Material Models Used in NairnMPM and NairnFEA

John Nairn

September 27, 2017

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 Plane Stress Equations

The plane stress stiffness equations for in-plane stresses are

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

The elements of the **Q** matrix are found from

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

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

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

$$Q_{xyxy} = G_{xy} \tag{1.7}$$

These elements 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()`.

In plane stress analysis, $\sigma_{zz} = 0$, but $\varepsilon_{zz} \neq 0$. The out-of-plane strain is found from the 3D stiffness matrix by solving the σ_{zz} equation for ε_{zz}:

$$\varepsilon_{zz} = -\frac{C_{13}}{C_{33}}(\varepsilon_{xx} - \varepsilon_{xx}^{(res)}) - \frac{C_{23}}{C_{33}}(\varepsilon_{yy} - \varepsilon_{yy}^{(res)}) + \varepsilon_{zz}^{(res)} \tag{1.8}$$

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 Plane Strain Equations

The plane strain stiffness equations for in-plane stresses are

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy} - \varepsilon_{yy}^{(res,r)} \\ \gamma_{xy} \end{pmatrix} \tag{1.9}$$

where residual strains now depend on reduced residual strains

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \varepsilon_{xx}^{(res)} + \nu_{zx}\varepsilon_{zz}^{(res)} \\ \varepsilon_{yy}^{(res)} + \nu_{zy}\varepsilon_{zz}^{(res)} \end{pmatrix} \tag{1.10}$$

which is equivalent to using reduced expansion properties

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \alpha_{xx}^{(r)}\Delta T + \beta_{xx}^{(r)}\Delta c \\ \alpha_{yy}^{(r)}\Delta T + \beta_{xx}^{(r)}\Delta c \end{pmatrix} \tag{1.11}$$

The reduced expansion coefficients are

$$\alpha_{xx}^{(r)} = \alpha_{xx} + \nu_{zx}\alpha_{zz},\ \ \alpha_{yy}^{(r)} = \alpha_{yy} + \nu_{zy}\alpha_{zz},\ \ \beta_{xx}^{(r)} = \beta_{xx} + \nu_{zx}\beta_{zz},\ \ \beta_{yy}^{(r)} = \beta_{yy} + \nu_{zy}\beta_{zz} \tag{1.12}$$

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()`.

In plane strain analysis, $\varepsilon_{zz} = 0$, but $\sigma_{zz} \neq 0$. The out-of-plane stress is found from the 3D stiffness matrix by setting $\varepsilon_{zz} = 0$:

$$\begin{aligned}\sigma_{zz} &= C_{13}\big(\varepsilon_{xx} - (\alpha_{xx}^{(r)} - \nu_{zx}\alpha_{zz})\Delta T - (\beta_{xx}^{(r)} - \nu_{zx}\beta_{zz})\Delta c\big) \\ &\quad + C_{23}\big(\varepsilon_{yy} - (\alpha_{yy}^{(r)} - \nu_{zy}\alpha_{zz})\Delta T - (\beta_{yy}^{(r)} - \nu_{zy}\beta_{zz})\Delta c\big) - C_{33}\varepsilon_{zz}^{(res)}\end{aligned} \tag{1.13}$$

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:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & \texttt{C[1][3]} \\ \texttt{C[1][2]} & \texttt{C[2][2]} & \texttt{C[2][3]} \\ \texttt{C[1][3]} & \texttt{C[2][3]} & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy} - \varepsilon_{yy}^{(res)} \\ \gamma_{xx} - \varepsilon_{xy}^{(res)} \end{pmatrix} \tag{1.14}$$

where the rotated residual strains (which become reduced residual strains when in plane strain) are

$$\begin{pmatrix} \varepsilon_{xx}^{(res)} \\ \varepsilon_{yy}^{(res)} \\ \varepsilon_{xy}^{(res)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \texttt{alpha[3]}\Delta T + \texttt{beta[3]}\Delta c \end{pmatrix} \tag{1.15}$$

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

$$\begin{aligned}\varepsilon_{zz} &= \texttt{C[4][1]}(\varepsilon_{xx} - \varepsilon_{xx}^{(res)}) + \texttt{C[4][2]}(\varepsilon_{yy} - \varepsilon_{yy}^{(res)}) \\ &\quad + \texttt{C[4][3]}(\gamma_{xy} - \varepsilon_{xy}^{(res)}) + \varepsilon_{zz}^{(res)}\end{aligned} \tag{1.16}$$

where

$$\texttt{C[4][1]} = -\left(\frac{C_{13}}{C_{33}}\cos^2\theta + \frac{C_{23}}{C_{33}}\sin^2\theta\right) = \texttt{C13}\cos^2\theta + \texttt{C23}\sin^2\theta \tag{1.17}$$

$$\texttt{C[4][2]} = -\left(\frac{C_{13}}{C_{33}}\sin^2\theta + \frac{C_{23}}{C_{33}}\cos^2\theta\right) = \texttt{C13}\sin^2\theta + \texttt{C23}\cos^2\theta \tag{1.18}$$

$$\texttt{C[4][3]} = \left(\frac{C_{13}}{C_{33}} - \frac{C_{23}}{C_{33}}\right)\sin\theta\cos\theta = -(\texttt{C13} - \texttt{C23})\sin\theta\cos\theta \tag{1.19}$$

and CTE3 = alpha[4] = α_{zz} and CME3 = beta[4] = β_{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

$$\begin{aligned}\sigma_{zz} &= \texttt{C[4][1]}(\varepsilon_{xx} - (\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)})) + \texttt{C[4][2]}(\varepsilon_{yy} - (\varepsilon_{yy}^{(res,r)} - \texttt{alpha[6]}\varepsilon_{zz}^{(res)})) \\ &\quad + \texttt{C[4][3]}(\gamma_{xx} - (\varepsilon_{xy}^{(res,r)} - \texttt{alpha[7]}\varepsilon_{zz}^{(res)})) - \texttt{C[4][4]}\varepsilon_{zz}^{(res)} \end{aligned} \tag{1.20}$$

where

$$\rho\,\texttt{C[4][1]} = C_{13}\cos^2\theta + C_{23}\sin^2\theta = \texttt{C13}\cos^2\theta + \texttt{C23}\sin^2\theta \tag{1.21}$$

$$\rho\,\texttt{C[4][2]} = C_{13}\sin^2\theta + C_{23}\cos^2\theta = \texttt{C13}\sin^2\theta + \texttt{C23}\cos^2\theta \tag{1.22}$$

$$\rho\,\texttt{C[4][3]} = -(C_{13} - C_{23})\sin\theta\cos\theta = -(\texttt{C13} - \texttt{C23})\sin\theta\cos\theta \tag{1.23}$$

$$\rho\,\texttt{C[4][4]} = C_{33} \tag{1.24}$$

$$\texttt{alpha[5]} = \nu_{zx}\cos^2\theta + \nu_{zy}\sin^2\theta = \texttt{prop1}\cos^2\theta + \texttt{prop2}\sin^2\theta \tag{1.25}$$

$$\texttt{alpha[6]} = \nu_{zx}\sin^2\theta + \nu_{zy}\cos^2\theta = \texttt{prop1}\sin^2\theta + \texttt{prop2}\cos^2\theta \tag{1.26}$$

$$\texttt{alpha[7]} = -2\left(\nu_{zx} - \nu_{zy}\right)\sin\theta\cos\theta = -2(\texttt{prop1} - \texttt{prop2})\sin\theta\cos\theta \tag{1.27}$$

