymbol{\psi}) = \frac{\partial f}{\partial \boldsymbol{\sigma}} \quad \text{and} \quad H(\boldsymbol{\sigma}, \boldsymbol{\psi}) = -\frac{\partial f}{\partial \boldsymbol{\psi}} \tag{2.7}$$

Thus, the task is to solve

$$f\left(\boldsymbol{\sigma}+\mathbf{C}d\boldsymbol{\varepsilon}_{tot}-\lambda\mathbf{C}N(\boldsymbol{\sigma},\boldsymbol{\psi}),\boldsymbol{\psi}\left(\alpha+\lambda H(\boldsymbol{\sigma},\boldsymbol{\psi})\right)\right) = 0 \tag{2.8}$$

$$f\left(\boldsymbol{\sigma}+\mathbf{C}d\boldsymbol{\varepsilon}_{tot}-\lambda\mathbf{C}N(\boldsymbol{\sigma},\boldsymbol{\psi}),\boldsymbol{\psi}+\lambda\frac{\partial\psi}{\partial\boldsymbol{\alpha}}H(\boldsymbol{\sigma},\boldsymbol{\psi})\right) = 0 \tag{2.9}$$

For associative plasticity, this result becomes

$$f\left(\boldsymbol{\sigma}+\mathbf{C}d\boldsymbol{\varepsilon}_{tot}-\lambda\mathbf{C}\frac{\partial f}{\partial\boldsymbol{\sigma}},\boldsymbol{\psi}-\lambda\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\frac{\partial f}{\partial\boldsymbol{\psi}}\right)=0 \tag{2.10}$$

for λ. This solution will normally require numerical analysis.

2.1.1 Incremental Plasticity Problem

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

$$f(\boldsymbol{\sigma}_{n+1},\boldsymbol{\psi}_{n+1}) = 0 \tag{2.11}$$

$$d\boldsymbol{\varepsilon}_p = \lambda N(\boldsymbol{\sigma}_{n+1},\boldsymbol{\psi}_{n+1}) \tag{2.12}$$

$$d\boldsymbol{\varepsilon}_e = d\boldsymbol{\varepsilon}_{tot}-d\boldsymbol{\varepsilon}_p \tag{2.13}$$

$$\boldsymbol{\alpha}_{n+1} = \boldsymbol{\alpha}_n+\lambda H(\boldsymbol{\sigma}_{n+1},\boldsymbol{\psi}_{n+1}) \tag{2.14}$$

$$\boldsymbol{\sigma}_{n+1} = \boldsymbol{\sigma}_n+\mathbf{C}d\boldsymbol{\varepsilon}_e \tag{2.15}$$

$$\boldsymbol{\psi}_{n+1} = \boldsymbol{\psi}(\boldsymbol{\alpha}_{n+1}) \tag{2.16}$$

Ideally this problem is solved implicitly. For J_2 plasticity, these equations in 7 (or more) unknowns (for components of stress and plastic variables) can be reduced to a single equation for λ that can be solved implicitly. For most other problems some other numerical method is needed.

2.1.2 Explicit Integration

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

$$\boldsymbol{\sigma}^{(0)}=\boldsymbol{\sigma}_{trial} = \boldsymbol{\sigma}_n+\mathbf{C}d\boldsymbol{\varepsilon}_{tot} \tag{2.17}$$

$$d\boldsymbol{\varepsilon}_p^{(0)} = 0 \tag{2.18}$$

$$\boldsymbol{\lambda}^{(0)} = 0 \tag{2.19}$$

$$\boldsymbol{\alpha}^{(0)}=\boldsymbol{\alpha}_{trial} = \boldsymbol{\alpha}_n \tag{2.20}$$

$$\boldsymbol{\psi}^{(0)}=\boldsymbol{\psi}_{trial} = \boldsymbol{\psi}_n \tag{2.21}$$

$$f^{(0)}=f_{trial} = f(\boldsymbol{\varepsilon}_{e,trial},\boldsymbol{\psi}_{trial})>0 \tag{2.22}$$

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

$$f^{(k+1)}=f(\boldsymbol{\sigma}^{(k)}+d\boldsymbol{\sigma},\boldsymbol{\psi}^{(k)}+d\boldsymbol{\psi})=f^{(k)}+\frac{\partial f}{\partial\boldsymbol{\sigma}^{(k)}}d\boldsymbol{\sigma}+\frac{\partial f}{\partial\boldsymbol{\psi}^{(k)}}d\boldsymbol{\psi} \tag{2.23}$$

where stress differential is

$$d\boldsymbol{\sigma} = \boldsymbol{\sigma}^{(k+1)}-\boldsymbol{\sigma}^{(k)} \tag{2.24}$$

$$= \boldsymbol{\sigma}_n+\mathbf{C}d\boldsymbol{\varepsilon}_{tot}-\lambda^{(k+1)}\mathbf{C}N(\boldsymbol{\sigma}^{(k+1)},\boldsymbol{\psi}^{(k+1)})-\boldsymbol{\sigma}_n-\mathbf{C}d\boldsymbol{\varepsilon}_{tot}+\lambda^{(k)}\mathbf{C}N(\boldsymbol{\sigma}^{(k)},\boldsymbol{\psi}^{(k)}) \tag{2.25}$$

$$\approx -d\lambda\,\mathbf{C}N(\boldsymbol{\sigma}^{(k)},\boldsymbol{\psi}^{(k)}) \tag{2.26}$$

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

$$\begin{aligned} d\boldsymbol{\psi} &= \boldsymbol{\psi}^{(k+1)} - \boldsymbol{\psi}^{(k)} \approx \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}}(\boldsymbol{\alpha}^{(k+1)} - \boldsymbol{\alpha}^{(k)}) && (2.27)\\ &= \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}}\left(\boldsymbol{\alpha}_n + \lambda^{(k+1)} H(\boldsymbol{\sigma}^{(k+1)}, \boldsymbol{\psi}^{(k+1)}) - \boldsymbol{\alpha}_n - \lambda^{(k)} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)})\right) && (2.28)\\ &\approx d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.29) \end{aligned}$$

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

$$f^{(k+1)} = f^{(k)} - d\lambda \left(\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) - \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \right) \tag{2.30}$$

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

$$d\lambda = \frac{f^{(k)}}{\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \cdot \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) - \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\alpha}^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)})} \tag{2.31}$$

For associative plasticity, the result is:

$$d\lambda = \frac{f^{(k)}}{\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \cdot \mathbf{C} \frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} + \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}^{(k)}} \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}}} \tag{2.32}$$

From the solved increment, update the variables using:

$$\begin{aligned} \lambda^{(k+1)} &= \lambda^{(k)} + d\lambda && (2.33)\\ d\boldsymbol{\varepsilon}_p^{(k+1)} &= d\boldsymbol{\varepsilon}_p^{(k)} + d\lambda N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.34)\\ \boldsymbol{\alpha}^{(k+1)} &= \boldsymbol{\alpha}^{(k)} + d\lambda H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.35)\\ \boldsymbol{\sigma}^{(k+1)} &= \boldsymbol{\sigma}^{(k)} - d\lambda \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.36)\\ \boldsymbol{\psi}^{(k+1)} &= \boldsymbol{\psi}^{(k)} + d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.37) \end{aligned}$$

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 $d\boldsymbol{\psi}$.

2.2 J_2 Flow Theory for Isotropic Materials

For a special case, consider an isotropic material with isotropic hardening, a single internal variable, α, and assume the plastic potential is a function only of $J_2 = (1/2)\|\mathbf{s}\|^2$ expressed as

$$f = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} K(\alpha) = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}(\sigma_y + \psi) \tag{2.38}$$

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, but not pressure). The plastic force, ψ, as function of α is

$$\psi = K(\alpha) - \sigma_y \tag{2.39}$$

The usual assumption for associative flow is to take

$$d\alpha = -\lambda \frac{\partial f}{\partial \psi} = \lambda \sqrt{\frac{2}{3}} \tag{2.40}$$

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.

In terms of the deviatoric stress

$$2J_2 = \|\mathbf{s}\|^2 = s_{xx}^2 + s_{yy}^2 + s_{zz}^2 + 2s_{xy}^2 + 2s_{xz}^2 + 2s_{yz}^2 \tag{2.41}$$

During plastic deformation, the plastic strain increment simplifies to

$$\lambda \frac{\partial f}{\partial \boldsymbol{\sigma}} = \lambda \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} = \lambda \mathbf{n} \tag{2.42}$$

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. Since $\|d\boldsymbol{\varepsilon}_p\| = \|\lambda(\partial f/\partial \boldsymbol{\sigma})\| = \lambda$, this assumption corresponds to

$$d\alpha = \sqrt{\frac{2}{3}} \|d\boldsymbol{\varepsilon}_p\| \tag{2.43}$$

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

$$\mathbf{s} = \mathbf{s}_{trial} - \lambda 2G\mathbf{n} = \left(1 - \frac{\lambda 2G}{\|\mathbf{s}_{trial}\|}\right)\mathbf{s}_{trial} \tag{2.44}$$

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

$$\|\mathbf{s}\| = \|\mathbf{s}_{trial}\| - \lambda 2G \qquad \text{and} \qquad \frac{\mathbf{s}}{\|\mathbf{s}\|} = \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} \tag{2.45}$$

which confirms that normal is independent of λ.

The required equation for finding λ thus simplifies to depend only on $\|\mathbf{s}_{trial}\|$, G, and hardening law:

$$f^{(k)} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} K(\alpha^{(k)}) = \|\mathbf{s}_{trial}\| - \lambda^{(k)} 2G - \sqrt{\frac{2}{3}} K(\alpha^{(k)}) = 0 \tag{2.46}$$

This can be solved by Newton's method using:

$$\frac{df^{(k)}}{d\lambda} = -2G - \sqrt{\frac{2}{3}} \frac{dK(\alpha^{(k)})}{d\lambda} = -2G - \frac{2}{3} \frac{dK(\alpha^{(k)})}{d\alpha} \tag{2.47}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)} \sqrt{\frac{2}{3}} \tag{2.48}$$

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 $f > 0$.
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 f; 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

$$f = \|\mathbf{s}_{trial}\| - \lambda 2G - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\left(\alpha^0 + \lambda\sqrt{\frac{2}{3}}\right)\right) = 0 \tag{2.49}$$

The analytical solution is

$$\lambda = \frac{\|\mathbf{s}_{trial}\| - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\alpha^0\right)}{2G + \frac{2E_p}{3}} \tag{2.50}$$

2.3 Plane Strain and Axisymmetric Analysis for J_2 Flow Theory, Isotropic Materials

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

$$\frac{\Delta V}{V} = d\varepsilon_{xx} + d\varepsilon_{yy} + d\varepsilon_{zz} - 3d\varepsilon^{(res)} \tag{2.51}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.52}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i = j = x, y, z \tag{2.53}$$

$$d\tau_{xy} = ds_{xy} = Gd\gamma_{xy} \tag{2.54}$$

where

$$d\varepsilon_{xx}^{(tot)} = d\varepsilon_{xx} - d\varepsilon^{(res)}, \quad d\varepsilon_{yy}^{(tot)} = d\varepsilon_{yy} - d\varepsilon^{(res)}, \quad \text{and} \quad d\varepsilon_{zz}^{(tot)} = d\varepsilon_{zz} - d\varepsilon^{(res)} \tag{2.55}$$

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

$$d\varepsilon^{(res)} = \alpha\Delta T + \beta\Delta c \tag{2.56}$$

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

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

$$ds_{ij} = ds_{ij}^{trial} - 2Gd\varepsilon_{ij}^{p} \tag{2.57}$$

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

$$d\varepsilon_{ij}^{e} = -d\varepsilon_{ij}^{p} \tag{2.58}$$

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 `VeriofyAndLoadProperties()`. 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.

2.4 Plane Stress Analysis for J_2 Flow Theory, Isotropic Materials

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

$$d\varepsilon_{zz}^{(tot)} = -\frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.59}$$

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

$$\frac{\Delta V}{V} = d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)} + d\varepsilon_{zz}^{(tot)} = \left(\frac{1-2\nu}{1-\nu}\right)\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.60}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.61}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i = j = x, y \tag{2.62}$$

$$ds_{zz}^{trial} = ds_{zz} = dP \tag{2.63}$$

$$d\tau_{xy}^{trial} = ds_{xy}^{trial} = Gd\gamma_{xy} \tag{2.64}$$

$$\tag{2.65}$$

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:

$$\texttt{psRed} = \left(\frac{1-2\nu}{1-\nu}\right) = \frac{1}{\frac{K}{2G}+\frac{2}{3}} \tag{2.66}$$

$$\texttt{psLr2G} = \frac{\nu}{1-\nu} = \frac{\frac{K}{2G}-\frac{1}{3}}{\frac{K}{2G}+\frac{2}{3}} \tag{2.67}$$

$$\texttt{psKred} = \frac{E}{3(1-\nu)} = K * \texttt{psRed} = \frac{K}{\frac{K}{2G}+\frac{2}{3}} \tag{2.68}$$

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. (2.60)). 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 $f > 0$, the process (following Simo and Hughes), effectively (or equivalently) revises f using squares to be

$$f = \|\mathbf{s}\|^2 - \frac{2}{3}K^2(\alpha) = \sigma\mathbf{P}\sigma - \frac{2}{3}K^2(\alpha) \tag{2.69}$$

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

$$\mathbf{P} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & 0 \\ -\frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{2.70}$$

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

$$(d\varepsilon^p_{xx}, d\varepsilon^p_{yy}, d\gamma^p_{xy}) = \lambda\frac{\partial f}{\partial \boldsymbol{\sigma}} = \lambda\mathbf{P}\sigma \tag{2.71}$$

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

$$d\boldsymbol{\varepsilon}_p = \lambda\begin{pmatrix} \frac{1}{3}(2\sigma_{xx} - \sigma_{yy}) & \tau_{xy} & 0 \\ \tau_{xy} & \frac{1}{3}(2\sigma_{yy} - \sigma_{xx}) & 0 \\ 0 & 0 & -\frac{1}{3}(\sigma_{xx} + \sigma_{yy}) \end{pmatrix} \tag{2.72}$$

This traceless tensor has inner product

$$\|d\boldsymbol{\varepsilon}_p\|^2 = \lambda^2\left(\frac{2}{3}(\sigma^2_{xx} + \sigma^2_{yy} - \sigma_{xx}\sigma_{yy}) + 2\tau^2_{xy}\right) = \lambda^2\sigma\mathbf{P}\sigma \tag{2.73}$$

$$= \lambda^2\left(s^2_{xx} + s^2_{yy} + s^2_{zz} + 2s^2_{xy}\right) \tag{2.74}$$

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

$$d\alpha = \sqrt{\frac{2}{3}}\lambda\sqrt{\sigma\mathbf{P}\sigma} \tag{2.75}$$

When $f > 0$, 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

$$\sigma^{trial}_{n+1} = \sigma_n + \mathbf{C}(d\varepsilon^{(tot)}_{xx}, d\varepsilon^{(tot)}_{yy}, d\gamma^{(tot)}_{xy}) \tag{2.76}$$

$$f\sigma_{n+1} = \sigma^{trial}_{n+1} - \mathbf{C}d\boldsymbol{\varepsilon}_p = \sigma^{trial}_{n+1} - \mathbf{C}\lambda\mathbf{P}\sigma_{n+1} \tag{2.77}$$

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

$$\mathbf{C} = \begin{pmatrix} \frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\ \frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & G \end{pmatrix} \quad \text{with} \quad \mathbf{C}^{-1} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & 0 \\ 0 & 0 & \frac{1}{G} \end{pmatrix} \tag{2.78}$$

Solving the second equation the required stress is:

$$\sigma_{n+1} = \left[\mathbf{C}^{-1} + \lambda \mathbf{P}\right]^{-1} \mathbf{C}^{-1} \sigma_{n+1}^{trial} \tag{2.79}$$

This general result applied to isotropic materials leads to

$$\sigma_{xx}^{(n+1)} + \sigma_{yy}^{(n+1)} = \frac{1}{1 + \frac{E}{3(1-\nu)}\lambda} \left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right) \tag{2.80}$$

$$-\sigma_{xx}^{(n+1)} + \sigma_{yy}^{(n+1)} = \frac{1}{1 + 2G\lambda} \left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right) \tag{2.81}$$

$$\tau_{xy}^{(n+1)} = \frac{\tau_{xy}^{trial}}{1 + 2G\lambda} \tag{2.82}$$

and

$$\|\mathbf{s}\|^2 = \sigma_{n+1} \mathbf{P} \sigma_{n+1} = \frac{\frac{1}{6}\left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2}{\left(1 + \frac{E}{3(1-\nu)}\lambda\right)^2} + \frac{\frac{1}{2}\left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2 + 2{\tau_{xy}^{trial}}^2}{(1 + 2G\lambda)^2} \tag{2.83}$$

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

$$f^{(k)} = \frac{1}{2}\|\mathbf{s}^{(k)}\|^2 - \frac{1}{3}K^2(\alpha^{(k)}) = 0 \tag{2.84}$$

$$\frac{df^{(k)}}{d\lambda} = -\left[\frac{E}{3(1-\nu)} \frac{\frac{1}{6}\left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2}{\left(1 + \frac{E}{3(1-\nu)}\lambda^{(k)}\right)^3} + 2G \frac{\frac{1}{2}\left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2 + 2{\tau_{xy}^{trial}}^2}{\left(1 + 2G\lambda^{(k)}\right)^3}\right] - \frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} \tag{2.85}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)}\sqrt{\frac{2}{3}}\|\mathbf{s}^{(k+1)}\| \tag{2.86}$$

A subclass of `IsoPlasticity` class 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

$$\texttt{psKred} = \frac{E}{3(1-\nu)} = \frac{K}{\frac{K}{2G} + \frac{2}{3}} \tag{2.87}$$

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

$$\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{xx}^{trial} + s_{yy}^{trial} - 2P_{final} \tag{2.88}$$

$$-\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{yy}^{trial} - s_{xx}^{trial} \tag{2.89}$$

$$s_{xx}^{(n+1)} = \sigma_{xx}^{(n+1)} + P_{final} \tag{2.90}$$

$$s_{yy}^{(n+1)} = \sigma_{yy}^{(n+1)} + P_{final} \tag{2.91}$$

$$s_{zz}^{(n+1)} = P_{final} \tag{2.92}$$

$$s_{xy}^{(n+1)} = \tau_{xy}^{(n+1)} \tag{2.93}$$

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:

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}\left(\sigma_Y + E_p\alpha^{(k)}\right)E_p\|\mathbf{s}^{(k)}\| \tag{2.94}$$

2.5 3D Analysis for J_2 Flow Theory, Isotropic Materials

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

2.6 Examples of J_2 Flow Theory Materials

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. Those 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.

2.6.1 VonMises Material with Linear Work Hardening

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha) = \sigma_y + E_p\alpha && (2.95)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}E_p && (2.96)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}(\sigma_y + E_p\alpha)E_p\|\mathbf{s}\| && (2.97)
\end{aligned}
$$

2.6.2 VonMises Material with Non-Linear Work Hardening

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha)^n && (2.98)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}\sigma_y\beta n(1+\beta\alpha)^{n-1} && (2.99)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}\sigma_y^2\beta n(1+\beta\alpha)^{2n-1}\|\mathbf{s}\| && (2.100)
\end{aligned}
$$

2.6.3 VonMises Material with Alternate Non-Linear Work Hardening

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha^n) && (2.101)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}\sigma_y\beta n\alpha^{n-1} && (2.102)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}\sigma_y^2\beta n\alpha^{n-1}(1+\beta\alpha^n)\|\mathbf{s}\| && (2.103)
\end{aligned}
$$

2.6.4 Johnson-Cook

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.104}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}\left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\left(1-(T^*)^m\right) \tag{2.105}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right)^2 \left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\|\mathbf{s}\| \tag{2.106}$$

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

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.107}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.108}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}Bn\alpha^{n-1}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)^2\left(1-(T^*)^m\right)^2\|\mathbf{s}\| \tag{2.109}$$

2.7 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:

$$f = \sqrt{F\left(\sigma_{yy}-\sigma_{zz}\right)^2+G(\sigma_{xx}-\sigma_{zz})^2+H\left(\sigma_{yy}-\sigma_{xx}\right)^2+2L{\tau_{yz}}^2+2M{\tau_{xz}}^2+2N{\tau_{xy}}^2} - g(\boldsymbol{\alpha}) \tag{2.110}$$

$$= \left[(G+H){\sigma_{xx}}^2+(F+H){\sigma_{yy}}^2+(F+G)\sigma_{zz}^2-2F\sigma_{yy}\sigma_{zz}-2G\sigma_{xx}\sigma_{zz} - 2H\sigma_{xx}\sigma_{yy}+2L{\tau_{yz}}^2+2M{\tau_{xz}}^2+2N{\tau_{xy}}^2\right]^{1/2}-g(\boldsymbol{\alpha}) \tag{2.111}$$

$$= \sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}-g(\boldsymbol{\alpha}) = \sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}-\frac{\sigma^Y_{ref}+\sqrt{\frac{2}{3}}\boldsymbol{\psi}(\boldsymbol{\alpha})}{\sigma^Y_{ref}} \tag{2.112}$$

where $\boldsymbol{\sigma}$ is stress in the material axis system, $g(\boldsymbol{\alpha})$ is a hardening function, $\boldsymbol{\psi}$ is plastic force for hard-

ening, σ^Y_{ref} is a reference tensile yield strength, and

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.113}$$

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

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 \\ -H & F+H & -F & 0 \\ -G & -F & F+G & 0 \\ 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.114}$$

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

$$A_{xxxx} = G+H,\ A_{xxyy} = A_{yyxx} = -H,\ A_{xxzz} = A_{zzxx} = -G,\ A_{yyyy} = F+H, \tag{2.115}$$

$$A_{yyzz} = A_{zzyy} = -F,\ A_{zzzz} = F+G,\ A_{yzyz} = \frac{L}{2},\ A_{xzxz} = \frac{M}{2},\ A_{xyxy} = \frac{N}{2} \tag{2.116}$$

such that

$$\mathbf{A}\boldsymbol{\sigma} = \begin{pmatrix} (G+H)\sigma_{xx} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + (F+H)\sigma_{yy} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + (F+G)\sigma_{zz} \end{pmatrix} \tag{2.117}$$

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:

$$(G+H) = \frac{1}{(\sigma^Y_{xx})^2} \qquad (F+H) = \frac{1}{(\sigma^Y_{yy})^2} \qquad (F+G) = \frac{1}{(\sigma^Y_{zz})^2} \tag{2.118}$$

$$F = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{yy})^2} + \frac{1}{(\sigma^Y_{zz})^2} - \frac{1}{(\sigma^Y_{xx})^2}\right) \qquad G = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{zz})^2} + \frac{1}{(\sigma^Y_{xx})^2} - \frac{1}{(\sigma^Y_{yy})^2}\right) \tag{2.119}$$

$$H = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{xx})^2} + \frac{1}{(\sigma^Y_{yy})^2} - \frac{1}{(\sigma^Y_{zz})^2}\right) \quad L = \frac{1}{2(\tau^Y_{yz})^2} \quad M = \frac{1}{2(\tau^Y_{xz})^2} \quad N = \frac{1}{2(\tau^Y_{xy})^2} \tag{2.120}$$

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:

$$F^2 + G^2 + H^2 - FH - GH - FG \geq 0 \tag{2.121}$$

$$F + G + H \geq \sqrt{F^2 + G^2 + H^2 - FH - GH - FG} \tag{2.122}$$

Substituting yield stresses, the conditions can be recast as

$$\left(\frac{1}{\sigma^Y_{xx}}-\frac{1}{\sigma^Y_{yy}}\right)^2 \le \frac{1}{(\sigma^Y_{zz})^2} \le \left(\frac{1}{\sigma^Y_{xx}}+\frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.123}$$

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

$$\left(\frac{1}{\sigma^Y_{zz}}-\frac{1}{\sigma^Y_{yy}}\right)^2 \le \frac{1}{(\sigma^Y_{xx})^2} \le \left(\frac{1}{\sigma^Y_{zz}}+\frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.125}$$

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:

$$\frac{\sigma^Y_{yy}}{(1+R)} \le \sigma^Y_{zz} \le \frac{\sigma^Y_{yy}}{|1-R|} \tag{2.126}$$

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

$$\frac{1}{\sigma^Y_{ref}} = \sqrt{F+G+H} = \sqrt{\frac{1}{2}\left(\frac{1}{(\sigma^Y_{xx})^2}+\frac{1}{(\sigma^Y_{yy})^2}+\frac{1}{(\sigma^Y_{yy})^2}\right)} \tag{2.127}$$

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

$$(G+H)=(F+H)=(F+G)=2F=2G=2H=\frac{1}{\sigma^2_Y}, \tag{2.128}$$

$$L=M=N=\frac{1}{2\tau^2_Y}=\frac{3}{2\sigma^2_Y}, \quad \text{and} \quad \sigma^Y_{ref}=\sqrt{\frac{2}{3}}\sigma_Y \tag{2.129}$$

leading to:

$$\begin{aligned} f &= \sqrt{\frac{\left(\sigma_{yy}-\sigma_{zz}\right)^2}{2\sigma^2_Y}+\frac{(\sigma_{xx}-\sigma_{zz})^2}{2\sigma^2_Y}+\frac{\left(\sigma_{yy}-\sigma_{xx}\right)^2}{2\sigma^2_Y}+\frac{3{\tau_{yz}}^2}{\sigma^2_Y}+\frac{3{\tau_{xz}}^2}{\sigma^2_Y}+\frac{3{\tau_{xy}}^2}{\sigma^2_Y}} - g(\boldsymbol{\alpha}) \\ &= \frac{1}{\sigma_Y}\sqrt{3J_2}-g(\boldsymbol{\alpha}) = \frac{1}{\sigma_Y}\sqrt{\frac{3}{2}}\left(\sqrt{2J_2}-\sqrt{\frac{2}{3}}(\sigma_Y+\psi)\right) \end{aligned} \tag{2.130}$$

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

$$\frac{d\boldsymbol{f}}{d\boldsymbol{\sigma}} = \frac{\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.131}$$

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

$$d\boldsymbol{\varepsilon}_p = \lambda d\boldsymbol{f} = \frac{\lambda\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.132}$$

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

$$d\boldsymbol{\varepsilon}_p = \frac{\lambda}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}}\begin{pmatrix} \frac{\sigma_{xx}}{(\sigma^Y_{xx})^2} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + \frac{\sigma_{yy}}{(\sigma^Y_{yy})^2} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + \frac{\sigma_{zz}}{(\sigma^Y_{zz})^2} \end{pmatrix} \tag{2.133}$$

The engineering plastic strain increment is

$$d\boldsymbol{\varepsilon}_p = \frac{\lambda}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}}\begin{pmatrix} \frac{\sigma_{xx}}{(\sigma^Y_{xx})^2} - H\sigma_{yy} - G\sigma_{zz} \\ -H\sigma_{xx} + \frac{\sigma_{yy}}{(\sigma^Y_{yy})^2} - F\sigma_{zz} \\ -G\sigma_{xx} - F\sigma_{yy} + \frac{\sigma_{zz}}{(\sigma^Y_{zz})^2} \\ \frac{\tau_{yz}}{(\tau^Y_{yz})^2} \\ \frac{\tau_{xz}}{(\tau^Y_{yx})^2} \\ \frac{\tau_{xy}}{(\tau^Y_{xy})^2} \end{pmatrix} \tag{2.134}$$

The usual assumption for associative flow is to take

$$d\alpha = -\lambda\frac{\partial f}{\partial \psi} = \frac{\lambda}{\sigma^Y_{ref}}\sqrt{\frac{2}{3}} \tag{2.135}$$

Solving for $\boldsymbol{\psi}$ gives

$$\boldsymbol{\psi} = \sigma^Y_{ref}\sqrt{\frac{3}{2}}(g(\boldsymbol{\alpha})-1) \quad \text{and} \quad \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}} = \sigma^Y_{ref}\sqrt{\frac{3}{2}}g'(\alpha) \tag{2.136}$$

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

$$\frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}}\frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}^{(k)}}\frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} = \frac{g'(\alpha)}{\sigma^Y_{ref}}\sqrt{\frac{2}{3}} \tag{2.137}$$

The hardening law currently implements is:

$$g(\alpha) = 1 + K\alpha^n, \quad g'(\alpha) = nK\alpha^{n-1}, \quad K_n = K_1\alpha^{1-n} \tag{2.138}$$

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, the value of K_n gives the value of K for new n to match the amount of hardening that occurs up to any specified α between the $n = 1$ and n laws. Compared to nonlinear hardening law defined by

$$\sigma_y = \sigma_{y0}(1 + K'\alpha_k) \quad \text{with} \quad \psi = \sigma_y = \sigma_{y0}K'\alpha^n \tag{2.139}$$

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

$$K = K'\frac{\sigma_{y0}}{\sigma^Y_{ref}}\sqrt{\frac{2}{3}} \quad (= K') \quad \text{and} \quad K = \frac{E_p}{\sigma^Y_{ref}}\sqrt{\frac{2}{3}} \quad \left(= \frac{E_p}{\sigma_{y0}}\right) \tag{2.140}$$

where second form is for linear hardening with plastic modulus E_p (and parenthetical forms are if material is isotropic too). Other hardening laws are easily implement such as

$$g(\alpha) = (1 + K\alpha)^n, \; g'(\alpha) = nK(1 + K\alpha)^{n-1}, \; g'(0) = nK \tag{2.141}$$

2.8 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:

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}_{tot} + \boldsymbol{c}_{excess} \tag{2.142}$$

The key terms are

$$\mathbf{C} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 & 0 \\ \texttt{C[4][1]} & \texttt{C[4][2]} & 0 & \texttt{C[4][4]} \\ 0 & 0 & \texttt{C[3][3]} & 0 \end{pmatrix} \tag{2.143}$$

$$d\boldsymbol{\varepsilon}_{tot} = \left(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)},\, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)},\, d\varepsilon_{zz} - \varepsilon_{zz}^{(res)},\, d\gamma_{xy}\right) \tag{2.144}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.145}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res)} \\ \gamma_{xy}^{(res)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \alpha_{zz}\Delta T + \beta_{zz}\Delta c \\ 0 \end{pmatrix} \tag{2.146}$$

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:

$$\boldsymbol{c}_{excess}[3] = \left(\texttt{C[4][1]alpha[5]} + \texttt{C[4][2]alpha[6]}\right)\varepsilon_{zz}^{(res)} \tag{2.147}$$

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:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx}, \quad d\varepsilon_{yy}^{(p)} = \lambda df_{yy}, \quad d\gamma_{xy}^{(p)} = \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(p)} = \lambda df_{zz} \tag{2.148}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(e)} = -\lambda df_{zz} \tag{2.149}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 \\ 0 & 0 & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\gamma_{xx}^{(e)} \end{pmatrix} \tag{2.150}$$

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

$$\begin{aligned} d\sigma_{zz} = {} & \texttt{C[4][1]}\left(d\varepsilon_{xx}^{(e)} - (\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)})\right) + \texttt{C[4][2]}\left(d\varepsilon_{yy}^{(e)} - (\varepsilon_{yy}^{(res,r)} - \texttt{alpha[6]}\varepsilon_{zz}^{(res)})\right) \\ & - \texttt{C[4][4]}(d\varepsilon_{zz}^{(e)} - \varepsilon^{(res)}) \end{aligned} \tag{2.151}$$