Again, CTE3 = alpha[4] = α_{zz} and CME3 = beta[4] = β_{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

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \varepsilon_{zz} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \gamma_{xz} \\ \gamma_{yz} \\ \gamma_{xy} \end{pmatrix} \tag{1.28}$$

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

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} Q_{xx} & Q_{xy} & 0 \\ Q_{xy} & Q_{xx} & 0 \\ 0 & 0 & Q_{xyxy} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)} \\ \gamma_{xx} \end{pmatrix} \tag{1.29}$$

with out-of-plane strain given by

$$\varepsilon_{zz} = -\frac{C_{12}}{C_{11}}(\varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)}) - \frac{C_{12}}{C_{11}}(\varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)}) + \frac{\Delta}{3} + \varepsilon^{(res)} \tag{1.30}$$

For the super-class Isotropic material, the needed terms are stored as C[1][1] = C[2][2] = Q_{xx}/ρ, C[1][2] = Q_{xy}/ρ, C[3][3] = Q_{xyxy}/ρ, C[4][1] = C[4][2]= $-C_{12}/C_{11}$, alpha[1] = alpha[2] = alpha[4] = CTE3 = α, beta[1] = beta[2] = beta[4] = CME3 = β, 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

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \tau_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} - \frac{\Delta}{3}(1+\nu) - \varepsilon^{(res,r)} \\ \varepsilon_{yy} - \frac{\Delta}{3}(1+\nu) - \varepsilon^{(res,r)} \\ \gamma_{xx} \end{pmatrix} \tag{1.31}$$

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:

$$\sigma_{zz} = C_{12}\left(\varepsilon_{xx} - \frac{\Delta}{3} - \varepsilon^{(res)}\right) + C_{12}\left(\varepsilon_{yy} - \frac{\Delta}{3} - \varepsilon^{(res)}\Delta T\right) - C_{11}\left(\frac{\Delta}{3} + \varepsilon^{(res)}\right) \tag{1.32}$$

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

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:

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

$$\boldsymbol{\lambda}^{(0)} = 0 \tag{2.18}$$

$$\boldsymbol{\alpha}^{(0)}=\boldsymbol{\alpha}_{trial} = \boldsymbol{\alpha}_n \tag{2.19}$$

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

$$f^{(0)}=f_{trial} = f(\boldsymbol{\varepsilon}_{e,trial},\boldsymbol{\psi}_{trial})>0 \tag{2.21}$$

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

$$f^{(k+1)}=f(\boldsymbol{\sigma}^{(k)}+d\boldsymbol{\sigma},\boldsymbol{\psi}^{(k)}+d\boldsymbol{\psi})=f^{(k)}+\frac{\partial f}{\partial\boldsymbol{\sigma}^{(k)}}d\boldsymbol{\sigma}+\frac{\partial f}{\partial\boldsymbol{\psi}^{(k)}}d\boldsymbol{\psi} \tag{2.22}$$

where stress differential is

$$d\boldsymbol{\sigma} = \boldsymbol{\sigma}^{(k+1)}-\boldsymbol{\sigma}^{(k)} \tag{2.23}$$

$$= \boldsymbol{\sigma}_n+\mathbf{C}d\boldsymbol{\varepsilon}_{tot}-\lambda^{(k+1)}\mathbf{C}N(\boldsymbol{\sigma}^{(k+1)},\boldsymbol{\psi}^{(k+1)})-\boldsymbol{\sigma}_n-\mathbf{C}d\boldsymbol{\varepsilon}_{tot}+\lambda^{(k)}\mathbf{C}N(\boldsymbol{\sigma}^{(k)},\boldsymbol{\psi}^{(k)}) \tag{2.24}$$

$$\approx -d\lambda\,\mathbf{C}N(\boldsymbol{\sigma}^{(k)},\boldsymbol{\psi}^{(k)}) \tag{2.25}$$

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

$$\begin{aligned} d\boldsymbol{\psi} &= \boldsymbol{\psi}^{(k+1)} - \boldsymbol{\psi}^{(k)} \approx \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}}(\boldsymbol{\alpha}^{(k+1)} - \boldsymbol{\alpha}^{(k)}) && (2.26)\\ &= \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}}\left(\boldsymbol{\alpha}_n + \lambda^{(k+1)} H(\boldsymbol{\sigma}^{(k+1)}, \boldsymbol{\psi}^{(k+1)}) - \boldsymbol{\alpha}_n - \lambda^{(k)} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)})\right) && (2.27)\\ &\approx d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.28) \end{aligned}$$

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

$$f^{(k+1)} = f^{(k)} - d\lambda \left(\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) - \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}^{(k)}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) \right) \tag{2.29}$$

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

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

For associative plasticity, the result is:

$$d\lambda = \frac{f^{(k)}}{\frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} \cdot \mathbf{C} \frac{\partial f}{\partial \boldsymbol{\sigma}^{(k)}} + \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}} \frac{\partial \boldsymbol{\psi}_k}{\partial \boldsymbol{\alpha}^{(k)}} \frac{\partial f}{\partial \boldsymbol{\psi}^{(k)}}} \tag{2.31}$$

From the solved increment, update the variables using:

$$\begin{aligned} \lambda^{(k+1)} &= \lambda^{(k)} + d\lambda && (2.32)\\ \boldsymbol{\alpha}^{(k+1)} &= \boldsymbol{\alpha}^{(k)} + d\lambda H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.33)\\ \boldsymbol{\sigma}^{(k+1)} &= \boldsymbol{\sigma}^{(k)} - d\lambda \mathbf{C} N(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.34)\\ \boldsymbol{\psi}^{(k+1)} &= \boldsymbol{\psi}^{(k)} + d\lambda \frac{\partial \boldsymbol{\psi}}{d\alpha^{(k)}} H(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\psi}^{(k)}) && (2.35) \end{aligned}$$

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

$$f = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} K(\alpha) = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}(\sigma_y + \psi) \tag{2.36}$$

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

$$\psi = K(\alpha) - \sigma_y \tag{2.37}$$

The usual assumption for associative flow is to take

$$d\alpha = -\lambda \frac{\partial f}{\partial \psi} = \lambda \sqrt{\frac{2}{3}} \tag{2.38}$$

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

$$2J_2 = \|\mathbf{s}\|^2 = s_{xx}^2 + s_{yy}^2 + s_{zz}^2 + 2s_{xy}^2 + 2s_{xz}^2 + 2s_{yz}^2 \tag{2.39}$$

During plastic deformation, the plastic strain increment simplifies to

$$\lambda \frac{\partial f}{\partial \boldsymbol{\sigma}} = \lambda \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} = \lambda \mathbf{n} \tag{2.40}$$

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

$$d\alpha = \sqrt{\frac{2}{3}} \|d\boldsymbol{\varepsilon}_p\| \tag{2.41}$$

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

$$\mathbf{s} = \mathbf{s}_{trial} - \lambda 2G\mathbf{n} = \left(1 - \frac{\lambda 2G}{\|\mathbf{s}_{trial}\|}\right)\mathbf{s}_{trial} \tag{2.42}$$

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

$$\|\mathbf{s}\| = \|\mathbf{s}_{trial}\| - \lambda 2G \qquad \text{and} \qquad \frac{\mathbf{s}}{\|\mathbf{s}\|} = \frac{\mathbf{s}_{trial}}{\|\mathbf{s}_{trial}\|} \tag{2.43}$$

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:

$$f^{(k)} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} K(\alpha^{(k)}) = \|\mathbf{s}_{trial}\| - \lambda^{(k)} 2G - \sqrt{\frac{2}{3}} K(\alpha^{(k)}) = 0 \tag{2.44}$$

This can be solved by Newton's method using:

$$\frac{df^{(k)}}{d\lambda} = -2G - \sqrt{\frac{2}{3}} \frac{dK(\alpha^{(k)})}{d\lambda} = -2G - \frac{2}{3} \frac{dK(\alpha^{(k)})}{d\alpha} \tag{2.45}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)} \sqrt{\frac{2}{3}} \tag{2.46}$$

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

$$f = \|\mathbf{s}_{trial}\| - \lambda 2G - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\left(\alpha^0 + \lambda\sqrt{\frac{2}{3}}\right)\right) = 0 \tag{2.47}$$

The analytical solution is

$$\lambda = \frac{\|\mathbf{s}_{trial}\| - \sqrt{\frac{2}{3}}\left(\sigma_Y + E_p\alpha^0\right)}{2G + \frac{2E_p}{3}} \tag{2.48}$$

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

$$\frac{\Delta V}{V} = d\varepsilon_{xx} + d\varepsilon_{yy} + d\varepsilon_{zz} - 3d\varepsilon^{(res)} \tag{2.49}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.50}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i = j = x, y, z \tag{2.51}$$

$$d\tau_{xy} = ds_{xy} = Gd\gamma_{xy} \tag{2.52}$$

where

$$d\varepsilon_{xx}^{(tot)} = d\varepsilon_{xx} - d\varepsilon^{(res)}, \quad d\varepsilon_{yy}^{(tot)} = d\varepsilon_{yy} - d\varepsilon^{(res)}, \quad \text{and} \quad d\varepsilon_{zz}^{(tot)} = d\varepsilon_{zz} - d\varepsilon^{(res)} \tag{2.53}$$

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

$$d\varepsilon^{(res)} = \alpha\Delta T + \beta\Delta c \tag{2.54}$$

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

$$ds_{ij} = ds_{ij}^{trial} - 2Gd\varepsilon_{ij}^{p} \tag{2.55}$$

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

$$d\varepsilon_{ij}^{e} = -d\varepsilon_{ij}^{p} \tag{2.56}$$

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

$$d\varepsilon_{zz}^{(tot)} = -\frac{\nu}{1-\nu}\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.57}$$

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

$$\frac{\Delta V}{V} = d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)} + d\varepsilon_{zz}^{(tot)} = \left(\frac{1-2\nu}{1-\nu}\right)\left(d\varepsilon_{xx}^{(tot)} + d\varepsilon_{yy}^{(tot)}\right) \tag{2.58}$$

$$dP = -K\frac{\Delta V}{V} \tag{2.59}$$

$$ds_{ij}^{trial} = 2G\left(d\varepsilon_{ij}^{(tot)} - \frac{\Delta V}{3V}\right) \qquad \text{for } i = j = x, y \tag{2.60}$$

$$ds_{zz}^{trial} = ds_{zz} = dP \tag{2.61}$$

$$d\tau_{xy}^{trial} = ds_{xy}^{trial} = Gd\gamma_{xy} \tag{2.62}$$

$$\tag{2.63}$$

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:

$$\texttt{psRed} = \left(\frac{1-2\nu}{1-\nu}\right) = \frac{1}{\frac{K}{2G}+\frac{2}{3}} \tag{2.64}$$

$$\texttt{psLr2G} = \frac{\nu}{1-\nu} = \frac{\frac{K}{2G}-\frac{1}{3}}{\frac{K}{2G}+\frac{2}{3}} \tag{2.65}$$

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

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. (2.58)). 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

$$f = \|\mathbf{s}\|^2 - \frac{2}{3}K^2(\alpha) = \sigma\mathbf{P}\sigma - \frac{2}{3}K^2(\alpha) \tag{2.67}$$

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

$$\mathbf{P} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & 0 \\ -\frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 2 \end{pmatrix} \tag{2.68}$$

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

$$(d\varepsilon^p_{xx}, d\varepsilon^p_{yy}, d\gamma^p_{xy}) = \lambda\frac{\partial f}{\partial \boldsymbol{\sigma}} = \lambda\mathbf{P}\sigma \tag{2.69}$$

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

$$d\boldsymbol{\varepsilon}_p = \lambda \begin{pmatrix} \frac{1}{3}(2\sigma_{xx} - \sigma_{yy}) & \tau_{xy} & 0 \\ \tau_{xy} & \frac{1}{3}(2\sigma_{yy} - \sigma_{xx}) & 0 \\ 0 & 0 & -\frac{1}{3}(\sigma_{xx} + \sigma_{yy}) \end{pmatrix} \tag{2.70}$$

This traceless tensor has inner product

$$\|d\boldsymbol{\varepsilon}_p\|^2 = \lambda^2\left(\frac{2}{3}(\sigma^2_{xx} + \sigma^2_{yy} - \sigma_{xx}\sigma_{yy}) + 2\tau^2_{xy}\right) = \lambda^2\sigma\mathbf{P}\sigma \tag{2.71}$$

$$= \lambda^2\left(s^2_{xx} + s^2_{yy} + s^2_{zz} + 2s^2_{xy}\right) \tag{2.72}$$

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

$$d\alpha = \sqrt{\frac{2}{3}}\lambda\sqrt{\sigma\mathbf{P}\sigma} \tag{2.73}$$

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

$$\sigma^{trial}_{n+1} = \sigma_n + \mathbf{C}(d\varepsilon^{(tot)}_{xx}, d\varepsilon^{(tot)}_{yy}, d\gamma^{(tot)}_{xy}) \tag{2.74}$$

$$f\sigma_{n+1} = \sigma^{trial}_{n+1} - \mathbf{C}d\boldsymbol{\varepsilon}_p = \sigma^{trial}_{n+1} - \mathbf{C}\lambda\mathbf{P}\sigma_{n+1} \tag{2.75}$$

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

$$\mathbf{C} = \begin{pmatrix} \frac{E}{1-\nu^2} & \frac{\nu E}{1-\nu^2} & 0 \\ \frac{\nu E}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & G \end{pmatrix} \quad \text{with} \quad \mathbf{C}^{-1} = \begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & 0 \\ 0 & 0 & \frac{1}{G} \end{pmatrix} \tag{2.76}$$

Solving the second equation the required stress is:

$$\sigma_{n+1} = \left[\mathbf{C}^{-1} + \lambda \mathbf{P}\right]^{-1} \mathbf{C}^{-1} \sigma_{n+1}^{trial} \tag{2.77}$$