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

2.9 Anisotropic 2D Plane Stress Analysis

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

2.10 Anisotropic 3D Analysis - Material Axes

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

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}_{tot} \tag{2.152}$$

The key terms are

$$\mathbf{C} = \texttt{C[i][j]} \quad \text{for } \texttt{i} = 0,5 \text{ and } \texttt{j} = 0,5 \tag{2.153}$$

$$d\boldsymbol{\varepsilon}_{tot} = \left(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{zz}^{(res)}, d\gamma_{yz}, d\gamma_{xz}, d\gamma_{xy} \right) \tag{2.154}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{yz}, df_{xz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{yz}}, \frac{\partial f}{\tau_{xz}}, \frac{\partial f}{\tau_{xy}} \right) \tag{2.155}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[0]}\Delta T + \texttt{beta[0]}\Delta c \\ \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \end{pmatrix} \tag{2.156}$$

This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx},\ d\varepsilon_{yy}^{(p)} = \lambda df_{yy},\ d\varepsilon_{zz}^{(p)} = \lambda df_{zz}, \tag{2.157}$$

$$d\gamma_{yz}^{(p)} = \lambda df_{yz},\ d\gamma_{xz}^{(p)} = \lambda df_{xz},\ d\gamma_{xy}^{(p)} = \lambda df_{xy}, \tag{2.158}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\varepsilon_{zz}^{(e)} = d\varepsilon_{yy} - \lambda df_{zz} \tag{2.159}$$

$$d\gamma_{yz}^{(e)} = d\gamma_{yz} - \lambda df_{yz}, \quad d\gamma_{xz}^{(e)} = d\gamma_{xz} - \lambda df_{xz}, \quad \text{and} \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy} \tag{2.160}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \\ d\tau_{xz} \\ d\tau_{xy} \end{pmatrix} = \left(\texttt{C[i][j]} \quad \text{for } \texttt{i} = 0,5 \text{ and } \texttt{j} = 0,5 \right) \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\varepsilon_{zz}^{(e)} - \varepsilon_{zz}^{(res,r)} \\ d\gamma_{yz}^{(e)} \\ d\gamma_{xz}^{(e)} \\ d\gamma_{xy}^{(e)} \end{pmatrix} \tag{2.161}$$

2.11 More General Plasticity Methods

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

$$0 = \Delta\boldsymbol{\sigma} - \mathsf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_p) = \Delta\boldsymbol{\sigma} - \mathsf{C}d\boldsymbol{\varepsilon} + \lambda \mathsf{C} \nabla f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) \tag{2.162}$$

$$0 = f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) = f\left(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + \sqrt{\frac{3}{2}} \lambda \|\nabla f\| \right) \tag{2.163}$$

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:

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)}-\boldsymbol{x}^{(n)}\right)=-F(\boldsymbol{x}^{(n)}) \tag{2.164}$$

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

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)}-\boldsymbol{x}^{(n)}\right)=\begin{bmatrix} \mathsf{I}+\lambda\mathsf{C}\frac{d\nabla f}{d\Delta\boldsymbol{\sigma}} & \mathsf{C}\nabla f \\ \nabla f & \frac{df}{d\alpha}\frac{d\alpha}{d\lambda}\end{bmatrix}^{(n)}\begin{bmatrix}\delta\boldsymbol{\sigma}^{(n)}\\ \delta\lambda^{(n)}\end{bmatrix}=-\begin{bmatrix}\boldsymbol{p}^{(n)}\\ q^{(n)}\end{bmatrix} \tag{2.165}$$

where

$$\begin{aligned}\boldsymbol{p}^{(n)} &= \Delta\boldsymbol{\sigma}^{(n)}-\mathsf{C}d\boldsymbol{\varepsilon}+\lambda^{(n)}\mathsf{C}\nabla f(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)}) &(2.166)\\ q^{(n)} &= f\left(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)}\right) &(2.167)\\ d\alpha^{(n)} &= \sqrt{\frac{3}{2}}\lambda\left\|\nabla f(\boldsymbol{\sigma}+\Delta\boldsymbol{\sigma}^{(n)},\alpha+d\alpha^{(n)})\right\| &(2.168)\end{aligned}$$

The next iteration for stress and λ are

$$\begin{aligned}\Delta\boldsymbol{\sigma}^{(n+1)} &= \Delta\boldsymbol{\sigma}^{(n)}+\delta\boldsymbol{\sigma}^{(n)} &(2.169)\\ \delta\lambda^{(n+1)} &= \lambda^{(n)}+\delta\lambda^{(n)} &(2.170)\end{aligned}$$

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:

$$\delta\boldsymbol{\sigma}^{(n)}=-\boldsymbol{p}^{(n)}-\delta\lambda^{(n)}\mathsf{C}\nabla f \qquad \text{and} \qquad \delta\lambda^{(n)}=-\frac{q^{(n)}-\nabla f\cdot\boldsymbol{p}^{(n)}}{\nabla f\cdot\mathsf{C}\nabla f-\frac{df}{d\alpha}\frac{d\alpha}{d\lambda}} \tag{2.171}$$

For next increment:

$$\begin{aligned}\boldsymbol{p}^{(n+1)} &= \Delta\boldsymbol{\sigma}^{(n+1)}-\mathsf{C}d\boldsymbol{\varepsilon}+\lambda^{(n+1)}\mathsf{C}\nabla f &(2.172)\\ &= \Delta\boldsymbol{\sigma}^{(n)}-\boldsymbol{p}^{(n)}-\delta\lambda^{(n)}\mathsf{C}\nabla f-\mathsf{C}d\boldsymbol{\varepsilon}+(\lambda^{(n)}+\delta\lambda^{(n)})\mathsf{C}\nabla f &(2.173)\\ &= 0 &(2.174)\end{aligned}$$

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:

$$\Delta\boldsymbol{\sigma}^{(n)}=-\sum_{i=0}^{n}\delta\lambda^{(i)}\mathsf{C}\nabla f=-\lambda^{(n)}\mathsf{C}\nabla f \tag{2.175}$$

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

$$0=f\left(\boldsymbol{\sigma}+\mathsf{C}d\boldsymbol{\varepsilon}-\lambda^{(n)}\mathsf{C}\nabla f,\alpha+d\alpha^{(n)}\right)=f_{trial}-\lambda^{(n)}\left(\nabla f\cdot\mathsf{C}\nabla-\frac{df}{d\alpha}\frac{d\alpha}{d\lambda}\right) \tag{2.176}$$

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

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

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.

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. A recent fix to the code was to 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 track 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 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 $\mathbf{R}_n$:

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

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 a 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 $dT_{dS=0}$ is the temperature change that would occur for an isentropic 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} is temperature increase due to isentropic 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

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

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

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

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 this 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 the 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 required 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 methods. In anisotropic damage mechanics, which are based on small-strain elastic materials, the material's constitutive law is

$$\boldsymbol{\sigma} = (\mathsf{I} - \mathsf{D})\mathsf{C}_0(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{res}) \tag{5.1}$$

where D is an implemented damage tensor, C_0 is undamaged compliance tensor, and ε_{res} is residual stress (such as $\varepsilon_{res} - \boldsymbol{\alpha} dT$ for residual thermal stress. This law is supplement with an initiation criterion, which starts the damage process, and softening laws that control damage evolution.

5.2 Isotropic Softening Material

5.2.1 Damage Initiation

This material evolves as a standard isotropic, small strain material until the stress state reaches some friction condition. Once some critical stress state is reached, damage is initiated and the following sections described subsequent constitutive law modeling. For initiation of failure in an isotropic material, we define tension and shear strengths or mode I and mode II strengths as σ_I and σ_{II}. The damage evolution is controlled by mode I and mode II softening laws, $f_I(\delta_n)$ and $f_I I(\delta_s)$, that define proportional decrease in strength as a function of maximum experienced normal or shear cracking strain.

5.2.2 Post Damage Constitutive Law

This material uses the following damage tensor (which was originally proposed by Chaboche):

$$\mathsf{D} = \begin{bmatrix} d_n & 0 & 0 & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} d_n & 0 & 0 & 0 & 0 & 0 \\ \frac{\nu}{1-\nu} d_n & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{xz} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{xy} \end{bmatrix} \tag{5.2}$$

where d_n, d_{xy}, and d_{xz} are normal and two shear damage parameters. The damage parameters scale effective properties of the damaged, orthotropic material (with crack normal along the x axis) using

$E_{xx} = (1-d_n^*)E$, $\nu_{xz} = \nu_{xy} = (1-d_n^*)\nu$, $G_{xz} = (1-d_{xz})G$, $G_{xy} = (1-d_{xy})G$, and $C_{11} = (1-d_n)C_{0,11}$, where d_n and d_n^* are related by

$$d_n = \frac{d_n^*(1-\nu)}{1-\nu-2(1-d_n^*)\nu^2} \qquad \text{and} \qquad d_n^* = \frac{d_n(1+\nu)(1-2\nu)}{1-\nu-2d_n\nu^2} \tag{5.3}$$

For an elastic update account for residual stress (only thermal stress here, but for others replace $\boldsymbol{\alpha} dT$ to $d\boldsymbol{\varepsilon}_{res}$):

$$\begin{aligned} d\boldsymbol{\sigma} &= (\mathsf{I}-\mathsf{D})\mathsf{C}_0(d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT) && (5.4)\\ \mathsf{S}_0(\mathsf{I}-\mathsf{D})^{-1}d\boldsymbol{\sigma} &= d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT && (5.5)\\ \left(\mathsf{S}_0+\mathsf{S}_0(\mathsf{I}-\mathsf{D})^{-1}\mathsf{D}\right)d\boldsymbol{\sigma} &= d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT = d\boldsymbol{\varepsilon}_e-\boldsymbol{\alpha}dT+d\boldsymbol{\varepsilon}_c && (5.6)\\ d\boldsymbol{\varepsilon}_e-\boldsymbol{\alpha}dT &= \mathsf{S}_0 d\boldsymbol{\sigma} = (\mathsf{I}-\mathsf{S}_0\mathsf{D}\mathsf{C}_0)(d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT) = (\mathsf{I}-\mathsf{D}^T)(d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT) && (5.7)\\ d\boldsymbol{\varepsilon}_c &= d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT-(d\boldsymbol{\varepsilon}_e-\boldsymbol{\alpha}dT) = \mathsf{D}^T(d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT) && (5.8) \end{aligned}$$

The simplification to D^T follows because $\mathsf{S}_0\mathsf{D}$ is diagonal. By virtue of D^T, it is clear that $d\boldsymbol{\varepsilon}_c$ involves only xx, xz, and yz strains that physically correspond to crack opening displacement. It is also clear that input $d\boldsymbol{\varepsilon}$ can be replaced by $d\boldsymbol{\varepsilon}-\boldsymbol{\alpha}dT$; in other words, residual stresses are handled by doing calculations with effective strains.

For the update during damage loading, we start with

$$d\boldsymbol{\sigma} = \mathsf{C}_0 d\boldsymbol{\varepsilon}^* - d(\mathsf{D}\mathsf{C}_0\boldsymbol{\varepsilon}^*) = \mathsf{C}_0\left(\mathsf{I}-\mathsf{S}_0\frac{d(\mathsf{D}\mathsf{C}_0\boldsymbol{\varepsilon}^*)}{d\boldsymbol{\varepsilon}^*}\right)d\boldsymbol{\varepsilon}^* = \mathsf{C}_0(\mathsf{I}-\Delta)d\boldsymbol{\varepsilon}^* \tag{5.9}$$

where $\Delta = \mathsf{S}_0 d(\mathsf{D}\mathsf{C}_0\boldsymbol{\varepsilon}^*)/d\boldsymbol{\varepsilon}^*$ is the fourth-rank damage-strain partitioning tensor and $\boldsymbol{\varepsilon}^*$ is effective strain after subtracting residual strain. To track damage evolution, we partition the input strain into increments in elastic ($d\boldsymbol{\varepsilon}_e^*$) and cracking ($d\boldsymbol{\varepsilon}_c$) strain in the crack axis system where $d\boldsymbol{\varepsilon}^* = d\boldsymbol{\varepsilon}_e^* + d\boldsymbol{\varepsilon}_c$. Because the elastic strain is derived from undamaged properties, the strain partitioning reduces to:

$$d\boldsymbol{\varepsilon}_e^* = \mathsf{S}_0 d\sigma = (\mathsf{I}-\Delta)d\boldsymbol{\varepsilon}^* \qquad \text{and} \qquad d\boldsymbol{\varepsilon}_c = d\boldsymbol{\varepsilon}^* - d\boldsymbol{\varepsilon}_e = \Delta d\boldsymbol{\varepsilon}^* \tag{5.10}$$

Thus Δ relates the increment in cracking strain caused by an increment in global strain.

For an isotropic material and Chaboche form for D , we find Δ by first expanding:

$$\mathsf{D}\mathsf{C}_0\boldsymbol{\varepsilon}^* = \left(C_{0,11}d_n\varepsilon_n, \frac{C_{0,11}\nu}{1-\nu}d_n\varepsilon_n, \frac{C_{0,11}\nu}{1-\nu}d_n\varepsilon_n, 0, G_0 d_{xz}\gamma_{xz}, G_0 d_{xy}\gamma_{xy}\right) \tag{5.11}$$

where

$$\varepsilon_n = \varepsilon_{xx}^* + \frac{\nu}{1-\nu}\left(\varepsilon_{yy}^* + \varepsilon_{zz}^*\right) \tag{5.12}$$

is an effective normal strain on the crack. The full tensor evaluates to

$$\Delta = \begin{bmatrix} \frac{\partial(d_n\varepsilon_n)}{\partial\varepsilon_{xx}^*} & \frac{\partial(d_n\varepsilon_n)}{\partial\varepsilon_{yy}^*} & \frac{\partial(d_n\varepsilon_n)}{\partial\varepsilon_{zz}^*} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial(d_{xz}\gamma_{xz})}{\partial\gamma_{xz}} & \frac{\partial(d_{xz}\gamma_{xz})}{\partial\gamma_{xy}} \\ 0 & 0 & 0 & 0 & \frac{\partial(d_{yz}\gamma_{xy})}{\partial\gamma_{xz}} & \frac{\partial(d_{yz}\gamma_{xy})}{\partial\gamma_{xy}} \end{bmatrix} \tag{5.13}$$

Note that Δ describes anisotropic change in cracking strain and these elements apply to the crack axis system where the crack normal, $\hat{n} = (1,0,0)$ is in the x direction. The only assumptions in deriving Δ are that $\partial d_n/\partial \gamma_{ij} = \partial d_{xz}/\partial \varepsilon^*_{ii} = \partial d_{xy}/\partial \varepsilon^*_{ii} = 0$ (ii is component of normal strain and does not mean normal strains summed), which implies that crack sliding (caused by $d\gamma_{xz}$ of $d\gamma_{xy}$) changes only d_{xz} and d_{xy} and crack opening (caused by $d\varepsilon^*_{ii}$) changes only d_n. Physically, this response corresponds to the usual decoupling of mode I, mode II, and mode III fracture mechanisms. Finally, Δ is used to show that the only cracking strain increments (as full differentials) in the crack axis system are:

$$d\varepsilon_{c,xx} = d(d_n\varepsilon_n), \quad \gamma_{c,xz} = d(d_{xz}\gamma_{xz}), \quad \text{and} \quad d\gamma_{c,xy} = d(d_{xy}\gamma_{xy}) \tag{5.14}$$

Notice that this update reduces to the elastic case when the damage parameters are constant (*i.e.*, $\Delta \to \mathsf{D}^T$ for constants d's).

Normal Damage Evolution

During damage loading, the change in traction must compared to current allowed traction (which depends on extent of damage). The traction update during damage loading is:

$$d\boldsymbol{T} = d\sigma \cdot \hat{n} = \mathsf{C}_0(\mathsf{I}-\Delta)d\varepsilon^* \cdot \hat{n} = (d\sigma_{xx}, d\tau_{xy}, d\tau_{xz}) \tag{5.15}$$

where $\hat{n} = (1,0,0)$ is vector normal to the crack surface. The stress component updates are

$$\begin{pmatrix} d\sigma_{xx} \\ d\tau_{xy} \\ d\tau_{xz} \end{pmatrix} = \begin{pmatrix} C_{0,11}\left(d\varepsilon_n - d(d_n\varepsilon_n)\right) \\ G\left(d\gamma_{xy} - d\left(d_t\gamma_{xy}\right)\right) \\ G\left(d\gamma_{xz} - d\left(d_t\gamma_{xz}\right)\right) \end{pmatrix} \tag{5.16}$$

Defining the normal strain from total strain as $\varepsilon_n = \varepsilon^*_{xx} + \frac{\nu}{1-\nu}\left(\varepsilon^*_{yy} + \varepsilon^*_{zz}\right)$, the magnitude of the normal traction update (*i.e.*, mode I traction) is:

$$dT_n = C_{0,11}\left[d\varepsilon_n - d\left(d_n\varepsilon_n\right)\right] = \sigma_I f_I'(\delta_n)d\delta_n \tag{5.17}$$

where $\delta_n = \max(\varepsilon_{c,xx})$, and $\varepsilon_{c,xx}$ is the cracking strain normal to the crack surface. From the Δ matrix and assumming initial traction, T_n, was equal to current strength, $(\sigma_I f_I(\delta_n))$, the updates of these variables are $d\delta_n = d\varepsilon_{c,xx} = d\left(d_n\varepsilon_n\right)$. In other words, all the cracking strain goes into increasing δ_n. Therefore

$$\frac{d\varepsilon_n}{d\delta_n} = 1 + \varepsilon_{n0}f_I'(\delta_n) \qquad \text{or} \qquad \varepsilon_n = \delta_n + \varepsilon_{n0}f_I(\delta_n) \tag{5.18}$$

where $\varepsilon_{n0} = \sigma_I/C_{0,11}$ is the initiation normal strain. At initiation of failure, $\delta_n = 0$, $f_I(0) = 1$, and $\varepsilon_n = \varepsilon_{n0}$. At failure, $\delta_n = \delta_{max}$, $f_I(0) = 0$, $\varepsilon_n = \delta_n = \delta_{max}$, and the crack traction is zero. During monotonic damage propagation, the traction remains equal to the softening law and is given by:

$$T_n = (1-d_n)C_{0,11}\varepsilon_n = \sigma_I f_I(\delta_n) \tag{5.19}$$

The damage variable is

$$d_n = 1 - \frac{\varepsilon_{n0}}{\varepsilon_n}f_I(\delta_n) = 1 - \frac{\varepsilon_{n0}f_I(\delta_n)}{\delta_n + \varepsilon_{n0}f_I(\delta_n)} = \frac{\delta_n}{\delta_n + \varepsilon_{n0}f_I(\delta_n)} \tag{5.20}$$

The version with ε_n holds only during damage propagation, but the second holds always by using the current value of δ_n. When tracking energy dissipation, a differential of the damage variable is needed:

$$\frac{dd_n}{d\varepsilon_n} = \frac{\varepsilon_{n0}}{\varepsilon_n^2}f_I(\delta_n) - \frac{\varepsilon_{n0}}{\varepsilon_n}f_I'(\delta_n)\frac{d\delta_n}{d\varepsilon_n} = \frac{\varepsilon_{n0}}{\varepsilon_n^2}\left(f_I(\delta_n) - \frac{\varepsilon_n f_I'(\delta_n)}{1+\varepsilon_{n0}f_I'(\delta_n)}\right) \tag{5.21}$$

We also have $d\delta_n = d(d_n\varepsilon_n) = d_n d\varepsilon_n = \varepsilon_n dd_n$ to get

$$dd_n = \frac{1}{\varepsilon_n}(d\delta_n - d_n d\varepsilon_n) = \frac{1}{\varepsilon_n}\left(\frac{d\delta_n}{d\varepsilon_n} - d_n\right)d\varepsilon_n \tag{5.22}$$

and

$$\frac{dd_n}{d\varepsilon_n} = \frac{1}{\varepsilon_n}\left(\frac{1}{1+\varepsilon_{n0}f_I'(\delta_n)} - 1 + \frac{\varepsilon_{n0}}{\varepsilon_n}f_I(\delta_n)\right) = \frac{1}{\varepsilon_n}\left(\frac{\varepsilon_{n0}}{\varepsilon_n}f_I(\delta_n) - \frac{\varepsilon_{n0}f_I'(\delta_n)}{1+\varepsilon_{n0}f_I'(\delta_n)}\right) \tag{5.23}$$

which is same results as before.

— Alternate View Using a Differential Equation

Rearranging Eq. (5.22) gives a differential equation:

$$\frac{dd_n}{d\varepsilon_n} + \frac{d_n}{\varepsilon_n} = \frac{1}{\varepsilon_n}\frac{d\delta_n}{d\varepsilon_n} \tag{5.24}$$

$$p(\varepsilon_n) = \frac{1}{\varepsilon_n}, \quad \int \frac{d\varepsilon_n}{\varepsilon_n} = \ln\varepsilon_n, \quad e^{\int p(\varepsilon_n)\varepsilon_n} = \varepsilon_n \tag{5.25}$$

$$d_n = \frac{1}{\varepsilon_n}\left(\int \varepsilon_n \frac{1}{\varepsilon_n}\frac{d\delta_n}{d\varepsilon_n}d\varepsilon_n + (\text{const})\right) \tag{5.26}$$

$$d_n = \frac{1}{\varepsilon_n}(\delta_n + (\text{const})) = \frac{\delta_n}{\varepsilon_n} \tag{5.27}$$

The constant is zero because $d_n = 0$ when $\delta_n = 0$.

— Linear Softening

The above analysis shows that damage evolution can be tracked using either d_n or δ_n. The traditional approach in the literature is to track d_n. This parameter goes from 0 to 1 and directly describes evolving elastic properties. In contrast, δ_n from from 0 to δ_{max} and it decribes crack opening displacement and more directly related to energy dissipation. These two parameters are relative by Eq. (5.20). For general softening law, this equation requires numerical inversion of the softening law. But for linear softening law ($f_I(\delta_n) = 1 - \delta_n/\delta_{max}$), some analytical relations are possible:

$$d_n = \frac{\delta_n}{\delta_n + \varepsilon_{n0}\left(1 - \frac{\delta_n}{\delta_{max}}\right)} \quad \text{and} \quad \delta_n = \frac{\delta_{max}d_n\varepsilon_{n0}}{\delta_{max}(1-d_n) + d_n\varepsilon_{n0}} \tag{5.28}$$

For example, linear softening in terms of crack strain translates to nonlinear softening as a function of d_n:

$$f_I(d_n) = \frac{\delta_{max}(1-d_n)}{\delta_{max}(1-d_n) + d_n\varepsilon_{n0}} \tag{5.29}$$

$$\frac{d\delta_n}{d\varepsilon_n} = \frac{\delta_{max}\varepsilon_{n0}(\delta_{max}(1-d_n) + d_n\varepsilon_{n0}) - \delta_{max}d_n\varepsilon_{n0}(-\delta_{max} + \varepsilon_{n0})}{(\delta_{max}(1-d_n) + d_n\varepsilon_{n0})^2}\frac{dd_n}{d\varepsilon_n} \tag{5.30}$$

$$= \frac{\delta_{max}^2\varepsilon_{n0}}{(\delta_{max}(1-d_n) + d_n\varepsilon_{n0})^2}\frac{dd_n}{d\varepsilon_n} \tag{5.31}$$

$$= \frac{\varepsilon_{n0}}{\left(1 - d_n + \frac{d_n\varepsilon_{n0}}{\delta_{max}}\right)^2}\frac{dd_n}{d\varepsilon_n} \tag{5.32}$$

which translates to

$$\frac{dd_n}{d\varepsilon_n} + \frac{d_n}{\varepsilon_n} = \frac{\frac{\varepsilon_{n0}}{\varepsilon_n}}{\left(1 - d_n + \frac{d_n \varepsilon_{n0}}{\delta_{max}}\right)^2} \frac{dd_n}{d\varepsilon_n} \tag{5.33}$$

$$\frac{dd_n}{d\varepsilon_n} = \frac{d_n (\delta_{max}(1-d_n) + d_n \varepsilon_{n0})^2}{\varepsilon_{n0}\delta_{max}^2 - \varepsilon_n (\delta_{max}(1-d_n) + d_n \varepsilon_{n0})^2} \tag{5.34}$$

Update Shear Damage

— Shear Damage 2D

In 2D, the only shear damage is d_{xy} and shear damage updates by equations essentially the same as for normal damage update. In other words, during damage evolution (*i.e.*, for step when initial shear traction was equal to previous shear strength), the 2D shear cracking strain and damage variables are

$$\gamma_{xy} = \delta_{xy} + \gamma_{t0} f_{II}(\delta_{xy}) \tag{5.35}$$

and

$$d_{xy} = 1 - \frac{\gamma_{t0}}{\gamma_{xy}} f_{II}(\delta_{xy}) = 1 - \frac{\gamma_{t0} f_{II}(\delta_{xy})}{\delta_{xy} + \gamma_{t0} f_{II}(\delta_{xy})} = \frac{\delta_{xy}}{\delta_{xy} + \gamma_{t0} f_{II}(\delta_{xy})} \tag{5.36}$$

where $\gamma_{t0} = \sigma_{II}/G$ is the initiation tangential strain. For energy dissipation, the damage variable differential is

$$\frac{dd_{xy}}{d\gamma_{xy}} = \frac{\gamma_{t0}}{\gamma_{xy}^2} \left(f_{II}(\delta_{xy}) - \frac{\gamma_{xy} f'_{II}(\delta_{xy})}{1 + \gamma_{t0} f'_{II}(\delta_t)} \right) \tag{5.37}$$

— Shear Damage 3D

To update shear traction in 3D, we need a failure surface to couple to two shear directions perpendicular to the crack that describes maximum allowed tangential shear. The simplest model is to decoupled shear where shear stress in each direction is kept less than or equal to current shear strength in that direction. This failure surface is shown in Fig. 5.1. Point a is the initial stress, which is assumed to start on the current failure surface. Point b is the updated trial stress given by

$$\left(\tau_{xy}^{trial}, \tau_{xz}^{trial}\right) = \left(G_{xy}(1-d_{xy})(\gamma_{xy} + d\gamma_{xy}), G_{xz}(1-d_{xz})(\gamma_{xz} + d\gamma_{xz})\right) \tag{5.38}$$

$$= \left(\tau_{xy}^{(0)} + G_{xy}(1-d_{xy})d\gamma_{xy}, \tau_{xz}^{(0)} + G_{xz}(1-d_{xz})d\gamma_{xz}\right) \tag{5.39}$$

To anticipate future needs in aniostropic materials, G_{xy} and G_{xz} are initial shear moduli of an orthotropic material; for isotropic materials, they are both equal to G. Point c is the final state after damage evolution and falls on the new shifted failure surface. Because only τ_{xy} exceeds material's shear strength, the final point is:

$$\left(\tau_{xy}^{(0)} + G_{xy}(d\gamma_{xy} - d\delta_{xy}), \tau_{xz}^{trial}\right) = \left(\tau_0^{xy}\left(f_{xy}(\delta_{xy}) + (f'_{xy}(\delta_{xy})d\delta_{xy}\right), \tau_{xz}^{trial}\right) \tag{5.40}$$

where during damage evolution, $d\delta_{xy} = d_{xy}d\gamma_{xy} + \gamma_{xy}dd_{xy}$, $\tau_{xy}^{(0)} = G_{xy}(1-d_{xy})\gamma_{xy}$, and $f_{xy}(\delta)$ is softening law for G_{xy} (and equal to $f_{II}(\delta_{xy})$ for isotropic). Because we started on the failure surface where $\tau_{xy}^{(0)} = \tau_0^{xy} f_{xy}(\delta_{xy})$ with τ_0^{xy} shear strength in xy plane (or τ_0 for isotropic), the final equation is analogous to the normal damage update

$$\frac{d\gamma_{xy}}{d\delta_{xy}} = 1 + \gamma_{xy0} f'_{II}(\delta_{xy}) \tag{5.41}$$

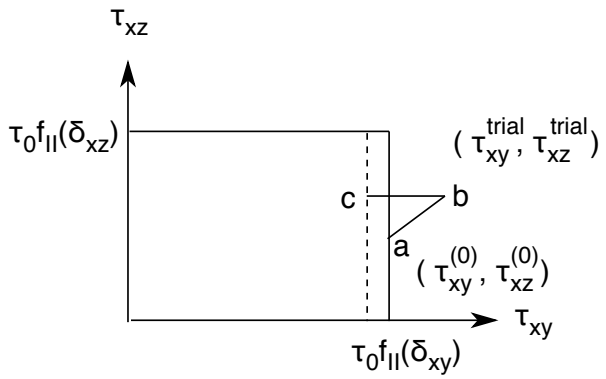

Figure 5.1: Decoupled shear. Point a is previous stress state on the surface. Point b is trial elastic update. Point c is final updated stress state.

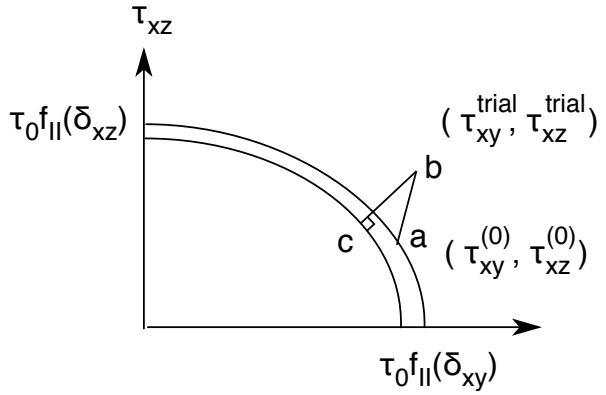

Figure 5.2: Decoupled shear. Point a is previous stress state on the surface. Point b is trial elastic update. Point c is final updated stress state.

where $\gamma_{xy0} = \tau_0^{xy}/G_{xy}$. All needed equations are given in previous section for 2D shear damage. If τ_{xz}^{trial} exceeds its strength (or $\tau_0^{xz} f_{xz}(\delta_{xz})$), it is returned to the surface by similar equation. A decoupled failure surface thus treats the two shear components independently.

— Shear Damage 3D Using Coupled Failure Surface

Decoupled shear, however, could lead to a $\left(\tau_{xy}, \tau_{xz}\right)$ stress state where maximum shear stress exceeds the shear strength of the material. It might be preferrable to couple shear deformation through a shear failure surface as shown in Fig. 5.2. Point's a and b are the same as in the decoupled case, but now point c will need to change damage in both direction (in general). Point c becomes:

$$\left(\tau_{xy}^{(0)} + G_{xy}(d\gamma_{xy} - d\delta_{xy}), \tau_{xz}^{(0)} + G_{xz}(d\gamma_{xz} - d\delta_{xz})\right) \tag{5.42}$$

It should fall on the failure surface, and by comparison to decoupled case, it probably should lie on the surface by returning from trial state along normal to the surface. The approach is like plasticity theory, but also describes the closest point on the new failure surface to the trial stress state, or, more physcially, the new point that minimizes the amount of dissipated energy.

We assume the shear failure surface is an ellipse (and therefore in the undamaged state, maximum shear stress in any direction causes failure when it exceeds shear strength of the material). Point c is

thus determined by solving damage evolution (assuming both directions are damaging) such that

$$\left(\frac{\tau_{xy}^{(0)}+G_{xy}(d\gamma_{xy}-d\delta_{xy})}{\tau_0^{xy}f_{xy}(\delta_{xy}+d\delta_{xy})}\right)^2+\left(\frac{\tau_{xz}^{(0)}+G_{xz}(d\gamma_{xz}-d\delta_{xz})}{\tau_0^{xy}f_{xz}(\delta_{xz}+d\delta_{xz})}\right)^2=1 \tag{5.43}$$

This single equation has two unknowns. If we require the return path to be along surface normal, then the vector from point c to b is:

$$\big(G_{xy}\gamma_{xy}dd_{xy},G_{xz}\gamma_{xz}dd_{xz}\big)=\big(G_{xy}\big(d\delta_{xy}-d_{xy}d\gamma_{xy}\big),G_{xz}\big(d\delta_{xz}-d_{xz}d\gamma_{xz}\big)\big) \tag{5.44}$$

which assumes point a was on the failure surface such that all new cracking strain contributes to increases in δ_{xy} and δ_{xz}. This vector should be parallel to normal vector on the new failure surface, which is

$$\hat{\boldsymbol{n}}\|\hat{\boldsymbol{n}}\|=\left(\frac{\tau_{xy}^{(0)}+G_{xy}(d\gamma_{xy}-d\delta_{xy})}{\big(\tau_0^{xy}f_{xy}(\delta_{xy}+d\delta_{xy})\big)^2},\frac{\tau_{xz}^{(0)}+G_{xz}(d\gamma_{xz}-d\delta_{xz})}{\big(\tau_0^{xz}f_{xz}(\delta_{xz}+d\delta_{xz})\big)^2}\right) \tag{5.45}$$

For a second equation, take dot product of vector perpendicular to vector from c to b with $\hat{\boldsymbol{n}}\|\hat{\boldsymbol{n}}\|$ to get

$$\frac{\left(\frac{\tau_{xy}^{(0)}}{G_{xy}}+(d\gamma_{xy}-d\delta_{xy})\right)(d_{xz}d\gamma_{xz}-d\delta_{xz})}{\big(\tau_n^{xy}f_{xy}(\delta_{xy}+d\delta_{xy})\big)^2}-\frac{\left(\frac{\tau_{xz}^{(0)}}{G_{xz}}+(d\gamma_{xz}-d\delta_{xz})\right)(d_{xy}d\gamma_{xy}-d\delta_{xy})}{\big(\tau_n^{xz}f_{xz}(\delta_{xz}+d\delta_{xz})\big)^2}=0 \tag{5.46}$$

For scaling of the two equations, it is best to keep $G_{xy}G_{xz}$ in both terms, which is done be defining the normalized stresses:

$$\tau_n^{xy}=\frac{\tau_0^{xy}}{\sqrt{G_{xy}G_{xz}}}\qquad\text{and}\qquad\tau_n^{xz}=\frac{\tau_0^{xz}}{\sqrt{G_{xy}G_{xz}}} \tag{5.47}$$

— One Axis Shear Damage

If $d\gamma_{xy}<0$ or $d\gamma_{xz}<0$, that direction should not damage so we accept its trial update. For this "uniaxial" case we return along the one direction that does damage. For example, assume $d\gamma_{xz}<0$, then we seek to find

$$\left(\frac{\tau_{xy}^{(0)}+G_{xy}(d\gamma_{xy}-d\delta_{xy})}{\tau_0^{xy}f_{xy}(\delta_{xy}+d\delta_{xy})}\right)^2+\left(\frac{\tau_{xz}^{(trial)}}{\tau_0^{xy}f_{xz}(\delta_{xz})}\right)^2=1 \tag{5.48}$$

This equation can be solved by Newton's method or analytically for linear softening.

5.2.3 Energy Dissipation

The damage energy dissipation rate is

$$d\Omega=\sigma\cdot d\varepsilon-d\Psi\qquad\text{where}\quad\Psi=\frac{1}{2}(\mathsf{I}-\mathsf{D})\mathsf{C}_0\varepsilon\cdot\varepsilon \tag{5.49}$$

is the stored elastic energy (note: papers call it Helmholz, but that would need $-ST$ as well and would need to account for heat caused by energy dissipation). The result is

$$d\Omega=\frac{1}{2}\big(d\mathsf{D}\mathsf{C}_0\big)\varepsilon\cdot\varepsilon \tag{5.50}$$

Evaluating $\left(d\mathrm{DC}_0\right)$ leads to

$$d\Omega = \frac{1}{2}\begin{bmatrix} C_{0,11}\varepsilon_n\, dd_n \\ C_{0,11}\frac{\nu}{1-\nu}\varepsilon_n\, dd_n \\ C_{0,11}\frac{\nu}{1-\nu}\varepsilon_n\, dd_n \\ 0 \\ G\gamma_{xz}\, dd_{xz} \\ G\gamma_{xy}\, dd_{xy} \end{bmatrix} \cdot \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{bmatrix} = \frac{1}{2}C_{0,11}\varepsilon_n^2 dd_n + \frac{1}{2}G\gamma_{xz}^2 dd_{xz} + \frac{1}{2}G\gamma_{xy}^2 dd_{xy} \tag{5.51}$$

The result should be equivalent to:

$$d\Omega = \boldsymbol{\sigma}\cdot d\boldsymbol{\delta} \tag{5.52}$$

which is based on my notes for irreversible thermodynamics in elastic-damage (or plastic) materials. But unlike for plastic materials, where is strain increment is any plastic strain, here it must only be cracking strain that is causing damage (*i.e.*, $d\boldsymbol{\delta} = (d\delta_n, 0, 0, 0, d\delta_{xz}, d\delta_{yz})$).

During damage loading, the energy dissipation reduces to

$$\begin{aligned} d\Omega &= \frac{\sigma_I}{2}\left(f_I(\delta) - \frac{\varepsilon_n f_I'(\delta)}{1+\varepsilon_{n0}f_I'(\delta)}\right)d\varepsilon_n + \frac{\sigma_{II}}{2}\left[\left(\frac{d\delta_{xz}}{d\gamma_{xz}} - d_{xz}\right)d\gamma_{xz} + \left(\frac{d\delta_{xy}}{d\gamma_{xy}} - d_{xy}\right)d\gamma_{xy}\right] && (5.53)\\ &= \frac{d\overline{G}_I}{d\varepsilon_n}d\varepsilon_n + \frac{d\overline{G}_{II,1}}{d\gamma_{xy}}d\gamma_{xy} + \frac{d\overline{G}_{II,2}}{d\gamma_{xz}}d\gamma_{xz} && (5.54)\end{aligned}$$

where $\overline{G}_I$ and $\overline{G}_{II}$ are the mode I and mode II dissipation energies per unit volume. The total mode I energy density dissipated up to current crack opening strain (and similar for mode II) is

$$\overline{G}_I = \frac{\sigma_I}{2}\int_{\varepsilon_{n0}}^{\varepsilon_n}\left(f_I(\delta) - \varepsilon_n f_I'(\delta)\frac{d\delta}{d\varepsilon_n}\right)d\varepsilon_n \tag{5.55}$$

Integrating the second term by parts gives

$$\begin{aligned} \overline{G}_I &= \sigma_I\int_{\varepsilon_{n0}}^{\varepsilon_n} f_I(\delta)d\varepsilon_n - \frac{\sigma_I}{2}\varepsilon_n f_I(\delta)|_{\varepsilon_{n0}}^{\varepsilon_n} && (5.56)\\ &= \sigma_I\int_{\varepsilon_{n0}}^{\varepsilon_n} f_I(\delta)d\varepsilon_n + \frac{\sigma_I\varepsilon_{n0}}{2} - \frac{\sigma_I\varepsilon_n f_I(\delta_n)}{2} && (5.57)\end{aligned}$$

The initial limit is ε_{n0} because the dissipated energy only occurs during damage loading. Converting to

integral over δ gives

$$\begin{aligned}
\overline{G}_I &= \sigma_I \int_0^{\delta_n} f_I(\delta)(1+\varepsilon_{n0} f_I'(\delta))d\delta + \frac{\sigma_I \varepsilon_{n0}}{2} - \frac{\sigma_I \varepsilon_n f_I(\delta_n)}{2} && (5.58)\\
&= \sigma_I \int_0^{\delta_n} f_I(\delta)d\delta + \sigma_I \varepsilon_{n0} \int_0^{\delta_n} f_I(\delta) f_I'(\delta)d\delta + \frac{\sigma_I \varepsilon_{n0}}{2} - \frac{\sigma_I \varepsilon_n f_I(\delta_n)}{2} && (5.59)\\
&= \sigma_I \int_0^{\delta_n} f_I(\delta)d\delta + \frac{\sigma_I \varepsilon_{n0}}{2} f_I(\delta)^2 |_0^{\delta_n} + \frac{\sigma_I \varepsilon_{n0}}{2} - \frac{\sigma_I \varepsilon_n f_I(\delta_n)}{2} && (5.60)\\
&= \sigma_I \int_0^{\delta_n} f_I(\delta)d\delta - \frac{\sigma_I \varepsilon_n f_I(\delta_n)}{2}\left(1 - \frac{\varepsilon_{n0}}{\varepsilon_n} f_I(\delta_n)\right) && (5.61)\\
&= \sigma_I \int_0^{\delta_n} f_I(\delta)d\delta - \frac{d_n \varepsilon_n \sigma_I f_I(\delta_n)}{2} && (5.62)\\
&= \sigma_I \left(\int_0^{\delta_n} f_I(\delta)d\delta - \frac{\delta_n f_I(\delta_n)}{2} \right) && (5.63)
\end{aligned}$$

The second term is energy released on unloading elastically from $\sigma_I f_I(\delta_n)$ to zero load over total cracking strain of δ_n. At failure, $f_I(\delta_n) = 0$ leading to the expected result for total energy released up to failure of:

$$\overline{G}_I = \sigma_I \int_0^{\delta_{max}} f_I(\delta)d\delta \qquad \text{and} \qquad \overline{G}_{II} = \sigma_{II} \int_0^{\delta_{max}} f_{II}(\delta)d\delta \tag{5.64}$$

This result ties total dissipated energy to area under the softening laws. During calculations, the current released energy density can come from the integrals or can be found incrementally with above relations.

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

$$G_{Ic} = \frac{V_p \rho \overline{\sigma}_I}{A_c} \int_0^{\delta_{max}} f_I(\delta)d\delta \tag{5.65}$$

where $\overline{\sigma}_I$ is a specific stress. Given toughness, V_p, and A_c, this equation can be solved to find the appropriate δ_{max}. For example, in linear softening:

$$G_{Ic} = \frac{V_p \rho \overline{\sigma}_I}{A_c} \frac{1}{2} \delta_{max} \qquad \text{or} \qquad \delta_{max} = 2G_{Ic} \frac{A_c}{V_p \rho \overline{\sigma}_I} \tag{5.66}$$

5.2.4 Failure and Post Failure

For mixed mode failure criterion using $\overline{G}_I$ and $\overline{G}_{II}$, which are released energy per unit volume (from previous section; that are not energy release rates, but the ratio is equal to ratio of energy release rates), a standard elliptical failure criterion is

$$\left(\frac{\overline{G}_I}{\overline{G}_{Ic}}\right)^m + \left(\frac{\overline{G}_{II}}{\overline{G}_{IIc}}\right)^n = 1 \tag{5.67}$$

Failure may also be induced by d_n or d_t reaching 1. When it fails, set $d_n = d_t = 1$, $\delta_n = \delta_{n,max}$, $\delta_t = \delta_{s,max}$, and $\sigma_{xx} = \tau_{xz} = \tau_{xy} = 0$ (but cracking strains are unchanged).

In post-failure updates, the normal stress is zero if not in contact, but my be negative if in compression. The stress update in the normal direction is

$$d\sigma_{xx} = C_{0,11}\left(d\varepsilon_n - d\varepsilon_{c,xx}\right) \tag{5.68}$$

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

$$d\varepsilon_{c,xx} = \begin{cases} d\varepsilon_n & \text{if } \varepsilon_{c,xx} > 0 \\ \max(d\varepsilon_n + \frac{\sigma_{xx}}{C_{0,11}}, 0) & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.69}$$

$$d\sigma_{xx} = \begin{cases} -\sigma_{xx} & \text{if } \varepsilon_{c,xx} > 0 \\ \min\left(-\sigma_{xx}, C_{0,11} d\varepsilon_n\right) & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.70}$$

The first case in each if 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

$$d\varepsilon_{c,xx} = \begin{cases} \max(d\varepsilon_n, -\varepsilon_{c,xx}) & \text{if } \varepsilon_{c,xx} > 0 \\ 0 & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.71}$$

$$d\sigma_{xx} = \begin{cases} -\sigma_{xx} \text{ or } C_{0,11}\left(d\varepsilon_n + \varepsilon_{c,xx}\right) & \text{if } \varepsilon_{c,xx} > 0 \\ C_{0,11} d\varepsilon_n & \text{if } \varepsilon_{c,xx} = 0 \end{cases} \tag{5.72}$$

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. The updates are always Subsequent updates can use elastic methods with zero stress increment in the crack plane stresses, but the cracking strains still update:

$$d\gamma_{c,xy} = d\gamma_{xy},\ d\gamma_{c,xz} = d\gamma_{xz},\ d\tau_{xy} - \tau_{xy},\ \text{and} d\tau_{xz} - \tau_{xz} \tag{5.73}$$

These update assume frictionless contact. It might be possible to model friction as well by comparing stick shear stress to friction stresses based on contact nomral stress.

5.2.5 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 particle start as undamaged, but they could alternatively be marked as damaged of failure. The followin steps depend on particle state.

1. From input ∇u, find $d\varepsilon$ in the initial configuration (using large rotation methods in chapter 3). In the process, find R_{n-1} and R_{tot} as rotation matrices to $(n-1)^{th}$ and n^{th} configurations and $d\mathsf{R} = \mathsf{R}_{tot}\mathsf{R}_{n-1}^T$ as the incremental rotation.

2. If the particle is undamaged, find trial stress update in the initial axes using

$$\boldsymbol{\sigma}^{(trial)} = \mathsf{R}_{n-1}^T \boldsymbol{\sigma}_{n-1}^{(p)} \mathsf{R}_{n-1} + \mathsf{C} d\boldsymbol{\varepsilon}_0 \tag{5.74}$$

   If failure criterion has not been reached, finish update by standard methods for a never-damaged, isotropic material material.

3. If the failure surface has been reached, mark the particle as "damaged," calculate (and store) rotation matrix, $\mathsf{R}_c^{(p)}$, as rotation from crack axis system where crack normal is along the x axis, to initial axes and calculate (and store) V_p/A_c. Note that A_c is intersection between the particle and a plane through the particle center with the determined crack normal. Proceed to update methods for a "damaged" particle.

4. For "damaged" and "failed" particles, update $\mathsf{R}_{tot} = \mathsf{R}_{tot}\mathsf{R}_c^{(p)}$ and $\mathsf{R}_{n-1} = \mathsf{R}_{n-1}\mathsf{R}_c^{(p)}$ to matrices that rotate from crack axis system to $(n-1)^{th}$ and n^{th} configurations. Next $d\boldsymbol{\varepsilon}$ and previous particle stress to the crack axis system:

$$d\boldsymbol{\varepsilon} = \mathsf{R}_c^{(p)^T} d\boldsymbol{\varepsilon} \mathsf{R}_c^{(p)} \quad \text{and} \quad \boldsymbol{\sigma}^{(0)} = \mathsf{R}_{n-1}^T \boldsymbol{\sigma}_{n-1}^{(p)} \mathsf{R}_{n-1} \tag{5.75}$$

5. Find strain increments

$$d\varepsilon_n = d\varepsilon_{xx}^* + \frac{\nu}{1-\nu}\left(\varepsilon_{yy}^* + \varepsilon_{zz}^*\right), \quad d\gamma_{xy} = d\varepsilon_{xy} + d\varepsilon_{yx}, \quad \text{and} \quad d\gamma_{xz} = d\varepsilon_{xz} + d\varepsilon_{zx} \tag{5.76}$$

6. First, if $d\varepsilon_n < 0$, the particle is unloading, set $d\varepsilon_{c,xx} = d_n d\varepsilon_n$ and proceed to final update for normal stresses. But, if $d\varepsilon_n > 0$, the update has to be checked if it is elastic or if it is propagating damage. A trial crack normal stress update assumes elastic loading such that $d\varepsilon_{c,xx}^{(trial)} = d_n d\varepsilon_n$, $d\sigma_{xx}^{(trial)} = C_{0,11}(1-d_n)d\varepsilon_n$, and $T_n^{(trial)} = \sigma_{xx} + d\sigma_{xx}^{(trial)}$. If $T_n^{(trial)} < \sigma_I f_I(\delta_n)$, then the update is elastic. Set $d\varepsilon_{c,xx} = d\varepsilon_{c,xx}^{(trial)}$ to update cracking strain, make no change to δ_n or d_n, and proceed to final update for normal stresses. But, this change cannot let $\varepsilon_{c,xx}$ become negative. If it does, change $d\varepsilon_{c,xx}$ to $-\varepsilon_{c,xx}$ to end up with zero crack opening strain after the update.

   If the trial update exceeds the current normal strength, then partition the step into two increments. The first normal increment brings the stress to the current traction while the second propagates with damage:

$$d\varepsilon_n^{(1)} = \frac{\sigma_I f_I(\delta_n) - \sigma_{xx}}{C_{0,11}(1-d_n)} \qquad \text{and} \qquad d\varepsilon_n^{(2)} = d\varepsilon_n - d\varepsilon_n^{(1)} = \frac{T_n^{(trial)} - \sigma_I f_I(\delta_n)}{C_{0,11}(1-d_n)} \tag{5.77}$$

   The normal crack opening strain update in the first increment is

$$d\varepsilon_{c,xx}^{(1)} = d_n d\varepsilon_n^{(1)} \tag{5.78}$$

   During this second phase, the increment in normal strain must equal

$$d\varepsilon_n^{(2)} = d\delta_n + \varepsilon_{n0}\left(f_I(\delta_n + d\delta_n) - f_I(\delta_n)\right) \tag{5.79}$$

   For small increments, this equation reduces to:

$$d\delta_n = \frac{1}{1 + \varepsilon_{n0} f_I'(\delta_n)} d\varepsilon_n^{(2)} \tag{5.80}$$

   For larger increments (which may occur if the softening is rapid or large negative stiffness), the equation has to be solved numerically to find δ_n. For Newton's methods, we need to solve

$$g(d\delta_n) = d\delta_n - d\varepsilon_n^{(2)} + \varepsilon_{n0}\left(f_I(\delta_n + d\delta_n) - f_I(\delta_n)\right) = 0 \tag{5.81}$$

   with

$$g'(d\delta_n) = 1 + \varepsilon_{n0} f_I'(\delta_n + d\delta_n) \tag{5.82}$$

For bracketing, we begin with

$$\begin{aligned} g(0) &= -d\varepsilon_n^{(2)} < 0 && (5.83)\\ g(d\varepsilon_n^{(2)}) &= \varepsilon_{n0}\big(f_I(\delta_n + d\varepsilon_n^{(2)}) - f_I(\delta_n)\big) < 0 && (5.84)\\ g(d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)) &= \varepsilon_{n0} f_I(\delta_n + d\varepsilon_n^{(2)} + \varepsilon_{n0} f_I(\delta_n)) \geq 0 && (5.85) \end{aligned}$$

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:

$$\begin{aligned} g(x) &= \frac{x - d\varepsilon_n^{(2)}}{b} + \frac{f_I(\delta_n + x)}{f_I(\delta)} - 1 = 0 && (5.86)\\ g'(x) &= \frac{1}{b} + \frac{f_I'(\delta_n + x)}{f_I(\delta)} && (5.87) \end{aligned}$$

where $b = \varepsilon_{n0} f_I(\delta_n)$ is the width of the bracket window. Over the window, the function will vary from

$$\frac{f_I(\delta_n + d\varepsilon_n^{(2)})}{f_I(\delta_n)} - 1 < g(x) < \frac{f_I(\delta_n + d\varepsilon_n^{(2)} + b)}{f_I(\delta_n)} \tag{5.88}$$

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:

(a) Use Newton's method with bracketing and the initial guess close to the lower limit of $d\varepsilon_n^{(2)}$

(b) 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.

(c) Standard Newton's method with bracketed uses midpoint if Newton's step is larger than half the current bracket. This option can be ignore for softening laws.

(d) The special case of linear softening with $f_I(\delta_n) = 1 - \delta_n/\delta_{max}$ can be solved explicitly:

$$d\varepsilon_n^{(2)} = d\delta_n - \varepsilon_{n0}\frac{d\delta_n}{\delta_{max}} \qquad \text{or} \qquad d\delta_n = \frac{d\varepsilon_n^{(2)}}{1 - \frac{\varepsilon_{n0}}{\delta_{max}}} \tag{5.89}$$

along with attention to surpassing the maximum crack strain.

7. For 2D problems, shear damage has only d_{xy}. It can update exactly like normal stress except uses γ_{xy} and $d\gamma_{xy}$ in place of ε_n and $d\varepsilon_n$, no contact calculations are needed, and must be prepared to handle either sign for shear stress. If shear stress is negative, change sign of strain updates, solves as for strain increments, and then change sign back.

8. For 3D problems, first temporarily change shear stresses to be positive and if sign change is needed, temporarily change sign of γ_{ij} and $d\gamma_{ij}$ as well. If $d\gamma_{xy} < 0$ and $d\gamma_{xz} < 0$, the update is elastic — proceed to final tasks with cracking strains $d\gamma_{c,ij} = d_{ij} d\gamma_{ij}$. If one or both are positive, the trial elastic stress update is:

$$T_t^{(trial)} = \left(\tau_{xy}^{(0)} + G_{xy}\left(1 - d_{xy}\right) d\gamma_{xy}, \tau_{xz}^{(0)} + G_{xz}\left(1 - d_{xz}\right) d\gamma_{xz}\right) \tag{5.90}$$

where $\tau_{xy}^{(0)} = G_{xy}\left(1-d_{xy}\right)\gamma_{xy}$, and $\tau_{xz}^{(0)} = G_{xz}\left(1-d_{xz}\right)\gamma_{xz}$ are stresses from prior time step. If trial traction is within elliptical failure surface, the update is elastic and cracking strains update by elastic equation — $d\gamma_{c,ij} = d_{ij}d\gamma_{ij}$. If trial state is outside failure surface go to one of the next two steps.

9. If either $d\gamma_{xy} \leq 0$ or $d\gamma_{xz} \leq 0$ (and it will never be both), only the positive direction causes damage (or we have uniaxial shear damage). First partition into elastic and damage components by solving

$$\frac{\tau_{xy}^{(0)} + \phi G_{xy}(1-d_{xy})d\gamma_{xy}}{\tau_0^{xy} f_{xy}(\delta_{xy})} = T_2 = \sqrt{1-\left(\frac{\tau_{xz}^{(trial)}}{\tau_0^{xz} f_{xz}(\delta_{xz})}\right)^2} \tag{5.91}$$

Solving for ϕ:

$$\phi = \frac{\tau_0^{xy} f_{xy}(\delta_{xy})T_2 - \tau_{xy}^{(0)}}{G_{xy}(1-d_{xy})d\gamma_{xy}} \tag{5.92}$$

and find

$$d\gamma_{xy}^{(1)} = \phi d\gamma_{xy}, \text{ and } d\gamma_{xy}^{(2)} = (1-\phi)d\gamma_{xy} \tag{5.93}$$

The equation for Newton's method (from Eq. (5.48) for xy shear damage only) with $x = d\delta_{xy}$ is:

$$g(x) = \left(\frac{T_1 - x}{\gamma_{xy0} f_{xy}}\right)^2 - T_2^2 \tag{5.94}$$

where $T_1 = \tau_{xy}^{(0)}/G_{xy} + (1-d_{xy})\gamma_{xy}^{(1)} + d\gamma_{xy}^{(2)}$, $\gamma_{xy0} = \tau_{xy0}/G_{xy}$, $f_{xy} = f_{xy}(\delta_{xy} + x)$. To avoid potential $f_{xy} = 0$ in denominator and eliminate squares, we can equivalently solve

$$g(x) = T_1 - x - \gamma_{xy0} f_{xy} T_2 \tag{5.95}$$

To make similar to normal stress, we note that

$$T_1 = \tau_{xy}^{(0)}/G_{xy} + (1-d_{xy})d\gamma_{xy}^{(1)} + d\gamma_{xy}^{(2)} = \gamma_{xy0} f_{xy}(\delta_{xy})T_2 + d\gamma_{xy}^{(2)} \tag{5.96}$$

leading to

$$g(x) = \frac{x - d\gamma_{xy}^{(2)}}{b} + \frac{f_{xy}(\delta_{xy} + x)}{f_{xy}(\delta_{xy})} - 1 \tag{5.97}$$

where $b = T_2\gamma_{xy0} f_{xy}(\delta_{xy})$. This equation is identical to single axis equation (see Eq,. (5.86)) except for addtion of T_2 into b. It can use the same code for solution and use exact result for linear elastic. The linear solution changes to

$$x = \frac{d\gamma_{xy}^{(2)}}{1 + T_2\gamma_{xy0} f'_{xy}} = \frac{d\gamma_{xy}^{(2)}}{1 - \frac{T_2\gamma_{xy0}\delta_{xy}}{\delta_{xy,max}}} \tag{5.98}$$

which is same as single-axis result (see Eq. (5.89)) except for added factor of T_2.

The cracking strain for axis that does not damage (xz above) uses elastic equation. For damage only in xz direction, interchage xy and xz in above equations.

10. If both $d\gamma_{xy} > 0$ or $d\gamma_{xz} > 0$, the first task is to partition into two increments along path from initial state to trial state:

$$d\gamma_{ij}^{(1)} = \phi d\gamma_{ij}, \text{ and } d\gamma_{ij}^{(2)} = (1-\phi)d\gamma_{ij} \qquad \text{for } ij = (xy, xz) \tag{5.99}$$

where fraction ϕ of this update brings stress state to the current failure surface, which is determined by solving:

$$1 = \left(\frac{\tau_{xy}^{(0)} + \phi G_{xy}(1-d_{xy})d\gamma_{xy}}{\tau_{xy0} f_{xy}}\right)^2 + \left(\frac{\tau_{xz}^{(0)} + \phi G_{xz}(1-d_{xz})d\gamma_{xz}}{\tau_{xz0} f_{xz}}\right)^2 \tag{5.100}$$

$$= \left(\frac{\tau_{xy}^{(0)}}{\tau_{xy0} f_{xy}}\right)^2 + \left(\frac{\tau_{xz}^{(0)}}{\tau_{xz0} f_{xz}}\right)^2 + 2\phi\left[\left(\frac{\tau_{xy}^{(0)} G_{xy}(1-d_{xy})d\gamma_{xy}}{\tau_{xy0}^2 f_{xy}^2}\right) + \left(\frac{\tau_{xz}^{(0)} G_{xz}(1-d_{xz})d\gamma_{xz}}{\tau_{xz0}^2 f_{xz}^2}\right)\right]$$
$$+ \phi^2\left[\left(\frac{G_{xy}(1-d_{xy})d\gamma_{xy}}{\tau_{xy0} f_{xy}}\right)^2 + \left(\frac{G_{xz}(1-d_{xz})d\gamma_{xz}}{\tau_{xz0} f_{xz}}\right)^2\right] \tag{5.101}$$

where $f_{xy} = f_{xy}(\delta_{xy})$ and $f_{xz} = f_{xz}(\delta_{xz})$. Solve for ϕ (a quadratic equation being careful to get stable root and watch for previous state on the failure surface (which should give $\phi = 0$). Next task is to solve for $d\delta_{xy}$ and $d\delta_{xz}$

Modify initial stresses in Eqs. (5.43) and (5.46) and then solve for incremental damage strain $d\gamma_{ij}^{(2)}$ for incremental strain. We need to solve two equations, $f_1(x_1, x_2) = 0$ and $f_2(x_1, x_2) = 0$, where $x_1 = d\delta_{xy}$, $x_2 = d\delta_{xz}$, and:

$$f_1 = f_{xz}^2\left(\frac{T_1 - x_1}{\gamma_{xy0}}\right)^2 + f_{xy}^2\left(\frac{T_2 - x_2}{\gamma_{xz0}}\right)^2 - f_{xy}^2 f_{xz}^2 \tag{5.102}$$

$$f_2 = \frac{f_{xz}^2(T_1 - x_1)(d_{xz}d\gamma_{xz} - x_2)}{\left(\tau_n^{xy}\right)^2} - \frac{f_{xy}^2(T_2 - x_2)(d_{xy}d\gamma_{xy} - x_1)}{\left(\tau_n^{xz}\right)^2} \tag{5.103}$$

where $d\gamma_{ij} = d\gamma_{ij}^{(2)}$, $T_1 = \tau_{xy}^{(0)}/G_{xy} + (1-d_{xy})\gamma_{xy}^{(1)} + d\gamma_{xy}^{(2)}$, $T_2 = \tau_{xz}^{(0)}/G_{xz} + (1-d_{xz})\gamma_{xz}^{(1)} + d\gamma_{xz}^{(2)}$, $\gamma_{ij0} = \tau_{ij0}/G_{ij}$, and now $f_{xy} = f_{xy}(\delta_{xy} + x_1)$, and $f_{xz} = f_{xz}(\delta_{xz} + x_2)$ (which differs from their use in ϕ equation). Note that two equation and by multilied through by $f_{xy}^2 f_{xz}^2$ to avoid possible zeros in the denominator near decohesion. To find Jacobian, we need

$$J_{11} = \frac{\partial f_1}{\partial x_1} = -\frac{2f_{xz}^2}{\gamma_{xy0}^2}(T_1 - x_1) + 2f_{xy}f'_{xy}\left(\left(\frac{T_2 - x_2}{\gamma_{xz0}}\right)^2 - f_{xz}^2\right) \tag{5.104}$$

$$J_{12} = \frac{\partial f_1}{\partial x_2} = -\frac{2f_{xy}^2}{\gamma_{xz0}^2}(T_2 - x_2) + 2f_{xz}f'_{xz}\left(\left(\frac{T_1 - x_1}{\gamma_{xy0}}\right)^2 - f_{xy}^2\right) \tag{5.105}$$

$$J_{21} = \frac{\partial f_2}{\partial x_1} = -\frac{f_{xz}^2(d_{xz}d\gamma_{xz} - x_2)}{\left(\tau_n^{xy}\right)^2} + \frac{f_{xy}(T_2 - x_2)}{\left(\tau_n^{xz}\right)^2}\left(f_{xy} - 2(d_{xy}d\gamma_{xy} - x_1)f'_{xy}\right) \tag{5.106}$$

$$J_{22} = \frac{\partial f_2}{\partial x_2} = \frac{f_{xy}^2(d_{xy}d\gamma_{xy} - x_1)}{\left(\tau_n^{xz}\right)^2} - \frac{f_{xz}(T_1 - x_1)}{\left(\tau_n^{xy}\right)^2}\left(f_{xz} - 2(d_{xz}d\gamma_{xz} - x_2)f'_{xz}\right) \tag{5.107}$$

where $f'_{xy} = f'_{xy}(\delta_{xy} + x_1)$ and $f'_{xz} = f'_{xz}(\delta_{xz} + x_2)$. The Newton method update is

$$(x_1^{(k+1)}, x_2^{(k+1)}) = (x_1^{(k)}, x_2^{(k)}) - J^{-1}(f_1^{(k)}, f_2^{(k)}) \tag{5.108}$$

The final cracking strains are

$$d\gamma_{c,ij} = d_{ij} d\gamma_{ij}^{(1)} + d\delta_{ij} \qquad \text{for } ij = (xy, xz) \tag{5.109}$$

The damage variables for an axis that damages could update using Eq. (5.22) as

$$dd_{ij} = \frac{1}{\gamma_{ij} + d\gamma_{ij}^{(1)}} \left(d\delta_{ij} - d_{ij} d\gamma_{ij}^{(2)} \right) \qquad \text{for } ij = (xy, xz) \tag{5.110}$$

but this can have problems when the denominator is close to zero (caused by coupled damage due to elliptical failure criterion). A more stable calculation is the universal result using the updated maximum cracking strain:

$$d_{ij} = \frac{\delta_{ij} + d\delta_{ij}}{\delta_{ij} + d\delta_{ij} + \gamma_{ij0} f_{ij}(\delta_{ij} + d\delta_{ij})} \qquad \text{for } ij = (xy, xz) \tag{5.111}$$

Numerical calculations confirm these are the same unless $\gamma_{ij} + d\gamma_{ij}^{(1)}$ is small and then the former can give very poor results.