This general result applied to isotropic materials leads to

$$\sigma_{xx}^{(n+1)} + \sigma_{yy}^{(n+1)} = \frac{1}{1+\frac{E}{3(1-\nu)}\lambda}\left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right) \tag{2.78}$$

$$-\sigma_{xx}^{(n+1)} + \sigma_{yy}^{(n+1)} = \frac{1}{1+2G\lambda}\left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right) \tag{2.79}$$

$$\tau_{xy}^{(n+1)} = \frac{\tau_{xy}^{trial}}{1+2G\lambda} \tag{2.80}$$

and

$$\|\mathbf{s}\|^2 = \sigma_{n+1}\mathbf{P}\sigma_{n+1} = \frac{\frac{1}{6}\left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2}{\left(1+\frac{E}{3(1-\nu)}\lambda\right)^2} + \frac{\frac{1}{2}\left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2 + 2\tau_{xy}^{trial\,2}}{(1+2G\lambda)^2} \tag{2.81}$$

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

$$f^{(k)} = \frac{1}{2}\|\mathbf{s}^{(k)}\|^2 - \frac{1}{3}K^2(\alpha^{(k)}) = 0 \tag{2.82}$$

$$\frac{df^{(k)}}{d\lambda} = -\left[\frac{E}{3(1-\nu)}\frac{\frac{1}{6}\left(\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2}{\left(1+\frac{E}{3(1-\nu)}\lambda^{(k)}\right)^3} + 2G\frac{\frac{1}{2}\left(-\sigma_{xx}^{trial} + \sigma_{yy}^{trial}\right)^2 + 2\tau_{xy}^{trial\,2}}{\left(1+2G\lambda^{(k)}\right)^3}\right] - \frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} \tag{2.83}$$

$$\alpha^{(k+1)} = \alpha^0 + \lambda^{(k+1)}\sqrt{\frac{2}{3}}\|\mathbf{s}^{(k+1)}\| \tag{2.84}$$

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

$$\texttt{psKred} = \frac{E}{3(1-\nu)} = \frac{K}{\frac{K}{2G}+\frac{2}{3}} \tag{2.85}$$

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

$$\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{xx}^{trial} + s_{yy}^{trial} - 2P_{final} \tag{2.86}$$

$$-\sigma_{xx}^{trial} + \sigma_{yy}^{trial} = s_{yy}^{trial} - s_{xx}^{trial} \tag{2.87}$$

$$s_{xx}^{(n+1)} = \sigma_{xx}^{(n+1)} + P_{final} \tag{2.88}$$

$$s_{yy}^{(n+1)} = \sigma_{yy}^{(n+1)} + P_{final} \tag{2.89}$$

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

$$s_{xy}^{(n+1)} = \tau_{xy}^{(n+1)} \tag{2.91}$$

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:

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}\left(\sigma_Y + E_p\alpha^{(k)}\right)E_p\|\mathbf{s}^{(k)}\| \tag{2.92}$$

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

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha) = \sigma_y + E_p\alpha && (2.93)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}E_p && (2.94)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}(\sigma_y + E_p\alpha)E_p\|\mathbf{s}\| && (2.95)
\end{aligned}
$$

2.6.2 VonMises Material with Non-Linear Work Hardening

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha)^n && (2.96)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}\sigma_y\beta n(1+\beta\alpha)^{n-1} && (2.97)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}\sigma_y^2\beta n(1+\beta\alpha)^{2n-1}\|\mathbf{s}\| && (2.98)
\end{aligned}
$$

2.6.3 VonMises Material with Alternate Non-Linear Work Hardening

$$
\begin{aligned}
K(\alpha) &= \sigma_y(1+\beta\alpha^n) && (2.99)\\
\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} &= \frac{2}{3}\sigma_y\beta n\alpha^{n-1} && (2.100)\\
\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} &= \sqrt{\frac{8}{27}}\sigma_y^2\beta n\alpha^{n-1}(1+\beta\alpha^n)\|\mathbf{s}\| && (2.101)
\end{aligned}
$$

2.6.4 Johnson-Cook

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.102}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}\left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\left(1-(T^*)^m\right) \tag{2.103}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right)^2 \left[Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_0}\right)+\frac{C}{\dot{\varepsilon}_p dt}(A+B\alpha^n)\right]\|\mathbf{s}\| \tag{2.104}$$

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

$$K(\alpha) = (A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.105}$$

$$\sqrt{\frac{2}{3}}\frac{dK(\alpha^{(k)})}{d\lambda} = \frac{2}{3}Bn\alpha^{n-1}\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)\left(1-(T^*)^m\right) \tag{2.106}$$

$$\frac{1}{3}\frac{dK^2(\alpha^{(k)})}{d\lambda} = \sqrt{\frac{8}{27}}Bn\alpha^{n-1}(A+B\alpha^n)\left(1+C\ln\frac{\dot{\varepsilon}_{p,min}}{\dot{\varepsilon}_0}\right)^2\left(1-(T^*)^m\right)^2\|\mathbf{s}\| \tag{2.107}$$

2.7 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:

$$d\boldsymbol{\sigma} = \mathbf{C}d\boldsymbol{\varepsilon}_{tot} + \boldsymbol{c}_{excess} \tag{2.108}$$

The key terms are

$$\mathbf{C} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 & 0 \\ \texttt{C[4][1]} & \texttt{C[4][2]} & 0 & \texttt{C[4][4]} \\ 0 & 0 & \texttt{C[3][3]} & 0 \end{pmatrix} \tag{2.109}$$

$$d\boldsymbol{\varepsilon}_{tot} = \left(d\varepsilon_{xx}-\varepsilon_{xx}^{(res,r)}, d\varepsilon_{yy}-\varepsilon_{yy}^{(res,r)}, d\varepsilon_{zz}-\varepsilon_{zz}^{(res)}, d\gamma_{xy}\right) \tag{2.110}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.111}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res)} \\ \gamma_{xy}^{(res)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \alpha_{zz}\Delta T + \beta_{zz}\Delta c \\ 0 \end{pmatrix} \tag{2.112}$$

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:

$$\boldsymbol{c}_{excess}[3] = \big(\texttt{C[4][1]alpha[5]} + \texttt{C[4][2]alpha[6]}\big)\varepsilon_{zz}^{(res)} \tag{2.113}$$

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:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx}, \quad d\varepsilon_{yy}^{(p)} = \lambda df_{yy}, \quad d\gamma_{xy}^{(p)} = \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(p)} = \lambda df_{zz} \tag{2.114}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(e)} = -\lambda df_{zz} \tag{2.115}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & 0 \\ 0 & 0 & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\gamma_{xx}^{(e)} \end{pmatrix} \tag{2.116}$$

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

$$\begin{aligned} d\sigma_{zz} \;=\; & \texttt{C[4][1]}\Big(d\varepsilon_{xx}^{(e)} - (\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)})\Big) + \texttt{C[4][2]}\Big(d\varepsilon_{yy}^{(e)} - (\varepsilon_{yy}^{(res,r)} - \texttt{alpha[6]}\varepsilon_{zz}^{(res)})\Big) \\ & - \texttt{C[4][4]}(d\varepsilon_{zz}^{(e)} - \varepsilon^{(res)}) \end{aligned} \tag{2.117}$$

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

2.8 Anisotropic 2D Plane Strain and Axisymmetric Analysis - Global Axes

In general plane strain or axisymmetric analysis, the matrix equation for update is:

$$d\boldsymbol{\sigma} = \mathbf{C}d\boldsymbol{\varepsilon}_{tot} + \boldsymbol{c}_{excess} \tag{2.118}$$