11. In calculations, the increment in dissipated energy due to any damage variable change is:

$$d\Omega_i = d\overline{G}_i = \overline{G}_i(\delta_i + d\delta_i) - \overline{G}_i(\delta_i) \tag{5.112}$$

Alternatively, the energy increment can be found from

$$d\Omega_n = C_{0,11} \left(\varepsilon_n + d\varepsilon_n^{(1)} \right) \left(d\delta_n - d_n d\varepsilon_n^{(2)} \right) \tag{5.113}$$

$$d\Omega_{ij} = G_{ij} \left(\gamma_{ij} + d\gamma_{ij}^{(1)} \right) \left(d\delta_{ij} - d_{ij} d\gamma_{ij}^{(2)} \right) \qquad \text{for } ij = (xy, xz) \tag{5.114}$$

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.

5.2.6 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:

$$d\varepsilon_n = d\varepsilon_{xx} - d\varepsilon_{res} + \frac{\nu}{1-\nu} d\varepsilon_{yy} - \frac{2\nu}{1-\nu} d\varepsilon_{res}, \tag{5.115}$$

or

$$d\varepsilon_n = d\varepsilon_{xx} + \frac{\nu}{1-\nu} d\varepsilon_{yy} - \frac{1+\nu}{1-\nu} d\varepsilon_{res}, \qquad \text{and} \qquad d\gamma_t = d\gamma_{xy} \tag{5.116}$$

The normal strain can be rewritten as:

$$d\varepsilon_n^{(r)} = d\varepsilon_{xx} - (1+\nu) d\varepsilon_{res} + \frac{\nu}{1-\nu} (d\varepsilon_{yy} - (1+\nu) d\varepsilon_{res}) = d\varepsilon_{xx}^{(r)} + \frac{\nu}{1-\nu} d\varepsilon_{yy}^{(r)} \tag{5.117}$$

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

$$d\varepsilon_{c,xx}^{(r)} = d\left(d_n \left(d\varepsilon_{xx}^{(r)} + \frac{\nu}{1-\nu} d\varepsilon_{yy}^{(r)} \right) \right), \quad d\gamma_{c,xy} = d(d_{xy}\gamma_{xy}), \quad \text{and} \quad d\gamma_{c,xz} = 0 \tag{5.118}$$

The normal stress updates become

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \end{pmatrix} = \begin{pmatrix} C_{0,11}(d\varepsilon_n^{(r)} - d\varepsilon_{c,xx}^{(r)}) \\ C_{0,11}\left(d\varepsilon_{yy}^{(r)} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(r)} - d\varepsilon_{c,xx}^{(r)}\right)\right) \\ C_{0,11}\left(-d\varepsilon_{res} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}^{(r)} + d\varepsilon_{yy} - 2d\varepsilon_{res}\right)\right) \end{pmatrix} \tag{5.119}$$

Here σ_{zz} is a separate calculation and uses total strain increments and a residual strain term.

Plane Stress

For plane stress, we begin with 3D solution but then impose $d\sigma_{zz} = 0$. The thickness stress update is

$$0 = d\sigma_{zz} = C_{0,11}\left(d\varepsilon_{zz} + \frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx} + d\varepsilon_{yy}\right)\right) \tag{5.120}$$

which implies

$$d\varepsilon_{zz} = -\frac{\nu}{1-\nu}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx} + d\varepsilon_{yy}\right) \tag{5.121}$$

The total normal strain on the crack becomes

$$\begin{aligned} d\varepsilon_n &= d\varepsilon_{xx} + \frac{\nu}{1-\nu}d\varepsilon_{yy} - \frac{\nu^2}{(1-\nu)^2}\left(d\varepsilon_{xx} - d\varepsilon_{c,xx} + d\varepsilon_{yy}\right) &(5.122)\\ &= \frac{(1-2\nu)}{(1-\nu)^2}d\varepsilon_{xx} - \frac{\nu^2}{(1-\nu)^2}d\varepsilon_{c,xx} + \frac{\nu(1-2\nu)}{(1-\nu)^2}d\varepsilon_{yy} &(5.123)\end{aligned}$$

The full in-plane stress update becomes

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \frac{E}{1-\nu^2}\left(d\varepsilon_{xx} + \nu d\varepsilon_{xyy} - d\varepsilon_{c,xx}\right) \\ \frac{E}{1-\nu^2}\left(d\varepsilon_{yy} + \nu\left(d\varepsilon_{xx} - d\varepsilon_{c,xx}\right)\right) \\ G\left(d\gamma_{xy} - d\gamma_{c,xy}\right) \end{pmatrix} \tag{5.124}$$

The problem here is anew coupling where $d\varepsilon_{c,xx} = d(d_n\varepsilon_n)$, but unlike for 3D and plane stress, ε_n depends on $\varepsilon_{c,xx}$. It may have a solution, but not sure yet. A potential approach is to start with plane stress from the beginning and define a plane stress D and Δ. The end result might be a new ε_n that work work out.

In plane stress, we use instead

$$\mathsf{D} = \begin{bmatrix} d_n & 0 & 0 \\ \nu d_n & 0 & 0 \\ 0 & 0 & d_{xy} \end{bmatrix} \quad \text{and} \quad \mathsf{C}_0 = \begin{bmatrix} \frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\ \frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & G \end{bmatrix} \tag{5.125}$$

The choice for new D follows from the *effective* compliance tensor and from that tensor $C_{0,12}/C_{0,11} = \nu$. For an isotropic material and this plane stress D , we find Δ by first expanding:

$$\mathsf{D}\mathsf{C}_0\boldsymbol{\varepsilon} = \left(C_{0,11}d_n\varepsilon_n, C_{0,11}\,\nu d_n\varepsilon_n, G_0 d_{xy}\gamma_{xy}\right) \tag{5.126}$$

where

$$\varepsilon_n^* = \varepsilon_{xx} + \nu\varepsilon_{yy} \qquad \text{and} \qquad C_{0,11}^* = \frac{E}{1-\nu^2} \tag{5.127}$$

and plane strain normal stress and stess tensor element. The full tensor evaluates to

$$\Delta = \begin{bmatrix} \frac{\partial(d_n\varepsilon_n^*)}{\partial\varepsilon_{xx}} & \frac{\partial(d_n\varepsilon_n^*)}{\partial\varepsilon_{yy}} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\partial(d_{yz}\gamma_{xy})}{\partial\gamma_{xy}} \end{bmatrix} \tag{5.128}$$

We can then proceed with standard analysis (being careful to define effective properties. The stress update becomes

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \frac{E}{1-\nu^2}\big(d\varepsilon_n^* - d\varepsilon_{c,xx}\big) \\ \frac{E}{1-\nu^2}\big(d\varepsilon_{yy} + \nu\big(d\varepsilon_{xx} - d\varepsilon_{c,xx}\big)\big) \\ G\big(d\gamma_{xy} - d\gamma_{c,xy}\big) \end{pmatrix} \tag{5.129}$$

where

$$d\varepsilon_{c,xx} = d(d_n\varepsilon_n^*) \qquad \text{and} \qquad d\gamma_{c,xy} = d(d_{yz}\gamma_{xy}) \tag{5.130}$$

which is same ad 3D version, but not have a path to implement softening the cracking strain decoupled from normal strain.

5.3 Isotropic Plastic Softening Material

The numerical strategy is to partition strain increment into elastic, plastic, and cracking strain along with updated stress state. The plasticity will use J_2 plasticity on the bulk material. The strain for this phase is total strain minus cracking strain. It can use standard plasticity methods. Once plasticity is done, the incremental plastic strain is subtracted from incremental total strain and the remaining incremental strain is input to softening calculations.

5.3.1 Plastic Phase

This phase assumes the material is damaged and imagines plasticity modeling under conditions of no damage evolution occurs in the current time step. When damage is present, but not evolving, the input strain can be partitioned into:

$$d\boldsymbol{\varepsilon}_{tot}^* = d\boldsymbol{\varepsilon}_e^* + d\boldsymbol{\varepsilon}_c \tag{5.131}$$

where e and c correspond to elastic strain increment on the bulk material and cracking strain increment, respectively. The superscript * indicates effective strains that account for residual stresses (*i.e.*, $d\boldsymbol{\varepsilon}^* = d\boldsymbol{\varepsilon}^* - d\boldsymbol{\varepsilon}_{res}$). For the plasticity phase, the cracking strain is subtracted from total strain to get trial elastic strain increment:

$$d\boldsymbol{\varepsilon}_{trial}^* = d\boldsymbol{\varepsilon}_{tot}^* - d\boldsymbol{\varepsilon}_c \tag{5.132}$$

where

$$d\boldsymbol{\varepsilon}_c = \mathsf{D}^T d\boldsymbol{\varepsilon}_{tot}^* \tag{5.133}$$

and the x direction cracking strain increment must look out for contact such that it is not less than minus the current cracking strain ($-\varepsilon_{c,xx}$). Because cracking strains are only clear in the crack axis system, this phase must be done in that configuration (prior to damage, this phase can use any configuration).

The plasticity calculations can then proceed by methods identical to standard isotropic material with J_2 plasticity with input trial elastic strain give by $d\boldsymbol{\varepsilon}_{trial}^*$ rather than total strain increment on this time step. The net result of the calculation will be to determine the plastic strain component of the trial elastic strain ($d\boldsymbol{\varepsilon}_p$) and a net reduction in trial stress caused by that plastic strain ($\boldsymbol{\sigma}_p = \mathsf{C}d\boldsymbol{\varepsilon}_p$). If plasticity occurs, the calculated incremental plastic strain (in current axes) and dissipated energy are

added to the particle. In addition, total work equal to $(\boldsymbol{\sigma}_{trial} - \boldsymbol{\sigma}_p) \cdot d\boldsymbol{\varepsilon}_p$ is added to particle energy. This work is added because the subsequent damage state will not include it in its work calculations.

When plasticity is done, calculate non-plasticity strain increment to provide as input to damage mechanics modeling:

$$d\boldsymbol{\varepsilon}_{damage} = d\boldsymbol{\varepsilon}_{tot} - d\boldsymbol{\varepsilon}_p = d\boldsymbol{\varepsilon}_{trial} + d\boldsymbol{\varepsilon}_c - d\boldsymbol{\varepsilon}_p \tag{5.134}$$

This strain increment is called $d\boldsymbol{\varepsilon}$ when input to the damage mechanics code

5.3.2 Predamage Phase

If the particle is not yet damaged, this phase uses the final stress in the plasticity phase ($\boldsymbol{\sigma} = \boldsymbol{\sigma}_{trial} - \boldsymbol{\sigma}_p$) to determine if damage has initiated. If it has not initiated, finish calculations by transferring final stress from plasticity phase stress to the particle (rotated to current configuration), updating work and residual energy, and calling code to increment heat energy. Note that the total work energy from the two phases will be

$$dW = (\boldsymbol{\sigma}_{trial} - \boldsymbol{\sigma}_p) \cdot d\boldsymbol{\varepsilon}_p + (\boldsymbol{\sigma}_{trial} - \boldsymbol{\sigma}_p) \cdot d\boldsymbol{\varepsilon}_{damage} = (\boldsymbol{\sigma}_{trial} - \boldsymbol{\sigma}_p) \cdot d\boldsymbol{\varepsilon}_{tot} \tag{5.135}$$

Note these are correctly using strain increments and not *effective* strain increments.

If damage has occurred, calculate normal and V_p/A_c and then proceed to damage phase. Also rotate $d\boldsymbol{\varepsilon}_{damage}$ into the crack axis system.

5.3.3 Damage Phase

The first step is to find an adjusted initial particle stress in the crack axis system after plasticity changes to stress by rotating current particle stress to crack axis system and subtracting $\boldsymbol{\sigma}_p$ from the plasticity phase (which will be in crack axis system when damaged). After finding adjusted initial particle stress in crack axis system, rotate $\boldsymbol{\sigma}_p$ from crack axis system to $(n-1)^{th}$ current configuration and subtract from stress currently stored on the particle. The damage evolution calculations will rotate this update particle stress to n^{th} configuration and add stress increment from damage mechanics calculations.

Because "plastic strain" on the particle for this material tracks total inelastic strain (*e.g.* sum of plastic strain and cracking strain), this material needs to separately tracking just cracking strain in three history variables on each particle. The next step is to read the history variables and get current cracking strain tensor in $\boldsymbol{\varepsilon}_{crack}$.

Finally, adjusted initial particle stress, $d\boldsymbol{\varepsilon}_{damage}$, $d\boldsymbol{\varepsilon}_{crack}$, $\boldsymbol{\varepsilon}_{crack}$, and any dissipated plastic energy are input to damage evolution calculations. These proceed by methods identical to isotropic softening materials (see section 5.2). The damage evolution will return the calculated increments in cracking strain, which need to be added to cracking strain history variables on this material. The damage evolution will update stresses, add work energy (to now get total work energy), residual energy, and dissipated damage energy to the particle. In addition, it will increment heat energy using thermal strain and sum of plastic and damage dissipated energy.

Chapter 6

Poroelasticity Materials

6.1 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 modeling 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 add adds a required undrained pressure change term.

6.2 Biot Poroelasticity Theory

Generalizing Biot (1941) poroelasticity theory to anisotropic materials, the strain and water increment, θ, are given by:

$$\boldsymbol{\varepsilon} = \mathsf{S}\boldsymbol{\sigma} + \boldsymbol{h}dp \tag{6.1}$$

$$\theta = \boldsymbol{h}\cdot\boldsymbol{\sigma} + \frac{dp}{R} \tag{6.2}$$

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:

$$\theta = dv = v - v_0 \qquad \text{and} \qquad dp = p - p_0 \tag{6.3}$$

When $v = v_0$ and $p = p_0$, total stress is zero: $\boldsymbol{\sigma} = 0$. For an orthotropic material in material axes:

$$\boldsymbol{h} = \left(\frac{1}{3H_x}, \frac{1}{3H_y}, \frac{1}{3H_z}, 0, 0, 0 \right) \tag{6.4}$$

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

$$\boldsymbol{\sigma} = \mathsf{C}(\boldsymbol{\varepsilon} - \boldsymbol{h}dp) = \mathsf{C}\boldsymbol{\varepsilon} - \boldsymbol{\alpha}dp \tag{6.5}$$

$$\theta = \boldsymbol{h} \cdot (\mathsf{C}\boldsymbol{\varepsilon} - \boldsymbol{\alpha}dp) + \frac{dp}{R} = \boldsymbol{\alpha} \cdot \varepsilon + \frac{dp}{Q} \tag{6.6}$$

where

$$\boldsymbol{\alpha} = \mathsf{C}\boldsymbol{h} \text{ (or } \boldsymbol{h} = \mathsf{S}\boldsymbol{\alpha}) \qquad \text{and} \qquad \frac{1}{Q} = \frac{1}{R} - \boldsymbol{h} \cdot \boldsymbol{\alpha} \tag{6.7}$$

$\boldsymbol{\alpha}$ 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 $dp = -R\boldsymbol{h} \cdot \Delta\boldsymbol{\sigma}$. The change in strain becomes:

$$\Delta\boldsymbol{\varepsilon} = \mathsf{S}\Delta\sigma - \boldsymbol{h}R\boldsymbol{h} \cdot \Delta\sigma \tag{6.8}$$

The change in normal strains become

$$\begin{pmatrix} \Delta\varepsilon_{xx} \\ \Delta\varepsilon_{yy} \\ \Delta\varepsilon_{zz} \end{pmatrix} = \begin{pmatrix} \frac{\Delta\sigma_{xx} - \nu_{xy}\Delta\sigma_{yy} - \nu_{xz}\Delta\sigma_{zz}}{E_{xx}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_x} \\ \frac{\nu_{yx}\Delta\sigma_{xx} + \Delta\sigma_{yy} - \nu_{yz}\Delta\sigma_{zz}}{E_{yy}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_y} \\ \frac{\nu_{zx}\Delta\sigma_{xx} - \nu_{zy}\Delta\sigma_{yy} + \Delta\sigma_{zz}}{E_{zz}} - \left(\frac{\Delta\sigma_{xx}}{3H_x} + \frac{\Delta\sigma_{yy}}{3H_y} + \frac{\Delta\sigma_{zz}}{3H_z} \right) \frac{R}{3H_z} \end{pmatrix} \tag{6.9}$$

The total change in volumetric strain becomes:

$$\begin{aligned} \Delta\varepsilon_{ii} &= \frac{1}{3}\left(\frac{3(1 - \nu_{xy} - \nu_{xz})}{E_{xx}} - \frac{Rh_{ii}}{H_x} \right)\Delta\sigma_{xx} + \frac{1}{3}\left(\frac{3(1 - \nu_{yx} - \nu_{yz})}{E_{yy}} - \frac{Rh_{ii}}{H_y} \right)\Delta\sigma_{yy} \\ &\quad + \frac{1}{3}\left(\frac{3(1 - \nu_{zx} - \nu_{zy})}{E_{zz}} - \frac{Rh_{ii}}{H_z} \right)\Delta\sigma_{zz} \qquad (6.10) \\ &= \boldsymbol{k}_u \cdot \frac{1}{3}\left(\Delta\sigma_{xx}, \Delta\sigma_{yy}, \Delta\sigma_{yy} \right) \qquad (6.11) \end{aligned}$$

where $\boldsymbol{k}_u$ is an anisotropic compressibility tensor (components from terms above) and

$$h_{ii} = \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z} \right) \tag{6.12}$$

For an aniostropic material, we consider $\Delta\sigma_{xx} = \Delta\sigma_{yy} = \Delta\sigma_{zz} = -P$ and we can write

$$\Delta\varepsilon_{ii} = \left(\frac{1}{K} - \frac{Rh_{ii}}{3H_x} - \frac{Rh_{ii}}{3H_y} - \frac{Rh_{ii}}{3H_x} \right)P \quad \text{or} \quad \frac{1}{K_u} = \frac{1}{K} - Rh_{ii}^2 \tag{6.13}$$

is the undrained bulk modulus and

$$\frac{1}{K}=\frac{1-\nu_{xy}-\nu_{xz}}{E_{xx}}+\frac{1-\nu_{yx}-\nu_{yz}}{E_{yy}}+\frac{1-\nu_{zx}-\nu_{zy}}{E_{zz}} \tag{6.14}$$

The other limit is the "drained" limit where $dp=0$. In this condition:

$$\boldsymbol{\varepsilon}=\mathsf{S}\boldsymbol{\sigma},\quad \boldsymbol{\sigma}=\mathsf{C}\boldsymbol{\varepsilon},\quad \text{and}\quad \theta=\boldsymbol{h}\cdot\boldsymbol{\sigma}=\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon} \tag{6.15}$$

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 $\boldsymbol{h}=\mathsf{S}\boldsymbol{\alpha}$ and then find Q from

$$R=\frac{1}{h_{ii}^2}\left(\frac{1}{K}-\frac{1}{K_u}\right)\quad\text{and}\quad\frac{1}{Q}=\frac{1}{R}-\boldsymbol{h}\cdot\boldsymbol{\alpha} \tag{6.16}$$

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:

$$\boldsymbol{\beta}=\boldsymbol{h}=\mathsf{S}\boldsymbol{\alpha}=\left(\frac{\alpha_x-\nu_{xy}\alpha_y-\nu_{xz}\alpha_z}{E_{xx}},\frac{\alpha_y-\alpha_x\nu_{yx}-\nu_{yz}\alpha_z}{E_{yy}},\frac{\alpha_z-\alpha_x\nu_{zx}-\nu_{zy}\alpha_z}{E_{zz}},0,0,0\right) \tag{6.17}$$

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. For pore pressure transport, a poroelasticity analysis will need to use K_u to find R (or actually Q)

$$Q=\frac{R}{1-R\boldsymbol{h}\cdot\boldsymbol{\alpha}}=\frac{\left(\frac{1}{K}-\frac{1}{K_u}\right)}{h_{ii}^2-\left(\frac{1}{K}-\frac{1}{K_u}\right)\boldsymbol{h}\cdot\boldsymbol{\alpha}}=\frac{K_u-K}{KK_uh_{ii}^2-(K_u-K)\boldsymbol{h}\cdot\boldsymbol{\alpha}} \tag{6.18}$$

For an isotropic material, $\alpha_x=\alpha_y=\alpha_z=\alpha$ leading to $h_x=h_y=h_z=\beta=\alpha/3K$ and $h_{ii}=1/H=\alpha/K$. To find R and Q, begin with undrained bulk modulus:

$$\frac{1}{K_u}=\frac{1}{K}-\frac{R}{H^2}\quad\text{or}\quad K_u=K\left(\frac{H^2}{H^2-KR}\right)=K\left(1+\frac{KR}{H^2-KR}\right) \tag{6.19}$$

The results for R and Q become:

$$\frac{1}{R}=\frac{\alpha^2}{K}\left(\frac{K_u}{K_u-K}\right)\quad\text{and}\quad Q=\frac{K_u-K}{\alpha^2} \tag{6.20}$$

Clearly, we need $\alpha>0$ and $K_u>K$.

6.2.1 Darcy's Law Flow

In a Darcy flow analysis, the fluid volume rate of change is

$$\frac{d\theta}{dt}=-\frac{1}{\eta}\nabla\cdot\mathsf{k}\nabla p \tag{6.21}$$

where k is Darcy tensor (units length^2) and η is viscosity of permeating fluid. Substituting equation for θ leads to:

$$\frac{1}{Q}\frac{dp}{dt}=-\frac{1}{\eta}\nabla\cdot\mathsf{k}\nabla p-\boldsymbol{\alpha}\cdot\frac{d\boldsymbol{\varepsilon}}{dt} \tag{6.22}$$

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:

$$C_T = \frac{1}{Q} \tag{6.23}$$

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

$$\Delta p_{ud} = -Q\boldsymbol{\alpha} \cdot \Delta\boldsymbol{\varepsilon} \tag{6.24}$$

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:

$$\Delta t_\sigma = \frac{\Delta x}{v_{max}}, \qquad \Delta t_p = \frac{\eta \Delta x^2}{2Qk_{max}}, \qquad \text{and} \qquad \frac{\Delta t_p}{\Delta t_\sigma} = \frac{\eta v_{max} \Delta x}{2Qk_{max}} \tag{6.25}$$

where Δx is cell size, v_{max} is maximum wave speed, and k_{max} is maximum permeability. For an isotropic material:

$$v_{max} = \sqrt{\frac{2G(1-\nu)}{\rho(1-2\nu)}} = \sqrt{\frac{3K(1-\nu)}{\rho(1+\nu)}} \quad \text{and} \quad \frac{\Delta t_p}{\Delta t_\sigma} = \frac{\eta \alpha^2 \Delta x}{2k(K_u - K)} \sqrt{\frac{3K(1-\nu)}{\rho(1+\nu)}} \tag{6.26}$$

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.

6.2.2 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:

$$\sigma_{zz} = (\lambda + 2G)\varepsilon_{zz} = \frac{\varepsilon_{zz}}{a} \tag{6.27}$$

where a defined in Biot's paper is

$$a = \frac{1}{\lambda + 2G} = \frac{1}{C_{zz}} = \frac{(1+\nu)(1-2\nu)}{E(1-\nu)} = \frac{(1-2\nu)}{2G(1-\nu)} \tag{6.28}$$

For generalizations here to an orthotropic material:

$$a = \frac{1}{C_{zz}} = \frac{1 - \nu_{yz}\nu_{zy} - \nu_{xz}\nu_{zx} - \nu_{xy}\nu_{yx} - 2\nu_{xz}\nu_{yx}\nu_{zy}}{E_{zz}(1 - \nu_{xy}\nu_{yx})} \tag{6.29}$$

6.2.3 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:

$$\boldsymbol{\varepsilon} = \mathsf{S}\sigma_s - \frac{\boldsymbol{k}_s' p}{3} \tag{6.30}$$

$$\theta - \theta_0 = \boldsymbol{h} \cdot \sigma_s - \frac{\theta_0}{K_s''} p \tag{6.31}$$

where

$$\boldsymbol{k}_s' = 3(\mathsf{S}\mathsf{I} - \boldsymbol{h}), \quad \frac{\theta_0}{K_s''} = h_{ii} - \frac{1}{R} \quad \text{and} \quad h_{ii} = \boldsymbol{h} \cdot \mathsf{I} = \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z}\right) \tag{6.32}$$

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:

$$p = \frac{K_s'' \boldsymbol{h} \cdot \sigma_s}{\theta_0} \tag{6.33}$$

In this "unstressed state", the total strain is

$$\boldsymbol{\varepsilon} = \mathsf{S}\sigma_s - \frac{\boldsymbol{k}_s' K_s'' \boldsymbol{h} \cdot \sigma_s}{3\theta_0} \tag{6.34}$$

Writing out expressions for an orthoropic material gives

$$\boldsymbol{k}_s' = \left(\frac{3(1 - \nu_{xy} - \nu_{xz})}{E_{xx}} - \frac{1}{H_x}, \frac{3(1 - \nu_{yx} - \nu_{yz})}{E_{yy}} - \frac{1}{H_y}, \frac{3(1 - \nu_{zx} - \nu_{zy})}{E_{zz}} - \frac{1}{H_z}, 0, 0, 0\right) \tag{6.35}$$

$$\frac{\theta_0}{K_s'} = \left(\frac{1}{R} - \frac{1}{3}\left(\frac{1}{H_x} + \frac{1}{H_y} + \frac{1}{H_z}\right)\right) \tag{6.36}$$

If the material is isotropic, the results become:

$$\boldsymbol{k}_s'' = \left(\frac{1}{K} - \frac{1}{H}\right)(1,1,1,0,0,0) = \frac{1}{K_s'}(1,1,1,0,0,0) \tag{6.37}$$

$$\frac{\theta_0}{3K_s''} = \frac{1}{R} - \frac{1}{H} \tag{6.38}$$

Here K_s' and K_s'' are terms defined by Rice (1976).

Chapter 7

Hyperelastic Materials

7.1 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:

$$\mathbf{F} = \begin{pmatrix} 1+\varepsilon_{xx} & \frac{1}{2}(\gamma_{xy}-\omega_{xy}) & \frac{1}{2}(\gamma_{xz}-\omega_{xz}) \\ \frac{1}{2}(\gamma_{xy}+\omega_{xy}) & 1+\varepsilon_{yy} & \frac{1}{2}(\gamma_{yz}-\omega_{yz}) \\ \frac{1}{2}(\gamma_{xz}+\omega_{xz}) & \frac{1}{2}(\gamma_{yz}+\omega_{yz}) & 1+\varepsilon_{zz} \end{pmatrix} \tag{7.1}$$

and should store the updated gradient back on strain and rotation tensors on each time step.

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 have information about elastic and plastic deformation, these 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

$$\frac{\boldsymbol{\sigma}}{\rho} = \frac{\boldsymbol{\sigma} J}{\rho_0} = \frac{\boldsymbol{\tau}}{\rho_0} \tag{7.2}$$

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.

7.2 Incremental Deformation Gradient

Each MPM time step requires evaluation of deformation gradient rate defined by

$$\frac{d\mathbf{F}}{dt} = \nabla \boldsymbol{v} \mathbf{F} \tag{7.3}$$

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

$$\mathbf{F}(t+\Delta t) = \exp(\Delta t \nabla \boldsymbol{v})\mathbf{F}(t) = \mathbf{dF}\,\mathbf{F}(t) \tag{7.4}$$

where

$$\mathbf{dF} = \exp(\Delta t \nabla \boldsymbol{v}) = \mathbf{F}(t+\Delta t)\mathbf{F}(t)^{-1} \tag{7.5}$$

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

$$\exp(\Delta t \nabla \boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \sum_{k=2}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{7.6}$$

where $\nabla u = \Delta t \nabla \boldsymbol{v}$ 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

$$\nabla u = \begin{pmatrix} \begin{bmatrix} du_{xx} & du_{xy} \\ du_{yx} & du_{yy} \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz} \end{pmatrix} \tag{7.7}$$

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

$$(\nabla u)^k = \begin{pmatrix} \mathsf{A}^k & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz}^k \end{pmatrix} \tag{7.8}$$

Let the characteristic polymer of A (of any dimension n) be

$$c(z) = \det(z\mathbf{I} - \mathsf{A}) = z^n - \sum_{k=0}^{n-1} c_k z^k \tag{7.9}$$

Because $c(\mathsf{A}) = 0$, the n^{th} power of A can be found from lower powers of A

$$\mathsf{A}^n = \sum_{k=0}^{n-1} c_k \mathsf{A}^k \tag{7.10}$$

For $n = 2$, these reduce to

$$c_0 = -\det(\mathsf{A}), \qquad c_1 = \mathrm{Tr}(\mathsf{A}), \qquad \text{and} \qquad \mathsf{A}^2 = c_0\mathbf{I} + c_1\mathsf{A} \tag{7.11}$$

Higher powers of A can be found by recursion to be

$$\mathsf{A}^k = \beta_{k,0}\mathbf{I} + \beta_{k,1}\mathsf{A} \tag{7.12}$$

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

$$\mathbf{dF}(k_{max}) = \begin{pmatrix} [\alpha_0\mathbf{I} + \alpha_1\mathsf{A}] & \begin{matrix}0\\0\end{matrix} \\ \begin{matrix}0 & 0\end{matrix} & 1 + du_{zz} + \sum_{k=2}^{k_{max}} \frac{du_{zz}^k}{k!} \end{pmatrix} \tag{7.13}$$

where

$$\alpha_0 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,0}}{k!} \qquad \text{and} \qquad \alpha_1 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,1}}{k!} \tag{7.14}$$

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

$$\exp(\Delta t\nabla\boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \frac{1}{2}(\nabla u)^2 + \sum_{k=3}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{7.15}$$

which can be reduced to

$$\exp(\Delta t\nabla\boldsymbol{v}) = \alpha_0\mathbf{I} + \alpha_1\nabla u + \alpha_2(\nabla u)^2 \tag{7.16}$$

$$\alpha_0 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,0}}{k!}, \qquad \alpha_1 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,1}}{k!}, \quad \text{and} \quad \alpha_2 = \frac{1}{2} + \sum_{k=3}^{k_{max}} \frac{\beta_{k,2}}{k!} \tag{7.17}$$

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

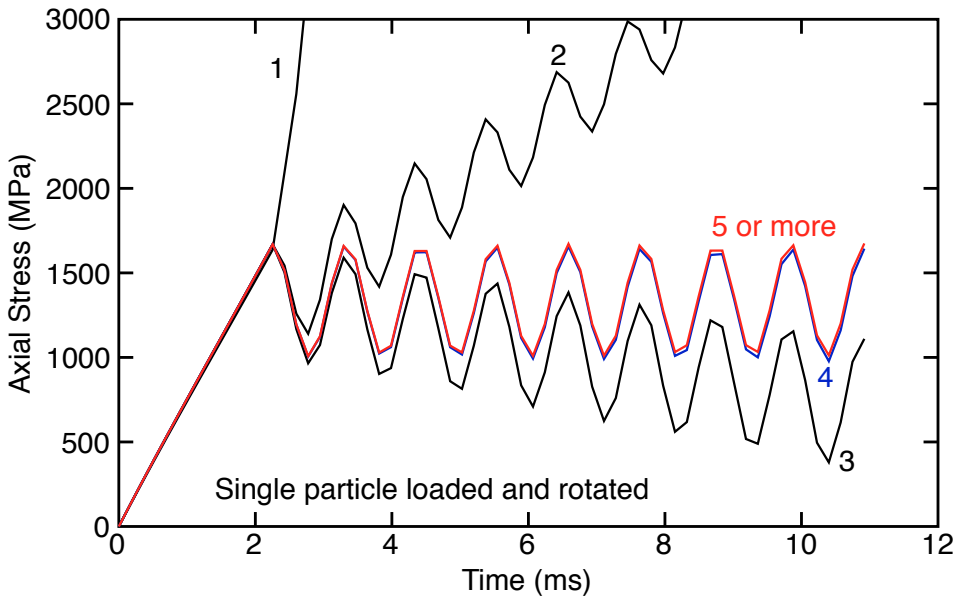

Figure 7.1: Calculation for a single particle loaded in tension, held, and then rotated. The different curves show k_{max} or the number of terms used to expand the matrix exponential in the incremental deformation gradient.

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. 7.1. 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.

7.3 Isotopic, Hyperelastic Materials

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:

$$I_1 = \mathrm{Tr}(\mathbf{B}) = B_{11} + B_{22} + B_{33} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \tag{7.18}$$

$$I_2 = \frac{1}{2}\left(I_1^2 - \mathbf{B}\cdot\mathbf{B}\right) = \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_1^2\lambda_3^2 \tag{7.19}$$

$$I_3 = \det(\mathbf{B}) = (\det(\mathbf{F}))^2 = J^2 = \lambda_1^2\lambda_2^2\lambda_3^2 \tag{7.20}$$

where λ_i are the principle stretches of the deformation. Sometimes modified invariants are used instead as $\overline{I_1} = I_1/J^{2/3}$ and $\overline{I_2} = I_2/J^{4/3}$. Next the strain energy is written as a function of these 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 Cauchy stress can be found from

$$\sigma_{ij} = \frac{1}{J}\sum_k F_{ik}\frac{\partial W}{\partial F_{jk}} \tag{7.21}$$

Using the key terms (adapted from "Applied Mechanics of Solids" by Alan Bower):

$$B_{ij} = \sum_k F_{ik}F_{jk}, \quad \frac{\partial B_{kl}}{\partial F_{ij}} = \delta_{ki}F_{lj} + \delta_{li}F_{kj} \tag{7.22}$$

$$I_1 = \sum_k\sum_l F_{kl}^2 = ||\mathbf{F}||_F^2, \quad I_2 = \frac{1}{2}\left(I_1^2 - \sum_k\sum_l B_{kl}^2\right) \tag{7.23}$$

$$\frac{\partial I_1}{\partial F_{ij}} = 2F_{ij}, \quad \frac{\partial I_2}{\partial F_{ij}} = 2\left(I_1F_{ij} - \sum_k B_{ik}F_{kj}\right), \quad \frac{\partial J}{\partial F_{ij}} = J(F_{ji})^{-1}, \quad \frac{\partial I_3}{\partial F_{ij}} = 2I_3(F_{ji})^{-1} \tag{7.24}$$

$$\frac{\partial \overline{I_1}}{\partial F_{ij}} = \frac{2}{J^{2/3}}\left(F_{ij} - \frac{I_1(F_{ij})^{-1}}{3}\right) = \frac{2F_{ij}}{J^{2/3}} - \frac{2\overline{I_1}(F_{ij})^{-1}}{3} \tag{7.25}$$

$$\frac{\partial \overline{I_2}}{\partial F_{ij}} = \frac{2\overline{I_1}F_{ij}}{J^{2/3}} - \frac{2\sum_k B_{ik}F_{kj}}{J^{4/3}} - \frac{4\overline{I_2}(F_{ij})^{-1}}{3} \tag{7.26}$$

the Cauchy stress can be found from

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\mathbf{B} + \frac{\partial W}{\partial I_2}\left(I_1\mathbf{B} - \mathbf{B}^2\right)\right] \tag{7.27}$$

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + 2\left[\frac{1}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{1}{J^{7/3}}\frac{\partial W}{\partial \overline{I_2}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right)\right] \tag{7.28}$$

$$\boldsymbol{\sigma} = \sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k}\boldsymbol{b}_k \otimes \boldsymbol{b}_k \tag{7.29}$$

where $\boldsymbol{b}_k$ is the eigenvector of $\mathbf{B}$ associated with eigenvalue λ_k^2. 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

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + 2\left[\frac{1}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\mathrm{dev}(\mathbf{B}) + \frac{1}{J^{7/3}}\frac{\partial W}{\partial \overline{I_2}}\mathrm{dev}(I_1\mathbf{B} - \mathbf{B}^2)\right] \tag{7.30}$$

The pressure ($P = -\mathrm{Tr}(\boldsymbol{\sigma})/3$) can be found (making use of $\mathrm{Tr}(\mathrm{dev}(\cdot)) = 0$) from three results as

$$P = -\frac{\partial W}{\partial J} - \frac{2}{3J}\left[\frac{\partial W}{\partial I_1}I_1 + \frac{\partial W}{\partial I_2}2I_2\right] \tag{7.31}$$

$$P = -\frac{\partial W}{\partial J} \tag{7.32}$$

$$P = -\frac{1}{3}\sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k} \tag{7.33}$$

with the last one assuming orthonormal eigenvectors. Thus the deviatoric Cauchy stresses are ($\mathbf{s} = \boldsymbol{\sigma} + P\mathbf{I}$):

$$\mathbf{s} = \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\text{dev}(\mathbf{B}) + \frac{\partial W}{\partial I_2}\text{dev}\left(I_1\mathbf{B} - \mathbf{B}^2\right)\right] \tag{7.34}$$

$$\mathbf{s} = \frac{2}{J}\left[\frac{1}{J^{2/3}}\frac{\partial W}{\partial \overline{I}_1}\text{dev}(\mathbf{B}) + \frac{1}{J^{4/3}}\frac{\partial W}{\partial \overline{I}_2}\text{dev}(I_1\mathbf{B} - \mathbf{B}^2)\right] \tag{7.35}$$

$$\mathbf{s} = \sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k}\text{dev}(\boldsymbol{b}_k \otimes \boldsymbol{b}_k) \tag{7.36}$$

In MPM, we track the Kirchoff stress $\boldsymbol{\tau} = J\boldsymbol{\sigma}$ given by

$$\tau_{kl} = \sum_j F_{kj}\frac{\partial W}{\partial F_{lj}} \tag{7.37}$$

To implement incremental elasticity, we would like to get the fourth rank tensor. For $W(I_1, I_2, J)$,

$$\frac{\partial W}{\partial F_{lj}} = \frac{\partial W}{\partial J}J(F_{jl})^{-1} + 2\frac{\partial W}{\partial I_1}F_{lj} + 2\frac{\partial W}{\partial I_2}\left(I_1 F_{lj} - \sum_m B_{lm}F_{mj}\right) \tag{7.38}$$

$$\tau_{kl} = \sum_j F_{kj}\frac{\partial W}{\partial F_{lj}} = J\frac{\partial W}{\partial J}\delta_{kl} + 2\left[\frac{\partial W}{\partial I_1}B_{kl} + \frac{\partial W}{\partial I_2}\left(I_1 B_{kl} - \sum_m B_{km}B_{ml}\right)\right] \tag{7.39}$$

Differentiation again gives:

$$\begin{aligned}\frac{\partial \tau_{kl}}{\partial F_{ij}} &= J(F_{ij})^{-1}\frac{\partial W}{\partial J}\delta_{kl} + J\frac{\partial^2 W}{\partial F_{ij}\partial J}\delta_{kl} + 2\frac{\partial^2 W}{\partial F_{ij}\partial I_1}B_{kl} + 2\frac{\partial W}{\partial I_1}(\delta_{ki}F_{lj} + \delta_{li}F_{kj}) \\ &\quad + 2\frac{\partial^2 W}{\partial F_{ij}\partial I_2}I_1 B_{kl} + 2\frac{\partial W}{\partial I_2}\frac{\partial I_1}{\partial F_{ij}}B_{kl} + 2\frac{\partial W}{\partial I_2}I_1(\delta_{ki}F_{lj} + \delta_{li}F_{kj}) \\ &\quad - \sum_n 2\frac{\partial^2 W}{\partial F_{ij}\partial I_2}B_{ln}F_{nm} - 2\frac{\partial W}{\partial I_2}\delta_{li}C_{mj} - 2\frac{\partial W}{\partial I_2}F_{lj}F_{im} - 2\frac{\partial W}{\partial I_2}B_{li}\delta_{mj}\end{aligned} \tag{7.40}$$

Finding the second derivatives, but for $W(I_1, J)$ only gives:

$$\frac{\partial^2 W}{\partial J\partial F_{ij}} = \frac{\partial}{\partial J}\left[\frac{\partial W}{\partial J}J(F_{ji})^{-1} + 2\frac{\partial W}{\partial I_1}F_{ij}\right] \tag{7.41}$$

$$= \frac{\partial^2 W}{\partial J^2}J(F_{ji})^{-1} + \frac{\partial W}{\partial J}(F_{ji})^{-1} + \frac{\partial W}{\partial J}J\frac{\partial (F_{ji})^{-1}}{\partial J} + 2\frac{\partial^2 W}{\partial J\partial I_1}F_{ij} + 2\frac{\partial W}{\partial I_1}\frac{\partial F_{ij}}{\partial J} \tag{7.42}$$

Alternatively, look direction at Cauchy pressure and deviatoric stress due to increments in J and B and $W(\overline{I_1}, J)$:

$$\frac{\partial P}{\partial J} = -\frac{\partial^2 W}{\partial J^2} \tag{7.43}$$

$$\frac{\partial s_{kl}}{\partial B_{ij}} = \frac{\partial}{\partial B_{ij}}\left[\frac{2}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right] \tag{7.44}$$

$$\begin{aligned} &= \frac{2}{J^{5/3}}\left[\left(\frac{\partial^2 W}{\partial B_{ij}\partial \overline{I_1}} - \frac{5}{3J}\frac{\partial J}{\partial B_{ij}}\frac{\partial W}{\partial \overline{I_1}}\right)\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right. \\ &\quad \left. + \frac{\partial W}{\partial \overline{I_1}}\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\frac{\partial I_1}{\partial B_{ij}}\delta_{kl}\right)\right]\end{aligned} \tag{7.45}$$

7.4 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

$$W(\overline{I_1},\overline{I_2},J) = \frac{G_1}{2}\left(\overline{I_1}-3\right)+\frac{G_2}{2}\left(\overline{I_2}-3\right)+\frac{K}{2}(J-1)^2 \tag{7.46}$$

where G_1, G_2, and K are material properties. For low strains, this material is equivalent for a linear elastic, isotropic material with shear modulus G_1+G_2 and bulk modulus K. If $G_2=0$, the material is one form or a neo-Hookean material (another form is given below). See below for alternate compressibility terms. Some hyperelastic rubber models assume incompressible materials, which corresponds to $K\rightarrow\infty$; such models do not work in dynamic code (because wave speed is infinite), although they can be used in membranes.

The Cauchy (or true stress) is found by differentiating the strain energy to get

$$\boldsymbol{\sigma} = \frac{G_1}{J^{5/3}}\left(\mathbf{B}-\frac{I_1}{3}\mathbf{I}\right)+\frac{G_2}{J^{7/3}}\left(I_1\mathbf{B}-\mathbf{B}^2-\frac{2I_2}{3}\mathbf{I}\right)+K(J-1)\mathbf{I} \tag{7.47}$$

The stress components can be divided into pressure, P, and deviatoric stress, $\mathbf{s}=\boldsymbol{\sigma}+P\mathbf{I}$, which explicitly evaluate to:

$$P = -K(J-1) \tag{7.48}$$

$$s_{xx} = G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}}+G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2-B_{xz}^2+2B_{yz}^2}{3J^{7/3}} \tag{7.49}$$

$$s_{yy} = G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}}+G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2+2B_{xz}^2-B_{yz}^2}{3J^{7/3}} \tag{7.50}$$

$$s_{zz} = G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}}+G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2-B_{xz}^2-B_{yz}^2}{3J^{7/3}} \tag{7.51}$$

$$s_{xy} = G_1\frac{B_{xy}}{J^{5/3}}+G_2\frac{B_{zz}B_{xy}-B_{xz}B_{yz}}{J^{7/3}} \tag{7.52}$$

$$s_{xz} = G_1\frac{B_{xz}}{J^{5/3}}+G_2\frac{B_{yy}B_{xz}-B_{xy}B_{yz}}{J^{7/3}} \tag{7.53}$$

$$s_{yz} = G_1\frac{B_{yz}}{J^{5/3}}+G_2\frac{B_{xx}B_{yz}-B_{xy}B_{xz}}{J^{7/3}} \tag{7.54}$$

7.4.1 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 $P=-K(J-1)$, $s_{xz}=s_{yz}=0$, and

$$s_{xx} = G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}}+G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{7.55}$$

$$s_{yy} = G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}}+G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{7.56}$$

$$s_{zz} = G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}}+G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2}{3J^{7/3}} \tag{7.57}$$

$$s_{xy} = G_1\frac{B_{xy}}{J^{5/3}}+G_2\frac{B_{zz}B_{xy}}{J^{7/3}} \tag{7.58}$$

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 ε_{zz} and other stresses.

In the presence of residual stresses (see details below), $\sigma_{zz} = 0$ is found by solving $f = 0$ where

$$f = -3J_{res}J_{eff}^2 P(J_{eff}) + G_1 J^{1/3}(2B_{zz} - \alpha_1) + \frac{G_2}{J^{1/3}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{7.59}$$

where $P(J_{eff})$ is the pressure model used, $\alpha_1 = B_{xx} + B_{yy}$, $\alpha_2 = B_{xx}B_{yy} - B_{xy}^2$, $J^2 = \det(\mathbf{B}) = B_{zz}\alpha_2$, and $J_{eff} = J/J_{res}$. More explicitly in B_{zz}, the function is

$$f = -3J_{res}J_{eff}^2 P(J_{eff}) + G_1 B_{zz}^{1/6}\alpha_2^{1/6}(2B_{zz} - \alpha_1) + \frac{G_2}{B_{zz}^{1/6}\alpha_2^{1/6}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{7.60}$$

For more efficient Newton's method, we need

$$\frac{df}{dB_{zz}} = -3J_{res}\frac{d\left(J_{eff}^2 P(J_{eff})\right)}{dJ_{eff}}\frac{dJ_{eff}}{dB_{zz}} + \frac{G_1 J^{1/3}(14B_{zz} - \alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1 B_{zz} + 2\alpha_2)}{6B_{zz}J^{1/3}} \tag{7.61}$$

where $J_{eff} = \sqrt{B_{zz}\alpha_2}/J_{res}$ and $B_{zz}(dJ_{eff}/dB_{zz}) = \sqrt{B_{zz}\alpha_2}/(2J_{res})$. The first term simplifies to:

$$\frac{df}{dB_{zz}} = -\frac{3J}{2B_{zz}}\frac{d\left(J_{eff}^2 P(J_{eff})\right)}{dJ_{eff}} + \frac{G_1 J^{1/3}(14B_{zz} - \alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1 B_{zz} + 2\alpha_2)}{6B_{zz}J^{1/3}} \tag{7.62}$$

For the pressure term above

$$-\frac{3J}{2B_{zz}}\frac{d\left(J_{eff}^2 P(J_{eff})\right)}{dJ_{eff}} = \frac{3J}{2B_{zz}}KJ_{eff}(3J_{eff} - 2) \tag{7.63}$$

Other pressure models are given below.

7.4.2 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

$$\mathbf{F} = \mathbf{F}^*\mathbf{F}^{res} = \mathbf{F}^*\lambda_{res}\mathbf{I} \tag{7.64}$$

where λ_{res} is total extension due to free thermal and moisture expansion:

$$\lambda_{res} = \exp(\alpha\Delta T + \beta\Delta c) \approx 1 + \alpha\Delta T + \beta\Delta c \tag{7.65}$$

where the approximation is for small ΔT and Δx. The stresses and energy, however, should be found using $\mathbf{F}^*$ instead of $\mathbf{F}$, where $\mathbf{F}^*$ is now deformation from the current free expansion volume instead of from the initial volume. The net effects are $\mathbf{F}^* = \mathbf{F}/\lambda_{res}$, $J_{eff} = |\mathbf{F}^*| = J/\lambda_{res}^3$, and $\mathbf{B}_{eff} = \mathbf{B}/\lambda_{res}^2$. In the above equations, the Cauchy stress is found by replacing J with J_{eff} in the pressure model and by multiplying all shear terms by $J_{res} = \lambda_{res}^3$, or explicitly by three equivalent forms:

$$\boldsymbol{\sigma} = \frac{J_{res}G_1}{J^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{J_{res}G_2}{J^{7/3}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{7.66}$$

$$\boldsymbol{\sigma} = \frac{G_1}{J_{eff}J^{2/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{G_2}{J_{eff}J^{4/3}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{7.67}$$

$$\boldsymbol{\sigma} = \frac{G_1}{J_{res}^{2/3}J_{eff}^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{G_2}{J_{res}^{4/3}J_{eff}^{7/3}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{7.68}$$

These results reduce to the proper low-strain thermoelastic relation at small strain. In this limit

$$\mathbf{B} \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad I_1 \approx 3 + 2\mathrm{Tr}(\boldsymbol{\varepsilon}), \quad \mathbf{B}^2 \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad J \approx 1 + \mathrm{Tr}(\boldsymbol{\varepsilon}), \quad \text{and} \quad \frac{1}{J_{res}} \approx 1 - 3\alpha\Delta T \tag{7.69}$$

leading to

$$\boldsymbol{\sigma} = G_1\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + G_2\left(2\boldsymbol{\varepsilon} + \left(I_1\left(1 - \frac{I_1}{3}\right) - 1 + \frac{\mathbf{B}\cdot\mathbf{B}}{3}\right)\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} \tag{7.70}$$

Using $\mathbf{B}\cdot\mathbf{B} \approx 3 + 4\mathrm{Tr}(\boldsymbol{\varepsilon})$ leads to

$$\begin{aligned} \boldsymbol{\sigma} &= (G_1 + G_2)\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} & (7.71)\\ &= \left[\left(K - \frac{2}{3}(G_1 + G_2)\right)\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3K\alpha\Delta T\right]\mathbf{I} + 2(G_1 + G_2)\boldsymbol{\varepsilon} & (7.72)\end{aligned}$$

which is the expected result where $G_1 + G_2$ is the low-strain shear modulus.

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_{eff} 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 $J_{eff,k+1} = dJ_{eff}J_{eff,k}$, which is

$$J_{eff,k+1} = \frac{V_{k+1}}{V_{sf,k+1}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}\frac{V_k}{V_{sf,k}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}J_{eff,k} = dJ_{eff}J_{eff,k} \tag{7.73}$$

which implies that

$$dJ_{eff} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}} = dJ/d\lambda_{res}^3 \tag{7.74}$$

where

$$d\lambda_{res} = \exp(\alpha dT + \beta dc) \approx 1 + \alpha dT + \beta dc \tag{7.75}$$

where dT and dc are temperature and concentration changes on the current time step.

7.4.3 Alternate Bulk Modulus Term

Besides the dilation energy term used above of

$$W = \frac{K}{2}(J-1)^2 \qquad \text{with} \qquad P = -K(J-1), \tag{7.76}$$

two alternative compressibility terms are:

$$W = \frac{K}{2}(\ln J)^2 \qquad \text{and} \qquad W = \frac{K}{2}\left(\frac{1}{2}(J^2-1) - \ln J\right) \tag{7.77}$$

which gives normal Cauchy pressure terms of

$$P = -K\frac{\ln J}{J} \qquad \text{and} \qquad P = -\frac{K}{2}\left(J - \frac{1}{J}\right) \tag{7.78}$$

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 the second one

above. This one correctly leads to inifinite positive stress as $J \to \infty$ and infinite negative stress as $J \to 0$. This later one is the default for this material in `NairnMPM`.

When implementing plane stress, the pressure term derivatives for these two new laws are:

$$\frac{d(J_{eff}^2 P(J_{eff}))}{dJ_{eff}} = -K\frac{d\left(J_{eff}\ln J_{eff}\right)}{dJ_{eff}} = -K(1+\ln J_{eff}) \tag{7.79}$$

$$\frac{d(J_{eff}^2 P(J_{eff}))}{dJ_{eff}} = -\frac{K}{2}\frac{d\left(J_{eff}^3 - J_{eff}\right)}{dJ_{eff}} = -\frac{K}{2}(3J_{eff}^2 - 1) \tag{7.80}$$

7.4.4 Tangent Bulk Modulus

The incremental bulk modulus is

$$\frac{1}{K(P)} = -\frac{d\ln V}{dP} = -\frac{d\ln J_{eff}}{dP} \qquad \text{or} \qquad K = -J_{eff}\frac{dP}{dJ_{eff}} \tag{7.81}$$

The various bulk moduli are:

$$P = -K_0(J_{eff}-1) \qquad \text{gives} \qquad K = K_0 J_{eff} \tag{7.82}$$

$$P = -K_0\frac{\ln J_{eff}}{J_{eff}} \qquad \text{gives} \qquad K = K_0\frac{1-\ln J_{eff}}{J_{eff}^2} \tag{7.83}$$

$$P = -\frac{K_0}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \qquad \text{gives} \qquad K = \frac{K_0}{2}\left(J_{eff} + \frac{1}{J_{eff}}\right) \tag{7.84}$$

If implementing increment pressure law, the result is:

$$P_n = P_{n-1} - K(J_{eff})d\ln J_{eff} = P_{n-1} - K(J_{eff})\ln dJ_{eff} \tag{7.85}$$

7.4.5 Tangent Shear Modulus

Assuming $G_2 = 0$, the deviatoric stress is

$$\mathsf{s} = \frac{J_{res}G_1}{J^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) \tag{7.86}$$

and the tangent shear modulus including residual stresses is

$$\frac{\partial s_{kl}}{\partial B_{ij}} = \frac{J_{res}G_1}{J^{5/3}}\left[\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\frac{\partial I_1}{\partial B_{ij}}\delta_{kl}\right) - \frac{5}{3J}\frac{\partial J}{\partial B_{ij}}\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right] \tag{7.87}$$

$$= \frac{J_{res}G_1}{J^{5/3}}\left[\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\delta_{ij}\delta_{kl}\right) - \frac{5}{6}(B_{ij})^{-1}\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right] \tag{7.88}$$

This form follows by using $\det(\mathbf{B}) = J^2$ and tensor calculus result for derivative of a determinant of a symmetric tensor:

$$\frac{\partial J^2}{\partial B_{ij}} = J^2(B_{ij})^{-1} = 2J\frac{\partial J}{B_{ij}} \qquad \text{or} \qquad \frac{\partial J}{\partial B_{ij}} = \frac{J}{2}(B_{ij})^{-1} \tag{7.89}$$

The normal and shear deviatoric stress increments are:

$$\frac{\partial s_{kk}}{\partial B_{ij}} = \frac{J_{res}G_1}{3J^{5/3}}\left[\left(3\delta_{ki}\delta_{kj}-\delta_{ij}\right)-\frac{5}{6}(B_{ij})^{-1}\left(3B_{kk}-I_1\right)\right] \tag{7.90}$$

$$\frac{\partial s_{kl}\ (k\neq l)}{\partial B_{ij}} = \frac{J_{res}G_1}{J^{5/3}}\left[\delta_{ki}\delta_{lj}-\frac{5}{6}(B_{ij})^{-1}\left(B_{kl}\right)\right] \tag{7.91}$$

Explicitly, for example:

$$\frac{3J^{5/3}}{J_{res}G_1}\frac{\partial s_{xx}}{\partial B_{ij}} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} - \frac{5}{6}\mathbf{B}^{-1}(2B_{xx}-B_{yy}-B_{zz}) \tag{7.92}$$

$$\frac{J^{5/3}}{J_{res}G_1}\frac{\partial s_{xy}}{\partial B_{ij}} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{5}{6}\mathbf{B}^{-1}B_{xy} \tag{7.93}$$

7.5 Neo-Hookean Material

Although using $G_2 = 0$ is 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:

$$W(I_1,I_2,J) = \frac{G}{2}(I_1-3-2\ln J)+\frac{\lambda}{2}(\ln J)^2 \tag{7.94}$$

where G is shear modulus and λ is the Lamé constant. The Cauchy stress (after accounting for residual stresses) is

$$\boldsymbol{\sigma} = \frac{\lambda \ln J_{eff}}{J_{eff}}\mathbf{I}+\frac{G}{J_{eff}}\left(\frac{\mathbf{B}}{J_{res}^{2/3}}-\mathbf{I}\right) \tag{7.95}$$

In the low strain limit, $J = 1+\mathrm{Tr}(\boldsymbol{\varepsilon})$, $J_{res} = 1+3\alpha\Delta T$, and $\mathbf{B} = \mathbf{I}+2\boldsymbol{\varepsilon}$. The stress simplifies to

$$\boldsymbol{\sigma} = \left(\lambda \mathrm{Tr}(\boldsymbol{\varepsilon})-(3\lambda+2G)\alpha\Delta T\right)\mathbf{I}+2G\boldsymbol{\varepsilon} \qquad \text{low strain} \tag{7.96}$$

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:

$$P = P(J_{eff})-\frac{G}{J_{eff}}\left(\frac{B_{xx}+B_{yy}+B_{zz}}{3J_{res}^{2/3}}-1\right) \tag{7.97}$$

$$s_{xx} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{xx}-B_{yy}-B_{zz}\right) \tag{7.98}$$

$$s_{yy} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{yy}-B_{xx}-B_{zz}\right) \tag{7.99}$$

$$s_{zz} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{zz}-B_{xx}-B_{zz}\right) \tag{7.100}$$

$$s_{ij} = \frac{J_{res}^{1/3}G}{J}B_{ij} \qquad \text{for } i\neq j \tag{7.101}$$

where $P(J_{eff})$ uses any pressure above except that K is replaced by λ. the Cauchy stresses are:

$$\sigma_{xx} = \frac{J_{res}^{1/3}G}{J}\left(B_{xx} - J_{res}^{2/3}\right) - P(J_{eff}) \tag{7.102}$$

$$\sigma_{yy} = \frac{J_{res}^{1/3}G}{J}\left(B_{yy} - J_{res}^{2/3}\right) - P(J_{eff}) \tag{7.103}$$

$$\sigma_{zz} = \frac{J_{res}^{1/3}G}{J}\left(B_{zz} - J_{res}^{2/3}\right) - P(J_{eff}) \tag{7.104}$$

$$\sigma_{ij} = \frac{J_{res}^{1/3}G}{J}B_{ij} \qquad \text{for } i \neq j \tag{7.105}$$

When doing plane stress calculations, one task is to solve for $\sigma_{zz} = 0$, which is equivalent to solving numerically for $f = 0$ give

$$f = -J_{res}^{2/3}J_{eff}P(J_{eff}) + G\left(B_{zz} - J_{res}^{2/3}\right) \tag{7.106}$$

$$\frac{df}{dB_{zz}} = G - \frac{J_{res}^{2/3}J_{eff}}{2B_{zz}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} \tag{7.107}$$

which used $J_{eff} = \sqrt{B_{zz}\alpha_2}/J_{res}$ with $\alpha_2 = B_{xx}B_{yy} - B_{xy}^2$ leading to $(dJ_{eff}/dB_{zz}) = J_{eff}/(2B_{zz})$. This equation can be solved analytically for two pressure models, but requires numerical solution for the third. The two analytical solutions are

$$B_{zz} = J_{res}^2\frac{\lambda + 2G}{\lambda\alpha_2 + 2GJ_{res}^{4/3}} \qquad \text{when} \quad J_{eff}P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff}^2 - 1\right) \tag{7.108}$$

and

$$\sqrt{B_{zz}} = J_{res}\frac{\lambda\sqrt{\alpha_2} + \sqrt{\lambda^2\alpha_2 + 4G\left(\lambda\alpha_2 + GJ_{res}^{4/3}\right)}}{2\left(\lambda\alpha_2 + GJ_{res}^{4/3}\right)} \tag{7.109}$$

when $P(J_{eff}) = -\lambda\left(J_{eff} - 1\right)$. A third pressure law has $P(J_{eff}) = -\lambda\ln J_{eff}/J_{eff}$ leading to

$$f = G\left(B_{zz} - J_{res}^{2/3}\right) + \lambda J_{res}^{2/3}\ln J_{eff} \tag{7.110}$$

$$\frac{df}{dB_{zz}} = G + \frac{\lambda J_{res}^{2/3}}{2B_{zz}} \tag{7.111}$$

7.5.1 Tangent Bulk Modulus

To support adiabatic heating (or state dependent wave speeds), we need K as a function of deformation. Using $K = -J_{eff}dP/dJ_{eff}$ gives The various bulk moduli are (using J for J_{eff}):

$$P(J_{eff}) = -\lambda(J-1) \qquad \text{gives} \qquad K = \lambda J + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{7.112}$$

$$P(J_{eff}) = -\lambda\frac{\ln J}{J} \qquad \text{gives} \qquad K = \lambda\frac{1-\ln J}{J^2} + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{7.113}$$

$$P(J_{eff}) = -\frac{\lambda}{2}\left(J - \frac{1}{J}\right) \qquad \text{gives} \qquad K = \frac{\lambda}{2}\left(J + \frac{1}{J}\right) + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{7.114}$$

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

$$G\left(1 - J^{2/3} + \frac{2}{3J^{1/3}}\right) = \frac{2G}{3}\left(\frac{1}{J^{1/3}} + \frac{3(1-J^{2/3})}{2}\right) \tag{7.115}$$

which appears to be the only way to evaluate K for a fixed particle state.