The key terms are

$$\mathbf{C} \;=\; \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & \texttt{C[1][3]} & 0 \\ \texttt{C[1][2]} & \texttt{C[2][2]} & \texttt{C[2][3]} & 0 \\ \texttt{C[4][1]} & \texttt{C[4][2]} & \texttt{C[4][3]} & \texttt{C[4][4]} \\ \texttt{C[1][3]} & \texttt{C[2][3]} & \texttt{C[3][3]} & 0 \end{pmatrix} \tag{2.119}$$

$$d\boldsymbol{\varepsilon}_{tot} \;=\; \Big(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)},\, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)},\, d\varepsilon_{zz} - \varepsilon_{zz}^{(res)},\, d\gamma_{xy} - \gamma_{xy}^{(res,r)}\Big) \tag{2.120}$$

$$d\boldsymbol{f} \;=\; (df_{xx}, df_{yy}, df_{zz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.121}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res)} \\ \gamma_{xy}^{(res,r)} \end{pmatrix} \;=\; \begin{pmatrix} \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \alpha_{zz}\Delta T + \beta_{zz}\Delta c \\ \texttt{alpha[3]}\Delta T + \texttt{beta[3]}\Delta c \end{pmatrix} \tag{2.122}$$

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:

$$\boldsymbol{c}_{excess}[3] = \big(\texttt{C[4][1]alpha[5]} + \texttt{C[4][2]alpha[6]} + \texttt{C[4][3]alpha[7]}\big)\varepsilon_{zz}^{(res)} \tag{2.123}$$

Note that in the code, `alpha[5]` to `alpha[7]` hold out-of-plane Poisson ratios (or rotated ratios) and not thermal expansion coefficient. This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx}, \quad d\varepsilon_{yy}^{(p)} = \lambda df_{yy}, \quad d\gamma_{xy}^{(p)} = \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(p)} = \lambda df_{zz} \tag{2.124}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy}, \quad \text{and} \quad d\varepsilon_{zz}^{(e)} = -\lambda df_{zz} \tag{2.125}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} \texttt{C[1][1]} & \texttt{C[1][2]} & \texttt{C[1][3]} \\ \texttt{C[1][2]} & \texttt{C[2][2]} & \texttt{C[2][3]} \\ \texttt{C[1][3]} & \texttt{C[2][3]} & \texttt{C[3][3]} \end{pmatrix} \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\gamma_{xx}^{(e)} - \gamma_{xy}^{(res,r)} \end{pmatrix} \tag{2.126}$$

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

$$\begin{aligned} d\sigma_{zz} \;=\; & \texttt{C[4][1]}\Big(d\varepsilon_{xx}^{(e)} - (\varepsilon_{xx}^{(res,r)} - \texttt{alpha[5]}\varepsilon_{zz}^{(res)})\Big) + \texttt{C[4][2]}\Big(d\varepsilon_{yy}^{(e)} - (\varepsilon_{yy}^{(res,r)} - \texttt{alpha[6]}\varepsilon_{zz}^{(res)})\Big) \\ & + \texttt{C[4][3]}\Big(d\gamma_{xx}^{(e)} - (\gamma_{xy}^{(res,r)} - \texttt{alpha[7]}\varepsilon_{zz}^{(res)})\Big) - \texttt{C[4][4]}(d\varepsilon_{zz}^{(e)} - \varepsilon^{(res)}) \end{aligned} \tag{2.127}$$

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

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}_{tot} \tag{2.128}$$

The key terms are

$$\mathbf{C} = \texttt{C[i][j]} \quad \text{for } \texttt{i} = 0,5 \text{ and } \texttt{j} = 0,5 \tag{2.129}$$

$$d\boldsymbol{\varepsilon}_{tot} = \left(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)}, d\varepsilon_{yy} - \varepsilon_{zz}^{(res)}, d\gamma_{yz}, d\gamma_{xz}, d\gamma_{xy}\right) \tag{2.130}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{yz}, df_{xz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{yz}}, \frac{\partial f}{\tau_{xz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.131}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[0]}\Delta T + \texttt{beta[0]}\Delta c \\ \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \end{pmatrix} \tag{2.132}$$

This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx},\ d\varepsilon_{yy}^{(p)} = \lambda df_{yy},\ d\varepsilon_{zz}^{(p)} = \lambda df_{zz}, \tag{2.133}$$

$$d\gamma_{yz}^{(p)} = \lambda df_{yz},\ d\gamma_{xz}^{(p)} = \lambda df_{xz},\ d\gamma_{xy}^{(p)} = \lambda df_{xy}, \tag{2.134}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\varepsilon_{zz}^{(e)} = d\varepsilon_{yy} - \lambda df_{zz} \tag{2.135}$$

$$d\gamma_{yz}^{(e)} = d\gamma_{yz} - \lambda df_{yz}, \quad d\gamma_{xz}^{(e)} = d\gamma_{xz} - \lambda df_{xz}, \quad \text{and} \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy} \tag{2.136}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \\ d\tau_{xz} \\ d\tau_{xy} \end{pmatrix} = \Big(\texttt{C[i][j]} \quad \text{for i} = 0,5 \text{ and j} = 0,5\Big) \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\varepsilon_{zz}^{(e)} - \varepsilon_{zz}^{(res,r)} \\ d\gamma_{yz}^{(e)} \\ d\gamma_{xz}^{(e)} \\ d\gamma_{xy}^{(e)} \end{pmatrix} \tag{2.137}$$

2.11 Anisotropic 3D Analysis - Global Axes

In 3D strain analysis, the matrix equation for update is

$$d\boldsymbol{\sigma} = \mathbf{C} d\boldsymbol{\varepsilon}_{tot} \tag{2.138}$$

The key terms are

$$\mathbf{C} = \texttt{C[i][j]} \quad \text{for i} = 0,5 \text{ and j} = 0,5 \tag{2.139}$$

$$d\boldsymbol{\varepsilon}_{tot} = \Big(d\varepsilon_{xx} - \varepsilon_{xx}^{(res,r)},\ d\varepsilon_{yy} - \varepsilon_{yy}^{(res,r)},\ d\varepsilon_{yy} - \varepsilon_{zz}^{(res)},\ d\gamma_{yz} - \gamma_{yz}^{(res,r)}, \\ d\gamma_{xz} - \gamma_{xz}^{(res,r)},\ d\gamma_{xy} - \gamma_{xy}^{(res,r)}\Big) \tag{2.140}$$

$$d\boldsymbol{f} = (df_{xx}, df_{yy}, df_{zz}, df_{yz}, df_{xz}, df_{xy}) = \left(\frac{\partial f}{\sigma_{xx}}, \frac{\partial f}{\sigma_{yy}}, \frac{\partial f}{\sigma_{zz}}, \frac{\partial f}{\tau_{yz}}, \frac{\partial f}{\tau_{xz}}, \frac{\partial f}{\tau_{xy}}\right) \tag{2.141}$$

$$\begin{pmatrix} \varepsilon_{xx}^{(res,r)} \\ \varepsilon_{yy}^{(res,r)} \\ \varepsilon_{zz}^{(res,r)} \\ \gamma_{yz}^{(res,r)} \\ \gamma_{xz}^{(res,r)} \\ \gamma_{xy}^{(res,r)} \end{pmatrix} = \begin{pmatrix} \texttt{alpha[0]}\Delta T + \texttt{beta[0]}\Delta c \\ \texttt{alpha[1]}\Delta T + \texttt{beta[1]}\Delta c \\ \texttt{alpha[2]}\Delta T + \texttt{beta[2]}\Delta c \\ \texttt{alpha[3]}\Delta T + \texttt{beta[3]}\Delta c \\ \texttt{alpha[4]}\Delta T + \texttt{beta[4]}\Delta c \\ \texttt{alpha[5]}\Delta T + \texttt{beta[5]}\Delta c \end{pmatrix} \tag{2.142}$$

This formulation is using engineering shear strains.