7.6 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

$$W = G(J_P)||\mathbf{F}_E - \mathsf{R}_E||_F^2 + \frac{\lambda(J_p)}{2}(J_E - 1)^2 \tag{7.116}$$

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

$$G(J_P) = G_0 e^{\xi(1-J_P)} \qquad \text{and} \qquad \lambda(\mathrm{J_P}) = \lambda_0 \mathrm{e}^{\xi(1-\mathrm{J_P})} \tag{7.117}$$

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

$$\begin{aligned} ||\mathbf{F} - \mathsf{R}||_F^2 &= \mathrm{Tr}\big((\mathbf{F} - \mathsf{R})^T(\mathbf{F} - \mathsf{R})\big) = \mathrm{Tr}\big((\mathsf{U} - \mathbf{I})^T R^T R(\mathsf{U} - \mathbf{I})\big) = ||\mathsf{U} - \mathbf{I}||_F^2 & (7.118)\\ &= ||\mathsf{Q}^T(\Lambda - \mathbf{I})\mathsf{Q}||_F^2 = ||\Lambda - \mathbf{I}||_F^2 = (\lambda_1 - 1)^2 + (\lambda_2 - 1)^2 + (\lambda_3 - 1)^2 & (7.119)\end{aligned}$$

The energy function is more practically written as

$$W(\lambda_1, \lambda_2, \lambda_3) = G(J_P)\sum_i (\lambda_i - 1)^2 + \frac{\lambda(J_p)}{2}(\lambda_1\lambda_2\lambda_3 - 1)^2 \tag{7.120}$$

where λ_i are the stretches of the elastic part of the deformation. 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

$$\begin{aligned} \boldsymbol{\sigma} &= \sum_k \left(\frac{2G(J_P)}{J_E}\lambda_k(\lambda_k - 1) + \lambda(J_p)(J_E - 1)\right)\boldsymbol{b}_k \otimes \boldsymbol{b}_k & (7.121)\\ P &= -\lambda(J_p)(J_E - 1) - \frac{2G(J_P)}{3J_E}\big(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 - \lambda_1 - \lambda_2 - \lambda_3\big) & (7.122)\end{aligned}$$

where $\boldsymbol{b}_k$ are eigenvectors of elastic $\mathbf{B}$ 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 $\mathbf{B}$:

$$\mathbf{F}_{n+1} = d\mathbf{F}\,\mathbf{F}_n, \qquad J_{n+1} = |d\mathbf{F}|J_n, \qquad \text{and} \qquad \mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{7.123}$$

2. Find eigenvalues and eigenvectors of $\mathbf{B}_{n+1}^{trial}$ as $(\lambda_{1,trial}^2, \lambda_{2,trial}^2, \lambda_{2,trial})$ and the matrix Q with eigenvectors on the columns.

3. If all $\lambda_{i,trial}^2$ 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 $J_E = J_{n+1}/J_P$.

4. If any $\lambda_{i,trial}^2$ exceeds the range, clamp them to that range and find $\mathbf{B}_{n+1} = \mathrm{Q}^T\Lambda\mathrm{Q}$ where Λ is diagonal matrix with the clamped values of λ_i on the diagonal, $J_E = \lambda_1\lambda_2\lambda_3$, and update J_P to $J_P = J/J_E$.

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).

7.6.1 Deformation Examples

This modified co-rotated, neo-Hookean material is not commonly documented in the literature on large deformation materials. Here are some special case deformation examples. For uniform dilation ($\lambda_i = 1+\varepsilon$, and eigenvectors $= \hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$) the pressure is:

$$P = -\left[\lambda(J_p)\left(1+\varepsilon+\frac{1}{3}\varepsilon^2\right) - \frac{2G(J_P)}{3(1+\varepsilon)^2}\right]3\varepsilon \tag{7.124}$$

For small ε, this result reduces to

$$P = -\left(\lambda(J_p) + \frac{2G(J_P)}{3}\right)3\varepsilon = -K\frac{\Delta V}{V} \tag{7.125}$$

as expected for small-strain, isotropic materials.

For constrained, uniaxial tension ($\lambda_1 = 1+\varepsilon$, $\lambda_2 = \lambda_3 = 1$, and eigenvectors $= \hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$):

$$\sigma_{xx} = \big(\lambda(J_p) + 2G(J_P)\big)\,\varepsilon \qquad \text{and} \qquad \sigma_{yy} = \sigma_{zz} = \lambda(J_p)\varepsilon \tag{7.126}$$

This result is the same as for small-strain, isotropic materials (*i.e.*, linear at all deformations and a weakness of this material).

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 $\hat{\boldsymbol{z}}$):

$$\sigma_{xx} = \frac{2G(J_P)}{\lambda\lambda_y}\lambda(\lambda-1) + \lambda(J_p)(\lambda\lambda_y - 1) \tag{7.127}$$

$$\sigma_{yy} = \frac{2G(J_P)}{\lambda}(\lambda_y - 1) + \lambda(J_p)(\lambda\lambda_y - 1) \tag{7.128}$$

Solving for zero stress in the y direction gives

$$\lambda_y = \frac{2G(J_P) + \lambda\lambda(J_p)}{2G(J_P) + \lambda^2\lambda(J_p)} \tag{7.129}$$

Substituting into axial stress gives

$$\sigma_{xx} = \frac{2G(J_P)(\lambda-1)}{1+\lambda^2\frac{\lambda(J_p)}{2G(J_P)}}\left(\frac{\lambda(J_p)}{2G(J_P)} + \frac{\left(1+\lambda^2\frac{\lambda(J_p)}{2G(J_P)}\right)^2}{1+\lambda\frac{\lambda(J_p)}{2G(J_P)}}\right) \tag{7.130}$$

For linear shear ($F_{ii} = 1$. $F_{xy} = \gamma$, rest zero, and $J = 1$), the eigenvalues and eigenvectors of $\mathbf{B}$ are

$$\lambda_1^2 = \frac{1}{2}\left(2+\gamma^2+\gamma\sqrt{4+\gamma^2}\right) \tag{7.131}$$

$$\lambda_2^2 = \frac{1}{2}\left(2+\gamma^2-\gamma\sqrt{4+\gamma^2}\right) \tag{7.132}$$

$$\lambda_3^2 = 1 \tag{7.133}$$

$$\boldsymbol{b}_1 = \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4+\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma+\sqrt{4+\gamma^2}\right),1,0\right) \tag{7.134}$$

$$\boldsymbol{b}_2 = \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4-\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma-\sqrt{4+\gamma^2}\right),1,0\right) \tag{7.135}$$

$$\boldsymbol{b}_3 = (0,0,1) \tag{7.136}$$

The Cauchy stress reduces to

$$\boldsymbol{\sigma} = 2G(J_P)\left(\lambda_1(\lambda_1-1)\boldsymbol{b}_1\otimes\boldsymbol{b}_1 + \lambda_2(\lambda_2-1)\boldsymbol{b}_2\otimes\boldsymbol{b}_2\right) \tag{7.137}$$

The algebra is messy. With the help of Mathematica, the stress terms reduce too

$$\sigma_{xx} = G(J_P)\left(2(1+\gamma^2) + \frac{k_1(\gamma-\sqrt{4+\gamma^2}) - k_2(\gamma+\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{7.138}$$

$$\sigma_{yy} = G(J_P)\left(2 - \frac{k_1(\gamma+\sqrt{4+\gamma^2}) - k_2(\gamma-\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{7.139}$$

$$\tau_{xy} = 2G(J_P)\left(\gamma + \frac{k_1-k_2}{\sqrt{8+2\gamma^2}}\right) \tag{7.140}$$

$$\sigma_{zz} = 0 \tag{7.141}$$

where

$$k_1 = \sqrt{2+\gamma^2-\gamma\sqrt{4+\gamma^2}} \qquad \text{and} \qquad k_2 = \sqrt{2+\gamma^2+\gamma\sqrt{4+\gamma^2}} \tag{7.142}$$

Expanding in γ and keeping only linear terms reduces to small strain result of $\tau_{xy} = G\gamma$ with all other stresses zero.

For hydrostatic compression ($\lambda_i = J^{1/3}$), the pressure is

$$P = -\frac{2G(J_P)}{J_E^{2/3}}(J_E^{1/3}-1) - \lambda(J_p)(J_E-1) \tag{7.143}$$

which leads to bulk modulus of:

$$K = -J_E\frac{dP}{dJ_E} = \lambda(J_p)J_E + \frac{2G(J_P)}{3}\frac{2-J_E^{1/3}}{J_E^{2/3}} \tag{7.144}$$

This result has the correct small-strain limit of:

$$\lim_{J_E\to 1} K = \lambda(J_p) + \frac{2G(J_P)}{3} \tag{7.145}$$

7.7 Mie-Grüniesen Equation of State

The Mie-Grüniesen Equation of State defines the pressure only and the Cauchy pressure is

$$P = \frac{\rho_0 C_0^2 \eta \left(1 - \frac{1}{2}\gamma_0 \eta\right)}{(1 - S_1\eta - S_2\eta^2 - S_3\eta^3)^2} + \rho_0 \gamma_0 U \tag{7.146}$$

where η is fraction compression and given by

$$\eta = 1 - \frac{\rho_0}{\rho} = 1 - \frac{V}{V_0} = 1 - J \tag{7.147}$$

and γ_0, C_0, and S_i are material properties and U is total internal energy. The above equation applies only in compression ($\eta > 0$). In tension, the pressure uses on of the Mooney-Rivlin pressure laws:

$$P = -\rho_0 C_0^2 (J_{eff} - 1) \tag{7.148}$$

The Kirchhoff pressure needed by MPM is

$$\frac{\tau}{\rho_0} = \frac{JP}{\rho_0} \tag{7.149}$$

This material model also causes a temperature change of

$$dT = -T\gamma_0 \frac{\rho_0}{\rho} \frac{V(t + \Delta t) - V(t)}{V} + \frac{dq}{C_v} \tag{7.150}$$

where dq is dissipated energy that is converted to heat. The first term simplifies to an isentropic temperature change of

$$dT_{dq=0} = -JT\gamma_0 \frac{V(t + \Delta t) - V(t)}{V} \tag{7.151}$$

The volume change relative to current volume can be found from

$$\frac{V(t + \Delta t) - V(t)}{V(t + \Delta t)} = 1 - \frac{1}{|dF|} \tag{7.152}$$

The temperature rise here, which is

$$dT_{dq=0} = -JT\gamma_0 \frac{\Delta V}{V} \qquad vs. \qquad dT_{dq=0} = -JT \frac{K}{K_0} \gamma_0 \frac{\Delta V}{V} \tag{7.153}$$

from above. The result here differs by a factor (K/K_0). In tension, this material uses the full law with $(K/K_0) = J_{eff}$. See Eq. (7.204) for comparable results in an ideal gas.

Noticing that

$$\frac{dT_{dq=0}}{T} = \gamma_0 d\eta \tag{7.154}$$

The temperature due to isoentropic heating alone can be integrated to

$$T = T_0 \exp(\gamma_0 \eta) \tag{7.155}$$

Thus the total temperature rise (assuming C_v is constant) is

$$dT = T_0 (\exp(\gamma_0 \eta) - 1)) + \frac{\Phi}{C_v} \tag{7.156}$$

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."

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 this equation of state, the denominator in pressure might become zero before η reaches 1. For example, Tungsten has $S_1 = 1.24$ and $S_2 = S_3 = 0$. The denominator becomes zero when

$$\eta = 1/1.24 = 0.806 \tag{7.157}$$

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. To avoid this situation, `NairnMPM/OSParticulas` prevents it. In compression, bulk modulus should monotonically increase. When compression strain is too high for given material parameters, the incremental bulk modulus may decrease or become negative. `NairnMPM/OSParticulas` prevents decreasing or negative bulk modulus by limiting bulk modulus to the peak value determined by the parameters or to a user-input maximum increase (`Kmax` with default of $20 * K_0$), whichever is lower. A warning is printed the first time the compression reaches the limiting value.

7.7.1 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:

$$3\alpha = \frac{\rho_0 \gamma_0 C_v}{K_0} \qquad \text{or} \qquad \gamma_0 = \frac{3K_0\alpha}{\rho_0 C_v} \tag{7.158}$$

which is same as defined above in Eq. (4.11).

Under free thermal expansion, $U = C_v \Delta T$. In small strain compression

$$P = -K_0 \frac{\Delta V}{V_0} + 3K_0 \alpha \Delta T \tag{7.159}$$

and for free thermal expansion, $P = 0$ which leads to

$$\frac{\Delta V}{V_0} = 3\alpha \Delta T \tag{7.160}$$

This volume change is the expected volume change for free thermal expansion.

7.8 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

$$P = JP(J_{eff}) \tag{7.161}$$

$$s_{xx}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{xx}^{trial} - B_{yy}^{trial} - B_{zz}^{trial}\right) \tag{7.162}$$

$$s_{yy}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{yy}^{trial} - B_{xx}^{trial} - B_{zz}^{trial}\right) \tag{7.163}$$

$$s_{zz}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{zz}^{trial} - B_{xx}^{trial} - B_{yy}^{trial}\right) \tag{7.164}$$

$$s_{ij}^{trial} = \frac{J_{res}G_1}{J^{2/3}}B_{ij}^{trial} \qquad \text{for } i \neq j \tag{7.165}$$

where $P(J_{eff})$ is any hyperelaastic pressure model, J is relative volume change, J_{res} is the volume change related to residual stresses, and $J_{eff} = J/J_{res}$. 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:

$$\mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{7.166}$$

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

$$\mathbf{s} = J_{res}G_1 \mathrm{dev}\,\overline{\mathbf{B}} \tag{7.167}$$

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

$$f_{trial} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}K(\alpha) \tag{7.168}$$

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:

$$\mathbf{B} = \mathbf{B}^{trial} - \frac{2}{3}\lambda\overline{I_1}\mathbf{n} \tag{7.169}$$

$$\mathbf{s} = \mathbf{s}^{trial} - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right)\mathbf{n} \tag{7.170}$$

$$\|\mathbf{s}\| = \|\mathbf{s}^{trial}\| - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right) \tag{7.171}$$

where $\mathbf{n}$ is normal defined from deviatoric stress tensor and

$$\overline{I_1} = \frac{B_{xx} + B_{yy} + B_{zz}}{J^{2/3}} \tag{7.172}$$

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

$$\overline{\mu} = \frac{J_{res}G\overline{I_1}}{3} \tag{7.173}$$

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. (7.163) 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 **s** and **B** on the particle.

7.9 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

$$PV = nRT \tag{7.174}$$

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:

$$\rho_0 = \frac{P_0}{T_0}\frac{M}{R} \tag{7.175}$$

We can now eliminate n and R to derive

$$P = P_0\frac{V_0}{V}\frac{T}{T_0} = P_0\frac{T}{T_0}\frac{1}{J} \tag{7.176}$$

where $J = \det\mathbf{F} = V/V_0$. The Cauchy stress due to this pressure is $-P\mathbf{I}$, which implies hyperelastic energy function determined from:

$$\boldsymbol{\sigma} = -P_0\frac{T}{T_0}\frac{1}{J}\mathbf{I} = \frac{dU(J)}{dJ}\mathbf{I} \qquad \text{or} \qquad U(J) = -P_i \ln J \tag{7.177}$$

where $P_i = P_0T/T_0$ is the initial pressure (when $J = 1$). This energy is equal to the energy per unit initial volume for isothermal compression or expansion of an ideal gas:

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\,dV = -\frac{P_0T}{T_0}\int_{V_0}^{V}\frac{1}{V}\,dV = -P_i \ln\frac{V}{V_0} = -P_i \ln J \tag{7.178}$$

For MPM calculations, the code needs a specific Kirchoff stress normalized to ρ_0 or

$$\boldsymbol{\tau}^{(s)} = -\frac{PJ}{\rho_0}\mathbf{I} = -\frac{P_0}{\rho_0}\frac{T}{T_0}\mathbf{I} \tag{7.179}$$

In coding, an incremental approach is preferred. If $\tau_n^{(s)}$ is any diagonal element of the specific Kirchoff stress tensor for time step n, then

$$\tau_{n+1}^{(s)} = -\frac{P_0}{\rho_0}\frac{T_{n+1}}{T_0} = -\frac{P_0}{\rho_0}\frac{T_n}{T_0}\frac{T_{n+1}}{T_n} = \tau_n^{(s)}\frac{T_{n+1}}{T_n} \tag{7.180}$$

Note that the Kirchoff stress remains constant for isothermal expansion and compression.

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

$$\frac{dU}{\rho_0 V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1} - V_n}{V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1}}{V_0}\left(1 - \frac{V_n}{V_{n+1}}\right) \tag{7.181}$$

Let deformation gradient for step $n+1$ be

$$\mathbf{F}_{n+1} = \mathbf{f}\cdot\mathbf{F}_n \quad \text{where} \quad \mathbf{f} = \exp(\Delta t\nabla \boldsymbol{v}) \quad \text{and} \quad J_{n+1} = \det\mathbf{f}\,J_n \tag{7.182}$$

which leads to

$$\frac{dU}{\rho_0 V_0} = -\frac{J_{n+1}}{2}\frac{P_n + P_{n+1}}{\rho_0}\left(1 - \frac{1}{\det f}\right) = -\frac{1}{2}\left(\frac{P_n}{\rho_n}\det f + \frac{P_{n+1}}{\rho_{n+1}}\right)\left(1 - \frac{1}{\det f}\right) \tag{7.183}$$

But, P/ρ is $-\tau^{(s)}$ leading to

$$\frac{dU}{\rho_0 V_0} = \frac{1}{2}\left(\tau_n^{(s)}\det f + \tau_{n+1}^{(s)}\right)\left(1 - \frac{1}{\det f}\right) \tag{7.184}$$

When gas particles are present, they have to be initialized to the pressure (or stress) of

$$\tau_i^{(s)} = -\frac{P_i}{\rho_0} = -\frac{P_0}{\rho_0}\frac{T}{T_0} \tag{7.185}$$

where T is the simulation reference temperature (need not be the gas reference temperature, which can be any desired reference condition). All simulations with gas particles must therefore specify a reference temperature in degrees Kelvin.

This material always needs heat capacity and needs thermal conductivity when doing conduction. Heat capacity 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

$$C_v = \frac{3}{2}\frac{P_0}{\rho_0 T_0} \tag{7.186}$$

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.

For wave speed calculations, the bulk modulus for adiabatic conditions is

$$K = -\frac{\frac{V}{V_0}}{\frac{d(V/V_0)}{dP}} = \gamma P = \frac{\gamma\rho RT}{M} \tag{7.187}$$

In terms of defined material properties, the wave speed reduces to

$$C = \sqrt{\frac{K}{\rho}} = \sqrt{\frac{5\rho_0 P_0 T}{3T_0}} \tag{7.188}$$

where T is particle temperature.

7.9.1 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:

$$\begin{aligned} P &= \frac{P_i}{1+\varepsilon_{xx}} && (7.189)\\ U &= 0 && (7.190)\\ w &= -P_i V_0 \ln(1+\varepsilon_{xx}) && (7.191)\\ q &= -w && (7.192)\\ S &= nR\ln(1+\varepsilon_{xx}) = \frac{P_0 V_0}{T_0}\ln(1+\varepsilon_{xx}) && (7.193) \end{aligned}$$

For adiabatic compression and expansion

$$\begin{aligned} P &= \frac{P_i}{(1+\varepsilon_{xx})^{\gamma}} && (7.194)\\ T &= \frac{T_i}{(1+\varepsilon_{xx})^{\gamma-1}} && (7.195)\\ U &= C_v(T-T_i) = \frac{3P_0V_0}{2T_0}T_i\left(\frac{1}{(1+\varepsilon_{xx})^{\gamma-1}}-1\right) && (7.196)\\ w &= U && (7.197)\\ q &= 0 && (7.198)\\ S &= -(\gamma-1)C_v\ln(1+\varepsilon_{xx}) + \frac{P_0V_0}{T_0}\ln(1+\varepsilon_{xx}) = 0 && (7.199) \end{aligned}$$

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:

$$\eta = 1 - \frac{T_2}{T_1} \qquad (7.200)$$

where T_1 is the hot reservoir and T_2 is the cold one.

7.9.2 Isothermal *vs.* Adiabatic *vs.* General Constitutive Law

Equation (7.172) can be rewritten as an increment in pressure from initial pressure P_0 at temperature T_0:

$$P - P_0 = \kappa_0\left[\left(\frac{J_{res}}{J}\right)-1\right] \qquad (7.201)$$

where κ_0 is the bulk modulus at P_0:

$$\frac{1}{\kappa_0} = -\frac{1}{V_0}\left(\frac{\partial V_0}{\partial P}\right)_T = \frac{1}{P_0} \qquad (7.202)$$

and

$$J = \frac{V(P,T)}{V(P_0,T_0)} = \frac{V}{V_0} \qquad \text{and} \qquad J_{res} = \frac{V(P_0,T)}{V(P_0.T_0)} = \frac{T}{T_0} \qquad (7.203)$$

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:

$$T = \frac{T_0}{J^{\gamma-1}} \qquad \text{and} \qquad J_{res} = \frac{1}{J^{\gamma-1}} \tag{7.204}$$

Two special cases of the general law, therefore, are:

$$P - P_0 = \kappa_0 \left[\left(\frac{1}{J} \right) - 1 \right] \qquad \text{isothermal} \tag{7.205}$$

$$P - P_0 = \kappa_0 \left[\left(\frac{1}{J} \right)^{\gamma} - 1 \right] \qquad \text{adiabatic} \tag{7.206}$$

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. For an ideal case undergoing in increment in volume of dV, the temperature change is

$$dT = -\frac{P dV}{C_v} = -\frac{nRT}{C_v} \frac{dV}{V} = -\frac{nRT}{C_v} \frac{\rho}{\rho_0} \frac{dV}{V_0} \tag{7.207}$$

In other words, all the work is converted into heat. Also notice that this result can be written

$$\frac{dT}{T} = \frac{nR}{C_v} \frac{1}{J} d\eta = \frac{\gamma_0}{J} d\eta = -\gamma_0 \frac{dJ}{J} \qquad \text{where} \qquad \eta = 1 - \frac{\rho_0}{\rho} = 1 - J \tag{7.208}$$

For a monatoic ideal gas $\gamma_0 = 2/3$; for a diatomic gas $\gamma_0 = 2/5$; for both $\gamma_0 = \gamma - 1$. This result is identical to the Mie-Grüniesen theory in Eq. (7.149) by using $K = P$, $3\alpha = 1/T$ and $C_v = (3/2)nR/(\rho V)$ (or $5/2$ for diatomic gas).

7.9.3 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 Wasls gas law is

$$\left(P - \frac{an^2}{V^2} \right) \left(\frac{V}{n} - b \right) = RT \tag{7.209}$$

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

$$P = \left(P_0 - a' \right) \left(\frac{1 - b'}{J - b'} \right) \frac{T}{T_0} + \frac{a'}{J^2} \tag{7.210}$$

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

$$U(J) = -\left[\left(P_i - a' \right) \left(1 - b' \right) \ln(J - b') - \frac{a'}{J} \right] \tag{7.211}$$

where P_i is the initial particle pressure (when $J = 1$) of

$$P_i = \left(P_0 - a'\right)\frac{T}{T_0} + a' \tag{7.212}$$

This energy is equal to the energy per unit initial volume for isothermal compression or expansion of a van der Waals gas:

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\,dV = -\int_1^J \left(\left(P_i - a'\right)\left(\frac{1-b'}{J-b'}\right) + \frac{a'}{J^2}\right) dJ \tag{7.213}$$

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

$$U = C_v(T - T_0) - \frac{a'}{\rho_0 J} \tag{7.214}$$

In hyperelastic code, an incremental form is

$$dU = C_v dT + \frac{a'}{\rho_0 J^2} dJ \tag{7.215}$$

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

$$\frac{ab}{V_0^2}n^3 - \frac{a}{V_0}n^2 - (P_0 b + RT_0)n + P_0 V_0 = 0 \tag{7.216}$$

This n is needed to find a', b' and C_v.

7.10 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:

$$V(P,T) = V(0,T)\left[1 - C\ln\left(1 + \frac{P}{B(T)}\right)\right] \tag{7.217}$$

where $C = 0.894$ 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

$$V(0,T) = A_0 + A_1 T + A_2 T^2 + \cdots \tag{7.218}$$

$$V(0,T) = V(0,T_0)e^{\beta(T-T_0)} \tag{7.219}$$

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

$$B(T) = B_0 e^{-B_1 T} \tag{7.220}$$

Note that bulk modulus from the Tait equation is

$$\frac{1}{K(P,T)} = -\frac{1}{V}\left(\frac{dV}{dP}\right)_T = \frac{C}{P+B(T)}\frac{1}{\left[1-C\ln\left(1+\frac{P}{B(T)}\right)\right]} = \frac{C}{P+B(T)}\frac{V(P,T)}{V(0,T)} \tag{7.221}$$

which shows that $B(T)$ is proportional to the temperature dependence of the zero-pressure bulk modulus:

$$B(T) = CK(0,T) \tag{7.222}$$

`NairnMPM` currently assumes temperature independent bulk modulus or assumes $B_1 = 0$. The pressure dependence to the thermal expansion coefficient is

$$\beta(P,T) = \frac{1}{V}\left(\frac{dV}{dT}\right)_P = \beta(0,T) - \frac{PB_1}{K(P,T)} \tag{7.223}$$

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

$$J = \frac{V(P,T)}{V(0,T_0)} \qquad \text{and} \qquad J_{res} = \frac{V(0,T)}{V(0,T_0)} = e^{\beta_0(T-T_0)} \tag{7.224}$$

as relative volumes. The constitutive law is rewritten as

$$\frac{J}{J_{res}} = 1 - C\ln\left(1+\frac{P}{CK_0}\right) \tag{7.225}$$

where K_0 is the zero-pressure bulk modulus. This equation can be solved for pressure:

$$P = CK_0\left[\exp\left(\frac{1-J^*}{C}\right)-1\right] \tag{7.226}$$

where $J^* = J/J_{res}$. This material is equivalent to a hyperelastic material with volumetric strain energy function of

$$U(J^*) = CK_0\left[C\exp\left(\frac{1-J^*}{C}\right)+J^*\right] \tag{7.227}$$

This energy function equals the energy per unit initial volume for isothermal compression or expansion of a Tait liquid.

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:

$$\tau = \eta\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T - \frac{2}{3}\mathrm{Tr}(\nabla\mathbf{v})\mathbf{I}\right) \tag{7.228}$$

where $\nabla\mathbf{v}$ is the velocity gradient and η is the viscosity. The total stress is given by $\sigma = -P\mathbf{I} + \tau$.

When the low-pressure bulk modulus is independent of temperature, the pressure dependent bulk modulus is

$$K(P,T) = \frac{P+CK_0}{C}J^* = K_0\exp\left(\frac{1-J^*}{C}\right)J^* \tag{7.229}$$

This results 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

$$dP = -K_0\exp\left(\frac{1-J^*}{C}\right)dJ^* = -K(P,T)d\ln J^* = -K(P,T)\ln dJ^* \tag{7.230}$$

Another option might to find finite dP and expand in a series:

$$\Delta P = CK_0\left[\exp\left(\frac{1-dJ^*J^*}{C}\right)-\exp\left(\frac{1-J^*}{C}\right)\right] \tag{7.231}$$

where $dJ^* = dJ/dJ_{res}$ is change in volume and residual stress term. Expanding in a series (using Mathematica):

$$\begin{aligned}\Delta P &= -K_0\exp\left(\frac{1-J^*}{C}\right)\left(\Delta J^*-\frac{(\Delta J^*)^2}{2C}+\frac{(\Delta J^*)^3}{6C^2}-\frac{(\Delta J^*)^4}{24C^3}+\cdots\right) &(7.232)\\ &= -K_0\exp\left(\frac{1-J^*}{C}\right)\left(\Delta J^*-\frac{\Delta J^*}{2C}\left(\Delta J^*-\frac{\Delta J^*}{3C}\left(\Delta J^*-\frac{(\Delta J^*)^2}{4C}+\cdots\right)\right)\right) &(7.233)\end{aligned}$$

where

$$\Delta J^* = \left(\frac{dJ}{dJ_{res}}-1\right)J^* \tag{7.234}$$

is the increment in J^* in the time step.

Chapter 8

Hyperelastic Membrane Modeling

This chapter looks at membrane modeling where deformation is limit to some membrane stress state. The implement is done using hyperelastic materials and done for both 2D (membrane is a "string") and 3D (membrane is a "sheet").

8.1 Hyperelastic 1D Membrane in a 2D Simulation

A membrane in a 2D simulation is a 1D path through the object (this notes are plane stress and plane strain only and will need to be updated for axisymnetry). Imagine a coordinate system with the fiber direction of the membrane initially along the x axis and the thickness direction along the y axis. In membrane models, it is assumed there is no shear deformation in the plane of the membrane — it has only stretches in fiber direction and thickness directions. As a result, the general deformation gradient is:

$$\mathbf{F} = \begin{pmatrix} \lambda_1 \cos\theta & \lambda_2 \sin\theta & 0 \\ -\lambda_1 \sin\theta & \lambda_2 \cos\theta & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \mathsf{R}[\lambda] \tag{8.1}$$

where λ_i are stretches in three orthogonal membrane directions (and they remain orthogonal) and θ is the clockwise rotation of the current fiber direction from the global, positive x axis direction. The first and second columns are vectors along the current fiber and thickness directions, respectively.

In an MPM time step, the membrane constitutive law will be provided an incremental deformation gradient, $\mathbf{dF}$ (as calculated above), but in general this deformation will not be compatible with a membrane deformation with zero shear. Instead, $\mathbf{dF}$ is just used to find new fiber vector:

$$\boldsymbol{m} = (\mathbf{dF}_{11}\mathsf{F}_{11} + \mathbf{dF}_{12}\mathsf{F}_{21}, \mathbf{dF}_{21}\mathsf{F}_{11} + \mathbf{dF}_{22}\mathsf{F}_{21}) \tag{8.2}$$

The magnitude of this vector is the new fiber stretch: $\lambda_1 = ||\boldsymbol{m}||$. A specific membrane material model should calculations λ_2 and λ_3 and then update the particle's deformation gradient to be:

$$\mathbf{F} = \begin{pmatrix} m_x & -\frac{\lambda_2}{\lambda_1} m_y & 0 \\ m_y & \frac{\lambda_2}{\lambda_1} m_x & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \tag{8.3}$$

For stresses and energy, membrane material classes find Kirchhoff stress in the unrotated membrane coordinates (which should only need the three λ_i stretches and ω). These stresses are rotated to the

MPM coordinates:

$$\boldsymbol{\tau} = \mathsf{R}\boldsymbol{\tau}\mathsf{R}^T = \mathsf{R}[\lambda]\big([\lambda]^{-1}\boldsymbol{\sigma}[\lambda]^{-T}\big)[\lambda]^T\mathsf{R}^T = \mathbf{F}\mathsf{S}\mathbf{F}^T \tag{8.4}$$

where $\mathbf{F}$ is the updated membrane deformation gradient on the particle and S is the second Poila-Kirchoff stress in the mebrane coordinates. The second Poila-Kirchoff stress will only have non-zero S_{11}, S_{12}, and S_{22} and it is found from $\mathsf{S} = [\lambda]^{-1}\boldsymbol{\tau}[\lambda]^{-T}$ or $S_{11} = \tau_{11}/\lambda_1^2$.

Work and residual energy updates can be done in the membrane coordinates:

$$dw = \tau_{11}du_{11} \qquad \text{and} \qquad dw_{res} = \tau_{11}du_{11}^{res} + \tau_{33}du_{33}^{res} \tag{8.5}$$

where du_{11} is element of the displacement gradient for this step and du_{res}^{ii} is incremental residual strain for this step. The displacement gradient can be found from the effective membrane incremental deformation gradient:

$$\mathbf{dF}_m = \exp(\nabla \boldsymbol{u}) = \begin{pmatrix} \frac{\lambda_1}{\lambda_1^{(n-1)}} & 0 & 0 \\ 0 & \frac{\lambda_2}{\lambda_2^{(n-1)}} & 0 \\ 0 & 0 & \frac{\lambda_2}{\lambda_2^{(n-1)}} \end{pmatrix} \quad \text{or} \quad du_{11} = \ln\frac{\lambda_1}{\lambda_1^{(n-1)}} \tag{8.6}$$

where $\lambda_1^{(n-1)}$ are the stretches at the start of the time step.

8.2 Hyperelastic 2D Membrane in a 3D Simulation

A membrane in a 3D simulation is a 2D surface through the object. Imagine a coordinate system with the two fiber directions of the membrane initially along the x and y axes and the thickness direction along the z axis. In membrane models, it is assumed the normal and shear stresses in the thickness direction of the membrane are zero — the membrane has only stretches and shear in the plane defined by the two fiber directions. As a result, the general deformation gradient can be written as:

$$\mathbf{F} = \mathsf{R}\begin{pmatrix} \lambda_1 & \lambda_2\cos\omega & 0 \\ 0 & \lambda_2\sin\omega & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \mathsf{R}[\lambda\omega] \tag{8.7}$$

where λ_i are stretches in three initially orthogonal membrane directions and ω is the angle between the deformed, in-plane fiber directions. The rotation matrix R rotates the positive x axis to the corresponding fiber axis in the deformed membrane.

In an MPM time step, the membrane constitutive law will be provided an incremental deformation gradient, $\mathbf{dF}$ (as calculated above), but in general this deformation will not be compatible with a membrane deformation where thickness direction should have stretch only and zero shear. Instead, $\mathbf{dF}$ is just used to find new fiber vectors from the first two columns of $\mathbf{dF}\cdot\mathbf{F}$. If these deformed vectors are $\boldsymbol{m_1}$ and $\boldsymbol{m_2}$ then the key deformation terms are:

$$\lambda_1 = ||\boldsymbol{m_1}||, \quad \lambda_2 = ||\boldsymbol{m_2}||, \quad \cos\omega = \frac{\boldsymbol{m_1}\cdot\boldsymbol{m_2}}{\lambda_1\lambda_2}, \quad \text{and} \quad \sin\omega = \frac{||\boldsymbol{m_1}\times\boldsymbol{m_2}||}{\lambda_1\lambda_2} \tag{8.8}$$

A specific membrane material model should calculate λ_3 for the thickness direction (to get zero thickness stress). The particle deformation gradient is updated with $\boldsymbol{m_1}$, $\boldsymbol{m_2}$ left intact as first two columns, but the third column of the provisional $\mathbf{dF}\cdot\mathbf{F}$ is changed to be $\lambda_3(\boldsymbol{m_1}\times\boldsymbol{m_2})/(\lambda_1\lambda_2)$. In this approach, the membrane normal vector remains normal to both $\boldsymbol{m_1}$ and $\boldsymbol{m_2}$.

For stresses and energy, membrane material classes finds Kirchhoff stress ($\boldsymbol{\tau}$) in the unrotated membrane coordinates (which should only need the three λ_i stretches and ω). These stresses are rotated to the MPM coordinates:

$$\boldsymbol{\tau}\ (\text{MPM}) = \mathsf{R}\boldsymbol{\tau}\mathsf{R}^T = \mathsf{R}[\lambda\omega]\big([\lambda\omega]^{-1}\boldsymbol{\tau}[\lambda\omega]^{-T}\big)[\lambda\omega]^T\mathsf{R}^T = \mathbf{F}\mathsf{S}\mathbf{F}^T \tag{8.9}$$

where $\mathbf{F}$ is the updated membrane deformation gradient on the particle and S is the second Poila-Kirchoff stress in the membrane coordinates. The second Poila-Kirchoff stress will only have non-zero S_{11}, S_{12}, and S_{22} and it is found from $\mathsf{S} = [\lambda\omega]^{-1}\boldsymbol{\tau}[\lambda\omega]^{-T}$ or:

$$\mathsf{S} = \begin{pmatrix} \frac{1}{\lambda_1} & -\frac{\cot\omega}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix} \begin{pmatrix} \tau_{11} & \tau_{12} & 0 \\ \tau_{12} & \tau_{y22} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_1} & 0 & 0 \\ -\frac{\cot\omega}{\lambda_1} & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix} \tag{8.10}$$

The result is

$$\mathsf{S} = \begin{pmatrix} \frac{1}{\lambda_1} & -\frac{\cot\omega}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix} \begin{pmatrix} \frac{\tau_{11}}{\lambda_1} - \frac{\tau_{12}\cot\omega}{\lambda_1} & \frac{\tau_{12}}{\lambda_2\sin\omega} & 0 \\ \frac{\tau_{12}}{\lambda_1} - \frac{\tau_{22}\cot\omega}{\lambda_1} & \frac{\tau_{22}}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{8.11}$$

which simplifies to

$$S_{11} = \frac{1}{\lambda_1^2}\left(\tau_{11} - 2\tau_{12}\cot\omega + \tau_{22}\cot^2\omega\right) \tag{8.12}$$

$$S_{22} = \frac{\tau_{22}}{\lambda_2^2\sin^2\omega} \tag{8.13}$$

$$S_{12} = \frac{(\tau_{12} - \tau_{22}\cot\omega)}{\lambda_1\lambda_2\sin\omega} \tag{8.14}$$

These can be inverted to

$$\tau_{11} = S_{11}\lambda_1^2 + 2S_{12}\lambda_1\lambda_2\cos\omega + S_{22}\lambda_2^2\cos^2\omega \tag{8.15}$$

$$\tau_{22} = S_{22}\lambda_2^2\sin^2\omega \tag{8.16}$$

$$\tau_{12} = S_{12}\lambda_1\lambda_2\sin\omega + S_{22}\lambda_2^2\cos\omega\sin\omega \tag{8.17}$$

The membrane deformation (or $[\lambda\omega]$) is tracked on the particle in the plastic strain. Work and residual energy updates can be done in the membrane coordinates:

$$dw = \tau_{11}du_{11} + \tau_{12}(du_{12} + du_{21}) + \tau_{22}du_{22} \tag{8.18}$$

$$dw_{res} = \tau_{11}du_{11}^{res} + \tau_{12}(du_{12}^{res} + (du_{12}^{res}) + \tau_{22}du_{22}^{res} \tag{8.19}$$

where du_{ij} are elements of the displacement gradient for this step and du_{res}^{ij} are incremental residual strains for this step. The displacement gradient can be found from the effective membrane incremental deformation gradient, which is defined by $[\lambda\omega] = \mathbf{dF}_m[\lambda\omega]_{n-1}$ giving

$$\mathbf{dF}_m = \exp(\nabla\boldsymbol{u}) = [\lambda\omega][\lambda\omega]_{n-1}^{-1} = \begin{pmatrix} \lambda_1 & \lambda_2\cos\omega & 0 \\ 0 & \lambda_2\sin\omega & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \begin{pmatrix} \frac{1}{M_{11}} & -\frac{M_{12}}{M_{11}M_{22}} & 0 \\ 0 & \frac{1}{M_{22}} & 0 \\ 0 & 0 & \frac{1}{M_{33}} \end{pmatrix} \tag{8.20}$$

$$= \begin{pmatrix} \frac{\lambda_1}{M_{11}} & \frac{\lambda_2\cos\omega}{M_{22}} - \frac{M_{12}\lambda_1}{M_{11}M_{22}} & 0 \\ 0 & \frac{\lambda_2\sin\omega}{M_{22}} & 0 \\ 0 & 0 & \frac{\lambda_3}{M_{33}} \end{pmatrix} \tag{8.21}$$

where $[\lambda\omega]_{n-1}$ is the membrane-coordinates deformation gradient at the start of the time step and M_{ij} are elements of $[\lambda\omega]_{n-1}$. Assuming that gradient of the displacement vector has non-zero elements the same places as $\mathbf{dF}_m$, the exponential can be evaluated:

$$\exp(\nabla \boldsymbol{u}) = \begin{pmatrix} e^{du_{11}} & \frac{du_{12}}{du_{11}}\left(e^{du_{22}} - e^{du_{11}}\right) & 0 \\ 0 & e^{du_{22}} & 0 \\ 0 & 0 & e^{du_{33}} \end{pmatrix} \tag{8.22}$$

From which

$$du_{11} = \ln \frac{\lambda_1}{M_{11}} \tag{8.23}$$

$$du_{22} = \ln \frac{\lambda_2 \sin\omega}{M_{22}} \tag{8.24}$$

$$du_{33} = \ln \frac{\lambda_3}{M_{33}} \tag{8.25}$$

$$du_{12} = \ln \frac{\lambda_1}{M_{11}} \frac{\frac{\lambda_2 \cos\omega}{M_{22}} - \frac{M_{12}\lambda_1}{M_{11}M_{22}}}{\frac{\lambda_2 \sin\omega}{M_{22}} - \frac{\lambda_1}{M_{11}}} \tag{8.26}$$

Alternatively, the incremental work can be written as

$$dw = \mathbf{S} \cdot \dot{\mathbf{E}}\, dt = \frac{1}{2}\mathbf{S} \cdot \dot{\mathbf{C}}\, dt \tag{8.27}$$

where $\mathbf{E}$ is Green-Lagrange strain. Evaluating $\dot{\mathbf{C}}$ and using $\dot{\mathbf{F}} = \nabla v \mathbf{F}$ gives

$$\dot{\mathbf{C}} = \dot{\mathbf{F}}^T\mathbf{F} + \mathbf{F}^T\dot{\mathbf{F}} = \mathbf{F}^T\left(\nabla v^T + \nabla v\right)\mathbf{F} \tag{8.28}$$

The energy increment (using tensors in the membrane coordinates) becomes

$$dw = \mathbf{S} \cdot [\lambda\omega]^T \left(\frac{1}{2}\left(\nabla u^T + \nabla u\right)\right)[\lambda\omega] \tag{8.29}$$

Expansion of this expression is identical to Eq. (8.18) (as it must be).

8.3 Membrane Material Tasks

Much of the work for membrane model is done by the `MemPoint2D.cpp`, `MemPointAS.cpp` and `MemPoint3D.cpp` classes. These classes do the following tasks:

1. Use **dF** to find λ_1 (2D), λ_1 and λ_3 (AS), or λ_1, λ_2, and ω (3D).
2. Call the material class, which will complete these calculations
   (a) For 2D and axisymmetric simulations, find λ_2, λ_3 (plane stress only), τ_{11} and $\tau_{33} = \tau_{zz}$. For 3D simulations, find λ_3, τ_{11}, τ_{12}, and τ_{22} (τ_{33} is zero, which may be used in the material model when finding the other quantities).
   (b) Alternatively, a membrane material can find S_{ij} in the membrane instead of τ_{ij} and then set `isPoila` variable to `true`.

(c) Call method to update residual energy (it is done in the material to be able to handle anisotropic materials).

(d) Call method to track temperature, entropy, and heat on the particle.

3. Find du_{ij} and increment work energy
4. Store $[\lambda]$ (2D) or $[\lambda\omega]$ (3D) in the particle plastic strain
5. Update $\mathbf{F}$ on the particle
6. Rotate membrane stress to MPM coordinates and store on the particle stresses.

The material class works in a simplified deformation system. In 2D plane stress simulations with fiber stretch λ_1, $J = \lambda_1\lambda_2\lambda_3$ and $\lambda_2 = \lambda_3 = \sqrt{J/\lambda_1}$ (assuming isotropic). The left Cauchy-Green deformation tensor in the membrane coordinates has non-zero elements $\mathsf{B}_{11} = \lambda_1^2$ and $\mathsf{B}_{22} = \mathsf{B}_{33} = J/\lambda_1$.

In 2D plane strain (or axisymmetric) simulations with fiber stretch λ_1, $J = \lambda_1\lambda_2\lambda_3$, $\lambda_3 = 1$ (plane strain) or is an input λ_3 (axisymmetric), and $\lambda_2 = J/(\lambda_1\lambda_3)$. The left Cauchy-Green deformation tensor in the membrane coordinates has non-zero elements $\mathsf{B}_{11} = \lambda_1^2$, $\mathsf{B}_{22} = J^2/(\lambda_1^2\lambda_3^2)$, and $\mathsf{B}_{33} = \lambda_3^2$.

In 3D simulations with fiber stretches λ_1 and λ_2, $J = \lambda_1\lambda_2\lambda_3\sin\omega$, and $\lambda_3 = J/(\lambda_1\lambda_2\sin\omega)$. The left Cauchy-Green deformation tensor in the membrane coordinates is

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} \lambda_1^2 + \lambda_2^2\cos^2\omega & \lambda_2^2\sin\omega\cos\omega & 0 \\ \lambda_2^2\sin\omega\cos\omega & \lambda_2^2\sin^2\omega & 0 \\ 0 & 0 & \lambda_3^2 \end{pmatrix} \tag{8.30}$$

and the right Cauchy-Green deformation tensor in the membrane coordinates is

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} = \begin{pmatrix} \lambda_1^2 & \lambda_1\lambda_2\cos\omega & 0 \\ \lambda_1\lambda_2\cos\omega & \lambda_2^2 & 0 \\ 0 & 0 & \lambda_3^2 \end{pmatrix} \tag{8.31}$$

Finally, in `NairnMPM`, the membrane deformation matrix ($[\lambda]$ or $[\lambda\omega]$), is tracked on the particle using the particle's plastic strain. Note that other Hyperelastic materials track $\mathbf{B}$ in the plastic strain and hyperelastic, plasticity materials track the elastic $\mathbf{B}$; plastic membranes will need an alternate method to store elastic deformation information.

8.4 Mooney-Rivlin Material as Membrane

8.4.1 Plane Stress Mooney-Rivlin Membrane

Using the deformation state for plane stress membrane and defining $\lambda = \lambda_1$) a Mooney-Rivlin material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + 2J_{res}G_1\frac{\lambda^2 - \frac{J}{\lambda}}{3J^{5/3}} + 2J_{res}G_2\frac{\lambda - \frac{J}{\lambda^2}}{3J^{4/3}} \tag{8.32}$$

$$\sigma_{22} = \sigma_{33} = -P(J_{eff}) + J_{res}G_1\frac{\frac{J}{\lambda} - \lambda^2}{3J^{5/3}} + J_{res}G_2\frac{\frac{J}{\lambda^2} - \lambda}{3J^{4/3}} \tag{8.33}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = J_{res}G_1\frac{\lambda^2 - \frac{J}{\lambda}}{3J^{5/3}} + J_{res}G_2\frac{\lambda - \frac{J}{\lambda^2}}{3J^{4/3}} \tag{8.34}$$

For Newton's method, solve $f = 0$ for J using

$$f = 3J_{res}J_{eff}^2 P(J_{eff}) + (J^{1/3}G_1 + J^{2/3}G_2)\left(\lambda^2 - \frac{J}{\lambda}\right) \tag{8.35}$$

$$\frac{df}{dJ} = 3\frac{d(J_{eff}^2 P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G_1}{3}\left(\frac{\lambda^2}{J} - \frac{4}{\lambda}\right) + \frac{J^{2/3}G_2}{3}\left(\frac{2\lambda}{J} - \frac{5}{\lambda^2}\right) \tag{8.36}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{J^{2/3}G_2}{\lambda}\right)\left(\lambda^2 - \frac{J}{\lambda}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{8.37}$$

and $\lambda_2 = \lambda_3 = \sqrt{J/\lambda}$. Normally dynamic code cannot model an incompressible material, but an incompressible membrane material can be modeled by setting $J = J_{res}$ and $J_{eff} = 1$ or:

$$\tau_{11} = \left(J_{res}^{1/3}G_1 + \frac{J_{res}^{2/3}G_2}{\lambda}\right)\left(\lambda^2 - \frac{J_{res}}{\lambda}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{8.38}$$

and $\lambda_2 = \lambda_3 = \sqrt{J_{res}/\lambda}$. Note that during free thermal expansion, $J_{res} = \lambda^3$ and all stresses are zero.

8.4.2 Plane Stress Mooney-Rivlin Membrane — Alternate Approach

In this alternate approach, the new fiber stretch is found by conserving the imposed incremental volume change, dJ, and then finding the new fiber stretch to keep the thickness stress equal to zero.

In 2D plane stress simulations with incremental fiber stretch $d\lambda$, $J = J_n = d\lambda d\lambda_2 d\lambda_3 J_{n-1}$ and $d\lambda_2 = d\lambda_3 = \sqrt{dJ/d\lambda}$. The left Cauchy-Green deformation tensor current membrane coordinates has non-zero elements $\mathsf{B}_{11} = \lambda_n^2$, $\mathsf{B}_{22} = \mathsf{B}_{33} = J/\lambda_n$, where $\lambda_n = d\lambda\lambda$ is the new fiber stretch in the n^{th} step. For a Mooney-Rivlin material (here neo-hookean only with $G_1 = G$ and $G_2 = 0$) the normal Cauchy stresses are:

$$\sigma_{11} = -P(J_{eff}) + 2J_{res}G\frac{\lambda_n^2 - \frac{J}{\lambda_n}}{3J^{5/3}} \tag{8.39}$$

$$\sigma_{22} = \sigma_{33} = -P(J_{eff}) + J_{res}G\frac{\frac{J}{\lambda_n} - \lambda_n^2}{3J^{5/3}} \tag{8.40}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by solving $\sigma_{yy} = 0$ for $d\lambda = \lambda_n/\lambda_{n-1}$, which is a cubic equation:

$$\lambda_n^3 + \frac{3J^{2/3}J_{eff}P(J_{eff})}{G}\lambda_n - J = 0 \tag{8.41}$$

This depressed cubic can be found analytically. When this approach was tried, the resulting membrane seemed too stiff and the stiffness was a strong function of the Poisson's ratio. This approach is not recommended for MPM membrane analysis.

8.4.3 Plane Strain and Axisymmetric Mooney-Rivlin Membrane

Using the deformation state for plane strain or axiymmetric membranes and defining $\lambda = \lambda_1$, a Mooney-Rivlin material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + J_{res}G_1\frac{2\lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2} - \lambda_3^2}{3J^{5/3}} + J_{res}G_2\frac{\lambda^2\lambda_3^2 + \frac{J^2}{\lambda_3^2} - 2\frac{J^2}{\lambda^2}}{3J^{7/3}} \tag{8.42}$$

$$\sigma_{22} = -P(J_{eff}) + J_{res}G_1\frac{2\frac{J^2}{\lambda^2\lambda_3^2} - \lambda^2 - \lambda_3^2}{3J^{5/3}} + J_{res}G_2\frac{\frac{J^2}{\lambda_3^2} + \frac{J^2}{\lambda^2} - 2\lambda^2\lambda_3^2}{3J^{7/3}} \tag{8.43}$$

$$\sigma_{33} = -P(J_{eff}) + J_{res}G\frac{2\lambda_3^2 - \lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2}}{3J^{5/3}} + J_{res}G_2\frac{\lambda^2\lambda_3^2 + \frac{J^2}{\lambda^2} - 2\frac{J^2}{\lambda_3^2}}{3J^{7/3}} \tag{8.44}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = J_{res}G_1\frac{\lambda_3^2 + \lambda^2 - 2\frac{J^2}{\lambda^2\lambda_3^2}}{3J^{5/3}} + J_{res}G_2\frac{2\lambda^2\lambda_3^2 - \frac{J^2}{\lambda_3^2} - \frac{J^2}{\lambda^2}}{3J^{7/3}} \tag{8.45}$$

For Newton's method, solve $f = 0$ for J using

$$\begin{aligned} f &= 3J_{res}J_{eff}^2P(J_{eff}) + J^{1/3}G_1\left(\lambda_3^2 + \lambda^2 - 2\frac{J^2}{\lambda^2\lambda_3^2}\right) + \frac{G_2}{J^{1/3}}\left(2\lambda^2\lambda_3^2 - J^2\left(\frac{1}{\lambda_3^2} + \frac{1}{\lambda^2}\right)\right) \\ \frac{df}{dJ} &= 3\frac{d(J_{eff}^2P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G_1}{3}\left(\frac{\lambda_3^2 + \lambda^2}{J} - \frac{14J}{\lambda^2\lambda_3^2}\right) - \frac{G_2}{3J^{1/3}}\left(\frac{2\lambda^2\lambda_3^2}{J} + 5J\left(\frac{1}{\lambda_3^2} + \frac{1}{\lambda^2}\right)\right) \end{aligned} \tag{8.46}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{G_2\lambda_3^2}{J^{1/3}}\right)\left(\lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2}\right) \tag{8.47}$$

$$\tau_{33} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{G_2\lambda^2}{J^{1/3}}\right)\left(\lambda_3^2 - \frac{J^2}{\lambda^2\lambda_3^2}\right) \tag{8.48}$$

and $\lambda_2 = J/(\lambda\lambda_3)$. Normally dynamic code cannot model an incompressible material, but a plane strain incompressible membrane material can be modeled by setting $J = J_{res}$ and $J_{eff} = 1$ or:

$$\tau_{11} = \left(J_{res}^{1/3}G_1 + \frac{G_2\lambda_3^2}{J_{res}^{1/3}}\right)\left(\lambda^2 - \frac{J_{res}^2}{\lambda^2\lambda_3^2}\right) \tag{8.49}$$

$$\tau_{33} = \left(J_{res}^{1/3}G_1 + \frac{G_2\lambda^2}{J_{res}^{1/3}}\right)\left(\lambda_3^2 - \frac{J_{res}^2}{\lambda^2\lambda_3^2}\right) \tag{8.50}$$

and $\lambda_2 = J_{res}/(\lambda\lambda_3)$. Note that during free plane strain thermal expansion, $J_{res} = \lambda^2$ and $\lambda_3 = 1$ such that in-plane stress will be zero but τ_{33} will be non-zero due to restraint in that direction. For axisymmetric free thermal expansion, $J_{res} = \lambda^3$ and $\lambda_3 = \lambda$ such that all stresses are zero.

8.4.4 3D Mooney-Rivlin Membrane

Using the deformation state for 3D membranes, a Mooney-Rivlin material has the normal Cauchy stresses:

$$\begin{aligned}\sigma_{11} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(2\lambda_1^2 + \lambda_2^2(2\cos^2\omega - \sin^2\omega) - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\ &\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega + \left(\lambda_1^2 + \lambda_2^2(\cos^2\omega - 2\sin^2\omega)\right)\frac{J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (8.51)\end{aligned}$$

$$\begin{aligned}\sigma_{22} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(\lambda_2^2(2\sin^2\omega - \cos^2\omega) - \lambda_1^2 - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \qquad (8.52) \\ &\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega - \left(2\lambda_1^2 + \lambda_2^2(2\cos^2\omega - \sin^2\omega)\right)\frac{J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (8.53)\end{aligned}$$

$$\begin{aligned}\sigma_{33} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(\frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega} - \lambda_1^2 - \lambda_2^2\right) \qquad (8.54) \\ &\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\frac{(\lambda_1^2 + \lambda_2^2)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega} - 2\lambda_1^2\lambda_2^2\sin^2\omega\right) \qquad (8.55)\end{aligned}$$

$$\sigma_{12} = \frac{J_{res}G_1}{J^{5/3}}\lambda_2^2\sin\omega\cos\omega + \frac{J_{res}G_2}{J^{1/3}}\frac{\cos\omega}{\lambda_1^2\sin\omega} \qquad (8.56)$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{33} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{J_{res}G_1}{3J^{5/3}}\left(\lambda_1^2 + \lambda_2^2 - \frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) + \frac{J_{res}G_2}{3J^{7/3}}\left(2\lambda_1^2\lambda_2^2\sin^2\omega - \frac{(\lambda_1^2 + \lambda_2^2)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (8.57)$$

For Newton's method, solve $f = 0$ for J using

$$\begin{aligned}f &= 3J_{res}J_{eff}^2P(J_{eff}) + J^{1/3}G_1\left(\lambda_1^2 + \lambda_2^2 - \frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\ &\quad + \frac{G_2}{J^{1/3}}\left(2\lambda_1^2\lambda_2^2\sin^2\omega - \frac{(\lambda_1^2 + \lambda_2^2)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (8.58) \\ \frac{df}{dJ} &= 3\frac{d(J_{eff}^2P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G}{3}\left(\frac{\lambda_1^2 + \lambda_2^2}{J} - \frac{14J}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\ &\quad - \frac{G_2}{3J^{1/3}}\left(\frac{2\lambda_1^2\lambda_2^2\sin^2\omega}{J} + \frac{5(\lambda_1^2 + \lambda_2^2)J}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (8.59)\end{aligned}$$

Given this J, the final results for Kirchhoff stresses are:

$$\tau_{11} = \frac{J^{1/3}G_1}{J_{eff}}\left(\lambda_1^2+\lambda_2^2\cos^2\omega-\frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)+\frac{G_2}{J_{eff}J^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{J^2}{\lambda_1^2}\right) \tag{8.60}$$

$$\begin{aligned}\tau_{22} &= \frac{J^{1/3}G_1}{J_{eff}}\left(\lambda_2^2\sin^2\omega-\frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)\\ &\quad+\frac{G_2}{J_{eff}J^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{\left(\lambda_1^2+\lambda_2^2\cos^2\omega\right)J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)\end{aligned} \tag{8.61}$$

$$\tau_{12} = \frac{J^{1/3}G_1}{J_{eff}}\lambda_2^2\sin\omega\cos\omega+\frac{G_2}{J_{eff}J^{1/3}}\frac{J^2\cos\omega}{\lambda_1^2\sin\omega} \tag{8.62}$$

and $\lambda_3 = J/(\lambda_1\lambda_2\sin\omega)$. Normally dynamic code cannot model an incompressible material, but a 3D incompressible membrane material can be modeled by setting $J = J_{res}$ and $J_{eff} = 1$ or:

$$\tau_{11} = J_{res}^{1/3}G_1\left(\lambda_1^2+\lambda_2^2\cos^2\omega-\frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)+\frac{G_2}{J_{res}^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{J_{res}^2}{\lambda_1^2}\right) \tag{8.63}$$

$$\begin{aligned}\tau_{22} &= J_{res}^{1/3}G_1\left(\lambda_2^2\sin^2\omega-\frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)\\ &\quad+\frac{G_2}{J_{res}^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{\left(\lambda_1^2+\lambda_2^2\cos^2\omega\right)J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)\end{aligned} \tag{8.64}$$

$$\tau_{12} = J_{res}^{1/3}G_1\lambda_2^2\sin\omega\cos\omega+\frac{G_2}{J_{res}^{1/3}}\frac{J_{res}^2\cos\omega}{\lambda_1^2\sin\omega} \tag{8.65}$$

and $\lambda_3 = J_{res}/(\lambda_1\lambda_2\sin\omega)$. Note that during free thermal expansion, $J_{res} = \lambda^3$, $\lambda_1 = \lambda_2 = \lambda$ and $\cos\omega = 0$, which leads to all stresses equal to zero.

8.5 Neo-Hookean Material as Membrane

8.5.1 Plane Stress Neo-Hookean Membrane

Using the deformation state for plane stress membrane, a neo-Hookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff})+\frac{G}{J_{eff}}\left(\frac{\lambda_1^2}{J_{res}^{2/3}}-1\right) \tag{8.66}$$

$$\sigma_{22}=\sigma_{33} = -P(J_{eff})+\frac{G}{J_{eff}}\left(\frac{J}{\lambda_1 J_{res}^{2/3}}-1\right) \tag{8.67}$$

where the $P(J_{eff})$ is the pressure model (using λ instead of K). The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1-\frac{J}{\lambda_1 J_{res}^{2/3}}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G}-\frac{J_{res}^{1/3}J_{eff}}{\lambda_1}+1=0 \tag{8.68}$$

For two models, this can be solved analytically:

$$J_{eff} = -\frac{J_{res}^{1/3}G}{\lambda\lambda_1} + \sqrt{1+\frac{2G}{\lambda}+\left(\frac{J_{res}^{1/3}G}{\lambda\lambda_1}\right)^2} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff}-\frac{1}{J_{eff}}\right) \tag{8.69}$$

$$J_{eff} = \frac{1}{2}\left(1-\frac{J_{res}^{1/3}G}{\lambda\lambda_1} + \sqrt{\frac{4G}{\lambda}+\left(1-\frac{J_{res}^{1/3}G}{\lambda\lambda_1}\right)^2}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff}-1\right) \tag{8.70}$$

Notice for incompressible ($\lambda\to\infty$), undeformed ($J_{res}^{1/3}=\lambda_1=1$), and free thermal expansion ($J_{res}^{1/3}=\lambda_1$) that $J_{eff}=1$. The last model (with $J_{eff}P(J_{eff}) = -\lambda\ln J_{eff}$) must be solved numerically for J using Newton's method with:

$$f = \lambda_1 J_{res}^{2/3} J_{eff} P(J_{eff}) + G\left(\lambda_1 J_{res}^{2/3} - J\right) = -\lambda\lambda_1 J_{res}^{2/3}\ln J_{eff} + G\left(\lambda_1 J_{res}^{2/3} - J\right) \tag{8.71}$$

$$\frac{df}{dJ} = \frac{\lambda_1}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - G = -\frac{\lambda\lambda_1 J_{res}^{2/3}}{J} - G \tag{8.72}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 - \frac{J}{\lambda_1}\right) \qquad \text{and} \qquad \tau_{33} = 0 \tag{8.73}$$

with $\lambda_2=\lambda_3=\sqrt{J/\lambda_1}$. Normally dynamic code cannot model an incompressible material, but an incompressible membrane material can be modeled by setting $J=J_{res}$ and $J_{eff}=1$ or:

$$\tau_{11} = \frac{G}{J_{res}^{2/3}}\left(\lambda_1^2 - \frac{J_{res}}{\lambda_1}\right) \qquad \text{and} \qquad \tau_{33} = 0 \tag{8.74}$$

with $\lambda_2=\lambda_3=\sqrt{J_{res}/\lambda_1}$. Note that during free thermal expansion, $J_{res}=\lambda_1^3$ and all stresses are zero.