The plastic strain increments are:

$$d\varepsilon_{xx}^{(p)} = \lambda df_{xx},\ d\varepsilon_{yy}^{(p)} = \lambda df_{yy},\ d\varepsilon_{zz}^{(p)} = \lambda df_{zz}, \tag{2.143}$$

$$d\gamma_{yz}^{(p)} = \lambda df_{yz},\ d\gamma_{xz}^{(p)} = \lambda df_{xz},\ d\gamma_{xy}^{(p)} = \lambda df_{xy}, \tag{2.144}$$

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

$$d\varepsilon_{xx}^{(e)} = d\varepsilon_{xx} - \lambda df_{xx}, \quad d\varepsilon_{yy}^{(e)} = d\varepsilon_{yy} - \lambda df_{yy}, \quad d\varepsilon_{zz}^{(e)} = d\varepsilon_{yy} - \lambda df_{zz} \tag{2.145}$$

$$d\gamma_{yz}^{(e)} = d\gamma_{yz} - \lambda df_{yz}, \quad d\gamma_{xz}^{(e)} = d\gamma_{xz} - \lambda df_{xz}, \quad \text{and} \quad d\gamma_{xy}^{(e)} = d\gamma_{xy} - \lambda df_{xy} \tag{2.146}$$

The specific stress increments are

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\sigma_{zz} \\ d\tau_{yz} \\ d\tau_{xz} \\ d\tau_{xy} \end{pmatrix} = \Big(\texttt{C[i][j]} \quad \text{for } \texttt{i} = 0,5 \text{ and } \texttt{j} = 0,5 \Big) \begin{pmatrix} d\varepsilon_{xx}^{(e)} - \varepsilon_{xx}^{(res,r)} \\ d\varepsilon_{yy}^{(e)} - \varepsilon_{yy}^{(res,r)} \\ d\varepsilon_{zz}^{(e)} - \varepsilon_{zz}^{(res,r)} \\ d\gamma_{yz}^{(e)} - \gamma_{yz}^{(res,r)} \\ d\gamma_{xz}^{(e)} - \gamma_{xz}^{(res,r)} \\ d\gamma_{xy}^{(e)} - \gamma_{xy}^{(res,r)} \end{pmatrix} \tag{2.147}$$

2.12 Quadratic Hill Criterion - Material Axes

The quadratic Hill yield criterion can implement anisotropic plasticity and hardening terms can be added to include aniostropic hardening as well. For 3D analysis, one version of Hill yield function with arbitrary hardening function (defined later) reduces to:

$$\begin{aligned} f &= \sqrt{F\left(\sigma_{yy}-\sigma_{zz}\right)^2 + G(\sigma_{xx}-\sigma_{zz})^2 + H\left(\sigma_{yy}-\sigma_{xx}\right)^2 + 2L{\tau_{yz}}^2 + 2M{\tau_{xz}}^2 + 2N{\tau_{xy}}^2} \\ &\quad - g(\boldsymbol{\alpha}) \qquad (2.148) \\ &= \Big[(G+H){\sigma_{xx}}^2 + (F+H){\sigma_{yy}}^2 + (F+G)\sigma_{zz}^2 - 2F\sigma_{yy}\sigma_{zz} - 2G\sigma_{xx}\sigma_{zz} \\ &\quad - 2H\sigma_{xx}\sigma_{yy} + 2L{\tau_{yz}}^2 + 2M{\tau_{xz}}^2 + 2N{\tau_{xy}}^2\Big]^{1/2} - g(\boldsymbol{\alpha}) \qquad (2.149) \\ &= \sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}} - g(\boldsymbol{\alpha}) \qquad (2.150) \end{aligned}$$

where $\boldsymbol{\sigma}$ is stress in the material axis system, $g(\boldsymbol{\alpha})$ is a hardening function, and

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.151}$$

For 2D, plane strain, $\boldsymbol{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \tau_{xy})$ and

$$\mathbf{A} = \begin{pmatrix} (G+H) & -H & -G & 0 \\ -H & F+H & -F & 0 \\ -G & -F & F+G & 0 \\ 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.152}$$

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

$$A_{xxxx} = G+H,\ A_{xxyy} = A_{yyxx} = -H,\ A_{xxzz} = A_{zzxx} = -G,\ A_{yyyy} = F+H, \tag{2.153}$$

$$A_{yyzz} = A_{zzyy} = -F,\ A_{zzzz} = F+G,\ A_{yzyz} = \frac{L}{2},\ A_{xzxz} = \frac{M}{2},\ A_{xyxy} = \frac{N}{2} \tag{2.154}$$

such that

$$\mathbf{A}\boldsymbol{\sigma} = \begin{pmatrix} (G+H)\sigma_{xx} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + (F+H)\sigma_{yy} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + (F+G)\sigma_{zz} \end{pmatrix} \tag{2.155}$$

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:

$$(G+H) = \frac{1}{(\sigma^Y_{xx})^2} \qquad (F+H) = \frac{1}{(\sigma^Y_{yy})^2} \qquad (F+G) = \frac{1}{(\sigma^Y_{zz})^2} \tag{2.156}$$

$$F = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{yy})^2} + \frac{1}{(\sigma^Y_{zz})^2} - \frac{1}{(\sigma^Y_{xx})^2}\right) \qquad G = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{zz})^2} + \frac{1}{(\sigma^Y_{xx})^2} - \frac{1}{(\sigma^Y_{yy})^2}\right) \tag{2.157}$$

$$H = \frac{1}{2}\left(\frac{1}{(\sigma^Y_{xx})^2} + \frac{1}{(\sigma^Y_{yy})^2} - \frac{1}{(\sigma^Y_{zz})^2}\right) \quad L = \frac{1}{2(\tau^Y_{yz})^2} \quad M = \frac{1}{2(\tau^Y_{xz})^2} \quad N = \frac{1}{2(\tau^Y_{xy})^2} \tag{2.158}$$

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:

$$F^2 + G^2 + H^2 - FH - GH - FG \geq 0 \tag{2.159}$$

$$F + G + H \geq \sqrt{F^2 + G^2 + H^2 - FH - GH - FG} \tag{2.160}$$

Substituting yield stresses, the conditions can be recast as

$$\left(\frac{1}{\sigma^Y_{xx}} - \frac{1}{\sigma^Y_{yy}}\right)^2 \leq \frac{1}{(\sigma^Y_{zz})^2} \leq \left(\frac{1}{\sigma^Y_{xx}} + \frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.161}$$

$$\left(\frac{1}{\sigma^Y_{xx}} - \frac{1}{\sigma^Y_{zz}}\right)^2 \leq \frac{1}{(\sigma^Y_{yy})^2} \leq \left(\frac{1}{\sigma^Y_{xx}} + \frac{1}{\sigma^Y_{zz}}\right)^2 \tag{2.162}$$

$$\left(\frac{1}{\sigma^Y_{zz}} - \frac{1}{\sigma^Y_{yy}}\right)^2 \leq \frac{1}{(\sigma^Y_{xx})^2} \leq \left(\frac{1}{\sigma^Y_{zz}} + \frac{1}{\sigma^Y_{yy}}\right)^2 \tag{2.163}$$

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

$$\frac{\sigma^Y_{yy}}{(1+R)} \leq \sigma^Y_{zz} \leq \frac{\sigma^Y_{yy}}{|1-R|} \tag{2.164}$$

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

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

$$(G+H) = (F+H) = (F+G) = 2F = 2G = 2H = \frac{1}{\sigma^2_Y}, \quad L = M = N = \frac{1}{2\tau^2_Y} = \frac{3}{2\sigma^2_Y} \tag{2.165}$$

leading to an isotropic material with $K(\alpha) = \sigma_Y + E_p\alpha$ if $g(\boldsymbol{\alpha}) = 1 + (E_p/\sigma_Y)\alpha$.

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

$$d\boldsymbol{f} = \left(df_{xx}, df_{yy}, df_{zz}, df_{yz}, df_{xz}, df_{xy}\right) = \frac{\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.166}$$

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

$$d\boldsymbol{\varepsilon}_p = \lambda d\boldsymbol{f} = \frac{\lambda\mathbf{A}\boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}} \tag{2.167}$$

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

$$d\boldsymbol{\varepsilon}_p = \frac{\lambda}{\sqrt{\boldsymbol{\sigma}\cdot\mathbf{A}\boldsymbol{\sigma}}}\begin{pmatrix} \frac{\sigma_{xx}}{(\sigma^Y_{xx})^2} - H\sigma_{yy} - G\sigma_{zz} & N\tau_{xy} & M\tau_{xz} \\ N\tau_{xy} & -H\sigma_{xx} + \frac{\sigma_{yy}}{(\sigma^Y_{yy})^2} - F\sigma_{zz} & L\tau_{yz} \\ M\tau_{xz} & L\tau_{yz} & -G\sigma_{xx} - F\sigma_{yy} + \frac{\sigma_{zz}}{(\sigma^Y_{zz})^2} \end{pmatrix} \tag{2.168}$$

or by direct evaluation of matrix equation in Eq. 2.166, we have

$$d\boldsymbol{\varepsilon}_p = \lambda\begin{pmatrix} df_{xx} & \frac{1}{2}df_{xy} & \frac{1}{2}df_{xz} \\ \frac{1}{2}df_{xy} & df_{yy} & \frac{1}{2}df_{yz} \\ \frac{1}{2}df_{xz} & \frac{1}{2}df_{yz} & df_{zz} \end{pmatrix} \tag{2.169}$$

In other words, df_{xy} found from contracted form gives engineering plastic strains (as desired).

We assume hardening is a function only of equivalent plastic strain and thus α is cumulative plastic strain. Perhaps a general anisotropic material would have something different, but this assumption is common in metals. The update in α is thus

$$d\alpha = \sqrt{\frac{2}{3}}\|d\boldsymbol{\varepsilon}_p\| = \lambda\sqrt{\frac{2}{3}\left(df^2_{xx} + df^2_{yy} + df^2_{zz} + \frac{1}{2}df^2_{yz} + \frac{1}{2}df^2_{xz} + \frac{1}{2}df^2_{xy}\right)} \tag{2.170}$$

The plastic internal variable is taken as $q = \alpha$ to give

$$dq = d\alpha = -\lambda h \tag{2.171}$$

which implies that

$$h = -\sqrt{\frac{2}{3}\left(df^2_{xx} + df^2_{yy} + df^2_{zz} + \frac{1}{2}df^2_{yz} + \frac{1}{2}df^2_{xz} + \frac{1}{2}df^2_{xy}\right)} \tag{2.172}$$

and

$$d\boldsymbol{f}^q\cdot\boldsymbol{h} = g'(\alpha)\sqrt{\frac{2}{3}\left(df^2_{xx} + df^2_{yy} + df^2_{zz} + \frac{1}{2}df^2_{yz} + \frac{1}{2}df^2_{xz} + \frac{1}{2}df^2_{xy}\right)} \tag{2.173}$$

Some possible hardening laws are

$$g(\alpha) = (1+K\alpha)^n,\ g'(\alpha) = nK(1+K\alpha)^{n-1},\ g'(0) = nK,\ K_n = \frac{(1+K_1\alpha)^{\frac{1}{n}} - 1}{\alpha} \tag{2.174}$$

$$g(\alpha) = 1 + K\alpha^n,\ g'(\alpha) = nK\alpha^{n-1}\ g'(0) = 0\ (n \neq 1),\ K_n = (K_1\alpha)^{\frac{1}{n}} \tag{2.175}$$

These two laws are identical when $n = 1$ and give linear hardening. If K_1 is the hardening term when $n = 1$ and then a new value of n is selected, the first law can preserve the initial slope, $g'(0)$, by keeping

the product constant or setting $K_n = K_1/n$; the second law will always have zero slope when $n \neq 1$ and thus cannot match the linear slope. The last equations for K_n give the value of K_n for new n to match the amount of hardening that occurs up to any specified α between the $n = 1$ and n laws.

The numerical solution uses the following iterative equations

$$\boldsymbol{\sigma}^{(k)} = \boldsymbol{\sigma}^{trial} - \lambda^{(k)}\mathbf{C}df(\sigma^{(k)}) \tag{2.176}$$

$$h^{(k)} = -\sqrt{\frac{2}{3}\left(df_{xx}^2 + df_{yy}^2 + df_{zz}^2 + \frac{1}{2}df_{yz}^2 + \frac{1}{2}df_{xz}^2 + \frac{1}{2}df_{xy}^2\right)} \tag{2.177}$$

$$f^{(k)} = f(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\alpha}^{(k)}) \tag{2.178}$$

$$\frac{df^{(k)}}{d\lambda} = -\left(df(\boldsymbol{\sigma}^{(k)}) \cdot \mathbf{C}df(\boldsymbol{\sigma}^{(k)}) - g'(\alpha)h^{(k)}\right) \tag{2.179}$$

$$\lambda^{(k+1)} = \lambda^{(k)} - \frac{f^{(k)}}{df^{(k)}/d\lambda} \tag{2.180}$$

$$\alpha^{(k+1)} = \alpha^0 - \lambda^{(k+1)}h^{(k)} \tag{2.181}$$

2.13 Quadratic Hill Criterion - Global Axes

The quadratic Hill yield criterion can implement anisotropic plasticity and hardening terms can be added to include aniostropic hardening as well. For 3D analysis, one version of Hill yield function with arbitrary hardening function (defined later) reduces to:

$$f = \sqrt{F\left(\overline{\sigma_{yy}} - \overline{\sigma_{zz}}\right)^2 + G\left(\overline{\sigma_{xx}} - \overline{\sigma_{zz}}\right)^2 + H\left(\overline{\sigma_{yy}} - \overline{\sigma_{xx}}\right)^2 + 2L\overline{\tau_{yz}}^2 + 2M\overline{\tau_{xz}}^2 + 2N\overline{\tau_{xy}}^2} - g(\boldsymbol{\alpha}) \tag{2.182}$$