8.5.2 Plane Strain and Axisymmetric Neo-Hookean Membrane

Using the deformation state for plane strain or axiymmetric membranes, a neo-Hookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_1^2}{J_{res}^{2/3}} - 1\right) \tag{8.75}$$

$$\sigma_{22} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_3^2} - 1\right) \tag{8.76}$$

$$\sigma_{33} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_3^2}{J_{res}^{2/3}} - 1\right) \tag{8.77}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22}=0$ for J or solving:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1-\frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_3^2}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G} - \frac{J_{res}^{4/3}J_{eff}^2}{\lambda_1^2\lambda_3^2} + 1 = 0 \tag{8.78}$$

For two models, this can be solved analytically:

$$J_{eff} = \sqrt{\frac{\lambda+2G}{\lambda+2G\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_3^2}}} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \tag{8.79}$$

$$J_{eff} = \frac{1}{2}\left(\frac{1+\sqrt{1+\frac{4G}{\lambda}\left(1+\frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^1\lambda_3^2}\right)}}{1+\frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^1\lambda_3^2}}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff}-1\right) \tag{8.80}$$

Notice for incompressible ($\lambda \to \infty$), undeformed ($J_{res}^{1/3} = \lambda_1 = \lambda_3 = 1$), and free thermal expansion ($J_{res}^{1/3} = \lambda_1 = \lambda_3$) that $J_{eff} = 1$. The last model (with $J_{eff}P(J_{eff}) = -\lambda \ln J_{eff}$) must be solved numerically for J using Newton's method with:

$$f = \lambda_1^2\lambda_3^2 J_{res}^{2/3} J_{eff} P(J_{eff}) + G\left(\lambda_1^2\lambda_3^2 J_{res}^{2/3} - J^2\right) \tag{8.81}$$

$$= -\lambda\lambda_1^2\lambda_3^2 J_{res}^{2/3} \ln J_{eff} + G\left(\lambda_1^2\lambda_3^2 J_{res}^{2/3} - J^2\right) \tag{8.82}$$

$$\frac{df}{dJ} = \frac{\lambda_1^2\lambda_3^2}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - 2GJ = -\frac{\lambda\lambda_1^2\lambda_3^2 J_{res}^{2/3}}{J} - 2GJ \tag{8.83}$$

Given the solved J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3} G\left(\lambda_1^2 - \frac{J^2}{\lambda_1^2\lambda_3^2}\right) \quad \text{and} \quad \tau_{33} = J_{res}^{1/3} G\left(\lambda_3^2 - \frac{J^2}{\lambda_1^2\lambda_3^2}\right) \tag{8.84}$$

and $\lambda_2 = J/(\lambda_1\lambda_3)$. Normally dynamic code cannot model an incompressible material, but a plane strain incompressible membrane material can be modeled by setting $J = J_{res}$ and $J_{eff} = 1$ or:

$$\tau_{11} = J_{res}^{1/3} G\left(\lambda_1^2 - \frac{J_{res}^2}{\lambda_1^2\lambda_3^2}\right) \quad \text{and} \quad \tau_{33} = J_{res}^{1/3} G\left(\lambda_3^2 - \frac{J_{res}^2}{\lambda_1^2\lambda_3^2}\right) \tag{8.85}$$

and $\lambda_2 = J_{res}/(\lambda_1\lambda_3)$. Note that during free plane strain thermal expansion, $J_{res} = \lambda_1^2$ and $\lambda_3 = 1$ such that in-plane stress will be zero but τ_{33} will be non-zero due to restraint in that direction. For axisymmetric free thermal expansion, $J_{res} = \lambda_1^3$ and $\lambda_3 = \lambda_1$ such that all stresses are zero.

8.5.3 3D Neo-Hookean Membrane

Using the deformation state for 3D membranes, a neo-Hookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_1^2 + \lambda_2^2\cos^2\omega}{J_{res}^{2/3}} - 1\right) \tag{8.86}$$

$$\sigma_{22} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_2^2\sin^2\omega}{J_{res}^{2/3}} - 1\right) \tag{8.87}$$

$$\sigma_{33} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega} - 1\right) \tag{8.88}$$

$$\sigma_{12} = \frac{G}{J_{eff}}\frac{\lambda_2^2\sin\omega\cos\omega}{J_{res}^{2/3}} \tag{8.89}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by solving $\sigma_{33} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1 - \frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G} - \frac{J_{res}^{4/3}J_{eff}^2}{\lambda_1^2\lambda_2^2\sin^2\omega} + 1 = 0 \tag{8.90}$$

For two models, this can be solved analytically:

$$J_{eff} = \sqrt{\frac{\lambda + 2G}{\lambda + 2G\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}}} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \tag{8.91}$$

$$J_{eff} = \frac{1}{2}\left(\frac{1 + \sqrt{1 + \frac{4G}{\lambda}\left(1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)}}{1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff} - 1\right) \tag{8.92}$$

Notice for incompressible ($\lambda \to \infty$), undeformed ($J_{res}^{1/3} = \lambda_1 = \lambda_3 = \sin\omega = 1$), and free thermal expansion ($J_{res}^{1/3} = \lambda_1 = \lambda_3$ and $\sin\omega = 1$) that $J_{eff} = 1$. The last model (with $J_{eff}P(J_{eff}) = -\lambda \ln J_{eff}$) must be solved numerically for J using Newton's method with:

$$f = J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega(J_{eff}P(J_{eff})) + G\left(J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega - J^2\right) \tag{8.93}$$

$$= -\lambda J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega(\ln J_{eff}) + G\left(J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega - J^2\right) \tag{8.94}$$

$$\frac{df}{dJ} = \frac{\lambda_1^2\lambda_2^2\sin^2\omega}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - 2GJ = -\frac{\lambda J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega}{J} - 2GJ \tag{8.95}$$

Given the solved J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 + \lambda_2^2\cos^2\omega - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{8.96}$$

$$\tau_{22} = J_{res}^{1/3}G\left(\lambda_2^2\sin^2\omega - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{8.97}$$

$$\tau_{12} = J_{res}^{1/3}G\lambda_2^2\sin\omega\cos\omega \tag{8.98}$$

and $\lambda_3 = J/(\lambda_1\lambda_2\sin\omega)$. Normally dynamic code cannot model an incompressible material, but a 3D incompressible membrane material can be modeled by setting $J = J_{res}$ and $J_{eff} = 1$ or:

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 + \lambda_2^2\cos^2\omega - \frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{8.99}$$

$$\tau_{22} = J_{res}^{1/3}G\left(\lambda_2^2\sin^2\omega - \frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{8.100}$$

$$\tau_{12} = J_{res}^{1/3}G\lambda_2^2\sin\omega\cos\omega \tag{8.101}$$

and $\lambda_3 = J_{res}/(\lambda_1\lambda_2\sin\omega)$. Note that during free thermal expansion, $J_{res} = \lambda_1^3$, $\lambda_2 = \lambda_1$, $\cos\omega = 0$, and $\sin\omega = 1$ such that all stresses are zero.

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

$$P = -K(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} - 3\varepsilon^{(res)}) \tag{9.1}$$

$$s_{ij} = \int_0^t 2G(t-\tau)\frac{de_{xy}}{d\tau}d\tau \tag{9.2}$$

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 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

$$d\alpha_k(\text{difference}) = \frac{(\Delta t)^2 de}{6\tau_k^2} + O[(\Delta t)^3] \tag{9.22}$$

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 (9.13). The dissipated energy (by midpoint rule) is

$$\Phi = \sum_{ij}\sum_{k=1}^{n} 2G_k(e_{ij}(t)-\alpha_{ij,k})d\alpha_{ij,k} = \sum_{ij}\sum_{k=1}^{n} 2G_k\left(e_{ij}+\frac{de_{ij}}{2}-\alpha_{ij,k}+\frac{d\alpha_{ij,k}}{2}\right)d\alpha_{ij,k} \tag{9.25}$$

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 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

$$g(t) = \gamma_0 + \sum_{k=1}^{n}\gamma_k e^{-t/\tau_k} \tag{9.35}$$

9.4.1 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.

9.5 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

$$\mathbf{F} = \begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \text{where} \qquad \dot{\varepsilon} = \frac{\Lambda - 1}{t_f} \tag{10.1}$$

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

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} (1+\dot{\varepsilon}t)^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.2}$$

and the relative volume change is

$$J = |\mathbf{F}| = (1+\dot{\varepsilon}t)^2 \tag{10.3}$$

To tested residual stress (here only thermal), we can all apply linear expansion using $\lambda_{res} = 1 + \dot{\varepsilon}_{res} t = e^{\alpha \Delta T}$, which corresponds to a temperature change ramp of

$$\Delta T = \frac{1}{\alpha} \ln(1 + \dot{\varepsilon}_{res} t) \quad \text{where} \quad \dot{\varepsilon}_{res} = \frac{\Lambda_{res} - 1}{t_f} \tag{10.4}$$

s 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

$$A(X,t) = \frac{d^2\chi(X,t)}{dt^2} = 0 \tag{10.7}$$

To get this same result for spatial velocity requires the material derivative

$$\frac{Dv(x,t)}{Dt} = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} + \frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} = 0 \tag{10.8}$$

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 change of coordinates:

$$\dot{\mathsf{F}} = \frac{dV(X,t)}{dX} = \frac{dv(x,t)}{dx}\frac{dx(X,t)}{dX} = \frac{dv(x,t)}{dx}\mathsf{F} \qquad \text{giving} \qquad \dot{F}_{11} = \dot{\varepsilon} \tag{10.10}$$

In this problem, the two are the same because $\dot{\mathsf{F}}$ is constant. Thus it is the same on all particles and in nodal coordinates is the same constant value (to extrapolate the constant to the particles). The spatial velocity gradient is the $\boldsymbol{\ell} = dv(x,t)/dx$ term, which in this example has:

$$l_{11} = \frac{\dot{\varepsilon}}{1+\dot{\varepsilon}t} \tag{10.11}$$

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 7.2). In this example:

$$\mathsf{F}(t+\Delta t)\mathsf{F}^{-1}(t) = \frac{1+\dot{\varepsilon}(t+\Delta t)}{1+\dot{\varepsilon}t} = 1 + \frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t} \tag{10.12}$$

$$\exp\left(\frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t}\right) \approx 1 + \frac{\dot{\varepsilon}\Delta t}{1+\dot{\varepsilon}t} \tag{10.13}$$

which is correct for small Δt.

10.2.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F})-3\big)\mathbf{I} + G(\mathbf{F}+\mathbf{F}^T-2\mathbf{I}) \tag{10.14}$$

where $\lambda = \nu E/((1+\nu)(1-2\nu))$ is the Lamé constant for the material. For constrained uniaxial tension, the stress is

$$\sigma_{ij} = (\lambda + 2G\delta_{i1})\dot{\varepsilon}t\,\delta_{ij} \tag{10.15}$$

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:

$$T_x = \pm(\lambda + 2G)\dot{\varepsilon}t \tag{10.16}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda\dot{\varepsilon}t \qquad \text{or} \qquad v_y = v_z = 0 \tag{10.17}$$

10.2.2 Neo-Hookean, Mooney-Rivlin Material

For a neo-Hookean version of a Mooney-Rivlin material (with $G_2 = 0$) with default pressure term and no residual stresses, the Cauchy stress is

$$\boldsymbol{\sigma} = \frac{K}{2}\left(J - \frac{1}{J}\right)\mathbf{I} + \frac{G_1}{J^{5/3}}\mathrm{dev}(\mathbf{F}\mathbf{F}^T) \tag{10.18}$$

where $\mathrm{dev}(\mathbf{F}\mathbf{F}^T)$ is the deviatoric part of the left Cauchy-Green tensor ($\mathbf{B}$) with diagonal elements $(1/3)(2(J^2-1), 1-J^2, 1-J^2)$. Under constrained uniaxial deformation:

$$\sigma_{xx} = \left(\frac{K}{2(1+\dot{\varepsilon}t)} + \frac{2G_1}{3(1+\dot{\varepsilon}t)^{5/3}}\right)(2+\dot{\varepsilon}t)\,\dot{\varepsilon}t \tag{10.19}$$

$$\sigma_{yy} = \left(\frac{K}{2(1+\dot{\varepsilon}t)} - \frac{G_1}{3(1+\dot{\varepsilon}t)^{5/3}}\right)(2+\dot{\varepsilon}t)\,\dot{\varepsilon}t \tag{10.20}$$

$$\sigma_{zz} = \sigma_{yy} \tag{10.21}$$

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 $T_z = \pm\sigma_{yy}$.

10.2.3 Neo-Hookean Material

For an alternate neo-Hookean material with default pressure term (`UJOption=0`) and residual stresses, the Cauchy stress is

$$P(J_{eff}) = \frac{\lambda}{2}\left(\frac{(1+\dot{\varepsilon}t)}{(1+\dot{\varepsilon}_{res}t)} - \frac{(1+\dot{\varepsilon}_{res}t)}{(1+\dot{\varepsilon}t)}\right) = \frac{\lambda}{2}\left(\frac{(1+\dot{\varepsilon}t)^2-(1+\dot{\varepsilon}_{res}t)^2}{(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\right) \tag{10.22}$$

$$\begin{aligned}
\sigma_{xx} &= \frac{(1+\dot{\varepsilon}_{res}t)^2 G}{(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\left((1+\dot{\varepsilon}t)^2-(1+\dot{\varepsilon}_{res}t)^2\right)+\frac{\lambda}{2}\left(\frac{(1+\dot{\varepsilon}t)^2-(1+\dot{\varepsilon}_{res}t)^2}{(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\right) \\
&= \frac{\lambda+2G(1+\dot{\varepsilon}_{res}t)^2}{2(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\left(2+(\dot{\varepsilon}+\dot{\varepsilon}_{res})t\right)(\dot{\varepsilon}-\dot{\varepsilon}_{res})t \qquad (10.23) \\
\sigma_{zz}=\sigma_{yy} &= \frac{(1+\dot{\varepsilon}_{res}t)^2 G}{(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\left(1-(1+\dot{\varepsilon}_{res}t)^2\right)+\frac{\lambda}{2}\left(\frac{(1+\dot{\varepsilon}t)^2-(1+\dot{\varepsilon}_{res}t)^2}{(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\right) \\
&= \frac{\lambda}{2(1+\dot{\varepsilon}t)(1+\dot{\varepsilon}_{res}t)}\left(2+(\dot{\varepsilon}+\dot{\varepsilon}_{res})t\right)(\dot{\varepsilon}-\dot{\varepsilon}_{res})t-\frac{(1+\dot{\varepsilon}_{res}t)G}{(1+\dot{\varepsilon}t)}(2+\dot{\varepsilon}_{res}t)\dot{\varepsilon}_{res}t \qquad (10.24)
\end{aligned}$$

Without residual expansion ($\dot{\varepsilon}_{res}=0$), the stresses become:

$$\begin{aligned}
\sigma_{xx} &= \frac{\lambda+2G}{2(1+\dot{\varepsilon}t)}(2+\dot{\varepsilon}t)\,\dot{\varepsilon}t \qquad (10.25) \\
\sigma_{zz}=\sigma_{yy} &= \frac{\lambda}{2(1+\dot{\varepsilon}t)}(2+\dot{\varepsilon}t)\,\dot{\varepsilon}t \qquad (10.26) \\
& \qquad (10.27)
\end{aligned}$$

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 $T_z=\pm\sigma_{yy}$.

For neo-Hookean material with alternate pressure term (`UJOption=2`) and no residual stresses, just the λ terms change. The Cauchy stresses become:

$$\begin{aligned}
\sigma_{xx} &= \frac{\lambda\ln(1+\dot{\varepsilon}t)+G(2+\dot{\varepsilon}t)\,\dot{\varepsilon}t}{(1+\dot{\varepsilon}t)} \qquad (10.28) \\
\sigma_{zz} &= \sigma_{yy}=\frac{\lambda\ln(1+\dot{\varepsilon}t)}{(1+\dot{\varepsilon}t)} \qquad (10.29)
\end{aligned}$$

10.2.4 Clamped Neohookean

For the neo-Hookean material in the elastic part of the Disney snow model (known as co-rotated neo-Hookean material), the eigenvalues of $\mathbf{B}$ are $1+\dot{\varepsilon}t$, 1, and 1 with eigenvectors $\hat{x}$, $\hat{y}$, and $\hat{z}$. The Cauchy stress is

$$\begin{aligned}
\sigma_{xx} &= \left(\lambda(J_p)+2G(J_p)\right)\dot{\varepsilon}t \qquad (10.30) \\
\sigma_{yy} &= \lambda(J_p)\dot{\varepsilon}t \qquad (10.31) \\
\sigma_{zz} &= \sigma_{yy} \qquad (10.32)
\end{aligned}$$

This result is identical to a low-strain, isotropic material, although these two models are not identical in all deformation states.

10.3 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

$$\mathbf{F}=\begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & 1+c\dot{\varepsilon}t & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (10.33)$$

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

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} (1+\dot{\varepsilon}t)^2 & 0 & 0 \\ 0 & (1+c\dot{\varepsilon}t)^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.34}$$

with volume change

$$J = |\mathbf{F}| = (1+\dot{\varepsilon}t)(1+c\dot{\varepsilon}t) \tag{10.35}$$

The large deformation mapping and its inverse are

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} X(1+\dot{\varepsilon}t) \\ Y(1+c\dot{\varepsilon}t) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \frac{x}{1+\dot{\varepsilon}t} \\ \frac{y}{1+c\dot{\varepsilon}t} \end{pmatrix} \tag{10.36}$$

The x and y components of material and spatial descriptions of velocity are

$$\begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \dot{\varepsilon}X \\ (c+c't)\dot{\varepsilon}Y \end{pmatrix} \tag{10.37}$$

and

$$\begin{pmatrix} v_x(x,t) \\ v_y(y,t) \end{pmatrix} = \begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \begin{pmatrix} \frac{\dot{\varepsilon}x}{1+\dot{\varepsilon}t} \\ \frac{(c+c't)\dot{\varepsilon}y}{1+c\dot{\varepsilon}t} \end{pmatrix} \tag{10.38}$$

The material velocity gradient is

$$\dot{\mathsf{F}} = \begin{pmatrix} \frac{dV_x(X,t)}{dX} & 0 \\ 0 & \frac{dV_y(X,t)}{dY} \end{pmatrix} = \begin{pmatrix} \dot{\varepsilon} & 0 \\ 0 & (c+c't)\dot{\varepsilon} \end{pmatrix} \tag{10.39}$$

The material acceleration comes from

$$\begin{pmatrix} A_x(\boldsymbol{X},t) \\ A_y(\boldsymbol{X},t) \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} V_x(\boldsymbol{X},t) \\ V_y(\boldsymbol{X},t) \end{pmatrix} = \begin{pmatrix} 0 \\ (2c'+c''t)\dot{\varepsilon}Y \end{pmatrix} \tag{10.40}$$

To get this same result for spatial velocity requires (and with $v_z = 0$) the material derivative

$$\frac{Dv_x}{Dt} = \frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} = -\frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} + \frac{\dot{\varepsilon}^2 xt}{(1+\dot{\varepsilon}t)^2} = 0 \tag{10.41}$$

$$\begin{aligned} \frac{Dv_y}{Dt} &= \frac{\partial v_y}{\partial t} + v_y\frac{\partial v_y}{\partial x} + v_y\frac{\partial v_y}{\partial y} = \frac{(2c'+c''t)\dot{\varepsilon}y(1+\dot{\varepsilon}t) - (c+c't)\dot{\varepsilon}^2 y}{(1+\dot{\varepsilon}t)^2} + \frac{(c+c't)\dot{\varepsilon}^2 y}{(1+\dot{\varepsilon}t)^2} \\ &= \frac{(2c'+c''t)\dot{\varepsilon}y}{(1+\dot{\varepsilon}t)} = (2c'+c''t)\dot{\varepsilon}Y \end{aligned} \tag{10.42}$$

10.3.1 Neo-Hookean Material

For an alternate neo-Hookean material using `UJOption=0` and no residual stresses ($J_{res} = 1$):

$$-P(J_{eff}) = \frac{\lambda}{2J}\left(J^2-1\right) = \frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2 - 1\right) \tag{10.43}$$

and the Cauchy stresses are:

$$\sigma_{xx} = \frac{G}{J}\left((1+\dot{\varepsilon}t)^2-1\right)+\frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) \tag{10.44}$$

$$\sigma_{yy} = \frac{G}{J}\left((1+c\dot{\varepsilon}t)^2-1\right)+\frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) \tag{10.45}$$

$$\sigma_{zz} = \frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2(1+c\dot{\varepsilon}t)^2-1\right) \tag{10.46}$$

$$\sigma_{ij} = 0 \qquad \text{for } i \neq j \tag{10.47}$$

We want zero in y direction stress., which reduces to:

$$(1+c\dot{\varepsilon}t)^2 = \frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G} \quad \text{or} \quad c = -\frac{1-\sqrt{\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}}}{\dot{\varepsilon}t} \tag{10.48}$$

Note that for small strain (t close to zero), this result reduces to

$$c = -\frac{\lambda}{\lambda+2G} = -\frac{\nu}{1-\nu} \tag{10.49}$$

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

$$\mathbf{F} = \begin{pmatrix} 1+\dot{\varepsilon}t & 0 & 0 \\ 0 & \sqrt{\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.50}$$

The particle Y velocities are now:

$$V_y(Y,t) = (c+c't)\dot{\varepsilon}t = -\lambda(1+\dot{\varepsilon}t)\,\dot{\varepsilon}Y\sqrt{\frac{\lambda+2G}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^3}} \tag{10.51}$$

The acceleration to provide as a body force is:

$$A_y(Y,t) = 2\lambda\left(\lambda(1+\dot{\varepsilon}t)^2-G\right)\dot{\varepsilon}^2Y\sqrt{\frac{\lambda+2G}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^5}} \tag{10.52}$$

Now substitute for Y to get

$$A_y(y,t) = \frac{2\lambda\left(\lambda(1+\dot{\varepsilon}t)^2-G\right)\dot{\varepsilon}^2y}{\left(\lambda(1+\dot{\varepsilon}t)^2+2G\right)^2} \tag{10.53}$$

For expected stresses and needed tractions, the pressure reduces to:

$$-P(J_{eff}) = \frac{\lambda}{2J}\left((1+\dot{\varepsilon}t)^2\frac{\lambda+2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}-1\right) \tag{10.54}$$

$$= \frac{\lambda}{2J}\left(\frac{(1+\dot{\varepsilon}t)^2(\lambda+2G)-\lambda(1+\dot{\varepsilon}t)^2-2G}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) \tag{10.55}$$

$$= \frac{G}{J}\left(\frac{\lambda\left((1+\dot{\varepsilon}t)^2-1\right)}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) \tag{10.56}$$

$$\tag{10.57}$$

and the Cauchy stresses become

$$\sigma_{xx} = \frac{G}{J}\left((1+\dot{\varepsilon}t)^2-1\right)\left(\frac{\lambda}{\lambda(1+\dot{\varepsilon}t)^2+2G}+1\right) \tag{10.58}$$

$$\sigma_{yy} = 0 \tag{10.59}$$

$$\sigma_{zz} = \frac{\lambda G}{J}\left(\frac{(1+\dot{\varepsilon}t)^2-1}{\lambda(1+\dot{\varepsilon}t)^2+2G}\right) \tag{10.60}$$

$$\sigma_{ij} = 0 \qquad \text{for } i \neq j \tag{10.61}$$

10.4 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 will be

$$\mathbf{F} = \begin{pmatrix} 1 & \Gamma\frac{t}{t_f} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} 1+\Gamma^2\frac{t^2}{t_f^2} & \Gamma\frac{t}{t_f} & 0 \\ \Gamma\frac{t}{t_f} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.62}$$

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:

$$\boldsymbol{T} = \left(\tau_{xy}, \sigma_{yy}, 0\right) \qquad \text{on } \pm y \tag{10.63}$$

$$\boldsymbol{T} = (0, 0, \sigma_{zz}) \qquad \text{on } \pm z \tag{10.64}$$

$$\tag{10.65}$$

On the initially $\pm x$ surface, the normal rotates to be

$$\hat{\boldsymbol{n}} = \left(\frac{1}{\sqrt{1+\gamma^2}}, \frac{-\gamma}{\sqrt{1+\gamma^2}}, 0\right) \tag{10.66}$$

where $\gamma = \Gamma t/t_f$. But since $\gamma = \tan\theta$, where θ is the current shear angle, this normal vector is also

$$\hat{\boldsymbol{n}} = (\cos\theta, -\sin\theta, 0) \tag{10.67}$$

For general stress state (but with $\sigma_{xz} = \sigma_{yz} = 0$), the traction will be

$$\boldsymbol{T} = \left(\sigma_{xx}\cos\theta - \sigma_{xy}\sin\theta, \sigma_{xy}\cos\theta - \sigma_{yy}\sin\theta, 0\right) \tag{10.68}$$

This traction can be divided into traction normal and tangential to the current surface:

$$T_n = \boldsymbol{T}\cdot\hat{\boldsymbol{n}} = \sigma_{xx}\cos^2\theta - 2\sigma_{xy}\cos\theta\sin\theta + \sigma_{yy}\sin^2\theta = \frac{\sigma_{xx} - 2\gamma\sigma_{xx} + \gamma^2\sigma_{yy}}{1+\gamma^2} \tag{10.69}$$

$$T_t = \boldsymbol{T}\cdot\hat{\boldsymbol{t}} = (\sigma_{xx}-\sigma_{yy})\cos\theta\sin\theta + \sigma_{xy}(\cos^2\theta - \sin^2\theta) \tag{10.70}$$

$$= \frac{\gamma(\sigma_{xx}-\sigma_{yy}) + \sigma_{xy}(1-\gamma^2)}{1+\gamma^2} \tag{10.71}$$

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 (when using CPDI). 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

$$\boldsymbol{v} = \left(\Gamma\frac{Y}{t_f}, 0, 0\right) \tag{10.72}$$

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.

10.4.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material for shear sliding can be written as

$$\boldsymbol{\sigma} = G(\mathbf{F} + \mathbf{F}^T - 2\mathbf{I}) \tag{10.73}$$

The only non-zero stress is the shear stress:

$$\sigma_{xy} = G\gamma = G\Gamma\frac{t}{t_f} \tag{10.74}$$

10.4.2 Neo-Hookean, Mooney-Rivlin Material

For a Mooney-Rivlin material, the Cauchy stress under sliding shear is found from elements of $\mathbf{B}$. In addition $J = 1$, which means pressure terms are zero. The final stresses are

$$\begin{aligned}
\sigma_{xx} &= \frac{J_{res}\gamma^2}{3}(2G_1 + G_2) && (10.75)\\
\sigma_{yy} &= -\frac{J_{res}\gamma^2}{3}(G_1 + 2G_2) && (10.76)\\
\sigma_{zz} &= \frac{J_{res}\gamma^2}{3}(-G_1 + G_2) && (10.77)\\
\tau_{xy} &= J_{res}\gamma(G_1 + G_2) && (10.78)
\end{aligned}$$

where J_{res} is set to one to generate a solution with no residual stresses.

10.4.3 Neo-Hookean Material

For an alternate Neo-Hookean material with no residual stresses, the Cauchy stress under sliding shear is found from elements of $\mathbf{B}$. In addition $J = 1$, which means pressure terms are zero (and result is independent of the `UJoption` setting). The final stresses are

$$\begin{aligned}
\sigma_{xx} &= G\gamma^2 && (10.79)\\
\sigma_{yy} = \sigma_{zz} &= 0 && (10.80)\\
\tau_{xy} &= G\gamma && (10.81)
\end{aligned}$$

On the $\pm y$ surfaces, the tractions are $T_x = \pm\tau_{xy}$ and $T_y = 0$. On the $\pm z$ surfaces, the traction are $T_z = 0$. The $\pm x$ surface have to account for rotations and can be done with normal and tangential tractions:

$$T_n = -\frac{G\gamma^2}{1+\gamma^2} \tag{10.82}$$

$$T_t = \frac{G\gamma}{1+\gamma^2} \tag{10.83}$$

or with tractions along x and y. Both work, but x and y tractions are more stable

10.4.4 Disney Snow Model

For the neo-Hookean material in the elastic part of the Disney snow model, the eigenvalues and eigenvectors of $\mathbf{B}$:

$$\lambda_1^2 = 1+\frac{1}{2}\gamma^2+\gamma\sqrt{1+\frac{1}{4}\gamma^2} \tag{10.84}$$

$$\lambda_2^2 = 1+\frac{1}{2}\gamma^2-\gamma\sqrt{1+\frac{1}{4}\gamma^2} \tag{10.85}$$

$$\lambda_3^2 = 1 \tag{10.86}$$

$$\tag{10.87}$$

10.5 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

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\frac{t^2}{t_f^2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.88}$$

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:

$$\boldsymbol{b} = \left(\frac{2(\Lambda-1)\frac{x}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{10.89}$$

To apply velocity boundary conditions, the applied velocity (in spatial nodal coordinates) should be

$$\boldsymbol{v} = \left(\frac{2(\Lambda-1)\frac{xt}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{10.90}$$

10.5.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F})-3\big)\mathbf{I} + G(\mathbf{F}+\mathbf{F}^T-2\mathbf{I}) \tag{10.91}$$

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

$$\sigma_{ij} = (\lambda + 2G\delta_{i1})(\Lambda-1)\frac{t^2}{t_f^2}\delta_{ij} \tag{10.92}$$

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:

$$T_x = \pm(\lambda+2G)(\Lambda-1)\frac{t^2}{t_f^2} \tag{10.93}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda(\Lambda-1)\frac{t^2}{t_f^2} \qquad \text{or} \qquad v_y = v_z = 0 \tag{10.94}$$

10.5.2 Neo-Hookean Material

For an alternate neo-Hookean material under constrained uniaxial deformation:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{\lambda+2G}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{10.95}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{10.96}$$

$$\sigma_{zz} = \sigma_{yy} \tag{10.97}$$

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 Sinusoidal Acceleration

If an object is stretched in uniaxial tension by sinusoidal function while be constrained in other two directions, the deformation gradient is:

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\sin\omega t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{10.98}$$

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

$$\chi(X,t) = x = X + v(X)t = X\left(1+(\Lambda-1)\sin\omega t\right) \quad \text{and} \quad \chi^{-1}(x,t) = X = \frac{x}{1+(\Lambda-1)\sin\omega t} \tag{10.99}$$

The x-components of material and spatial descriptions of velocity are

$$V(X,t) = \frac{d\chi(X,t)}{dt} = (\Lambda-1)X\omega\cos\omega t \quad \text{and} \quad v(x,t) = V(\chi^{-1}(x,t),t) = \frac{(\Lambda-1)x\omega\cos\omega t}{1+(\Lambda-1)\sin\omega t} \tag{10.100}$$

The material acceleration comes from

$$A(X,t) = \frac{d^2\chi(X,t)}{dt^2} = -(\Lambda-1)X\omega^2\sin\omega t \tag{10.101}$$

To get this same result for spatial velocity requires the material derivative

$$\frac{Dv(x,t)}{Dt} = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{(\Lambda-1)x\omega^2\sin\omega t}{1+(\Lambda-1)\sin\omega t} \tag{10.102}$$

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:

$$\boldsymbol{b} = \left(-\frac{(\Lambda-1)x\omega^2\sin\omega t}{1+(\Lambda-1)\sin\omega t}, 0, 0\right) \tag{10.103}$$

To apply velocity boundary conditions, the applied velocity (in spatial nodal coordinates) should be

$$\boldsymbol{v} = \left(\frac{(\Lambda-1)x\omega\cos\omega t}{1+(\Lambda-1)\sin\omega t}, 0, 0\right) \tag{10.104}$$

10.6.1 Neo-Hookean Material

For an alternate neo-Hookean material under constrained uniaxial deformation:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{(\lambda+2G)(\Lambda-1)\sin\omega t}{2(1+(\Lambda-1)\sin\omega t)}(2+(\Lambda-1)\sin\omega t) \tag{10.105}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda(\Lambda-1)\sin\omega t}{2(1+(\Lambda-1)\sin\omega t)}(2+(\Lambda-1)\sin\omega t) \tag{10.106}$$

$$\sigma_{zz} = \sigma_{yy} \tag{10.107}$$

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 $T_z = \pm\sigma_{yy}$.