$$= \Big[(G+H)\overline{\sigma_{xx}}^2 + (F+H)\overline{\sigma_{yy}}^2 + (F+G)\sigma_{zz}^2 - 2F\overline{\sigma_{yy}}\sigma_{zz} - 2G\overline{\sigma_{xx}}\sigma_{zz} - 2H\overline{\sigma_{xx}\sigma_{yy}} + 2L\overline{\tau_{yz}}^2 + 2M\overline{\tau_{xz}}^2 + 2N\overline{\tau_{xy}}^2\Big]^{1/2} - g(\boldsymbol{\alpha}) \tag{2.183}$$

$$= \sqrt{\overline{\boldsymbol{\sigma}}^T\mathbf{A}\overline{\boldsymbol{\sigma}}} - g(\boldsymbol{\alpha}) \tag{2.184}$$

where $\overline{\boldsymbol{\sigma}}^T = (\overline{\sigma_{xx}}, \overline{\sigma_{yy}}, \overline{\sigma_{zz}}, \overline{\tau_{yz}}, \overline{\tau_{xz}}, \overline{\tau_{xy}})$, $g(\boldsymbol{\alpha})$ is some hardening function of internal variables, and

$$\mathbf{A} = \begin{pmatrix} G+H & -H & -G & 0 & 0 & 0 \\ -H & F+H & -F & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 \\ 0 & 0 & 0 & 2L & 0 & 0 \\ 0 & 0 & 0 & 0 & 2M & 0 \\ 0 & 0 & 0 & 0 & 0 & 2N \end{pmatrix} \tag{2.185}$$

An overbar is the stress in the material coordinates. Defining $\mathbf{R}_\sigma$ as rotation matrix to rotate stress from material to the global axes, we have

$$\boldsymbol{\sigma} = \mathbf{R}_\sigma\overline{\boldsymbol{\sigma}} \qquad \text{or} \qquad \overline{\boldsymbol{\sigma}} = \mathbf{R}_\sigma^{-1}\boldsymbol{\sigma} = \mathbf{R}_\varepsilon^T\boldsymbol{\sigma} \tag{2.186}$$

In modeling, $\mathbf{R}_\sigma^{-1}$ is derived from $\boldsymbol{R}_{tot}^T\boldsymbol{\sigma}\boldsymbol{R}_{tot}$ where $\boldsymbol{R}_{tot}$ is 3×3 rotation matrix derived from initial orientation and it is output of polar decomposition of current deformation gradient (*i.e.*, $\boldsymbol{R}_{tot}$ rotates from material axes to analysis axes or $\boldsymbol{\sigma} = \boldsymbol{R}_{tot}\overline{\boldsymbol{\sigma}}\boldsymbol{R}_{tot}^T$). The corresponding equation in analysis axis coordinates for the yield function takes the form

$$f = \sqrt{\boldsymbol{\sigma}^T(\mathbf{R}_\sigma^{-1})^T\mathbf{A}\mathbf{R}_\sigma\boldsymbol{\sigma}} - g(\boldsymbol{\alpha}) = \sqrt{\boldsymbol{\sigma}\mathbf{A}'\boldsymbol{\sigma}} - g(\boldsymbol{\alpha}) \tag{2.187}$$

where $\mathbf{A}' = \mathbf{R}_\varepsilon \mathbf{A} \mathbf{R}_\varepsilon^T$ is the $\mathbf{A}$ matrix rotated using rotation matrix for transformation of strains in the contracted nomenclature. See the previous section for details on the elements of the $\mathbf{A}$ matrix in the material axis system.

The derivatives with respect to analyses axes are found by differentiating with respect to stress in the material axes and then rotating the result by strain rotation to the analysis axes. The result is

$$d\boldsymbol{f} = \frac{\mathbf{R}_\varepsilon \mathbf{A} \overline{\boldsymbol{\sigma}}}{\sqrt{\overline{\boldsymbol{\sigma}}^T \mathbf{A} \overline{\boldsymbol{\sigma}}}} \tag{2.188}$$

Substituting for $\overline{\boldsymbol{\sigma}}$ leads to

$$d\boldsymbol{f} = \frac{\mathbf{A}' \boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma}^T \mathbf{A}' \boldsymbol{\sigma}}} \tag{2.189}$$

as expected. The $d\boldsymbol{f}_{ij}$ found in contracted notation give the engineering plastic shear strain.

We assume hardening is a function only of equivalent plastic strain and thus α is cumulative plastic strain. Perhaps a general anisotropic material would have something different, but this assumption is common in metals. The update in alpha is thus

$$d\alpha = \sqrt{\frac{2}{3}} \|d\boldsymbol{\varepsilon}_p\| = \lambda \sqrt{\frac{2}{3}\left(d\boldsymbol{f}_{xx}^2 + d\boldsymbol{f}_{yy}^2 + d\boldsymbol{f}_{zz}^2 + \frac{1}{2} d\boldsymbol{f}_{yz}^2 + \frac{1}{2} d\boldsymbol{f}_{xz}^2 + \frac{1}{2} d\boldsymbol{f}_{xy}^2 \right)} \tag{2.190}$$

Thus the update vector is

$$\boldsymbol{h} = -\sqrt{\frac{2}{3}\left(d\boldsymbol{f}_{xx}^2 + d\boldsymbol{f}_{yy}^2 + d\boldsymbol{f}_{zz}^2 + \frac{1}{2} d\boldsymbol{f}_{yz}^2 + \frac{1}{2} d\boldsymbol{f}_{xz}^2 + \frac{1}{2} d\boldsymbol{f}_{xy}^2 \right)} \tag{2.191}$$

and

$$d\boldsymbol{f}^\alpha \cdot \boldsymbol{h} = g'(\alpha) \sqrt{\frac{2}{3}\left(d\boldsymbol{f}_{xx}^2 + d\boldsymbol{f}_{yy}^2 + d\boldsymbol{f}_{zz}^2 + \frac{1}{2} d\boldsymbol{f}_{yz}^2 + \frac{1}{2} d\boldsymbol{f}_{xz}^2 + \frac{1}{2} d\boldsymbol{f}_{xy}^2 \right)} \tag{2.192}$$

Some possible hardening laws are

$$g(\alpha) = (1 + K\alpha)^n,\ g'(\alpha) = nK(1 + K\alpha)^{n-1},\ g'(0) = nK,\ K_n = \frac{(1 + K_1\alpha)^{\frac{1}{n}} - 1}{\alpha} \tag{2.193}$$

$$g(\alpha) = 1 + K\alpha^n,\ g'(\alpha) = nK\alpha^{n-1}\ g'(0) = 0\ (n \neq 1),\ K_n = (K_1\alpha)^{\frac{1}{n}} \tag{2.194}$$

These two laws are identical when $n = 1$ and give linear hardening. If K_1 is the hardening term when $n = 1$ and then a new value of n is selected, the first law can preserve the initial slope, $g'(0)$, by keeping the product constant or setting $K_n = K_1/n$; the second law will always have zero slope when $n \neq 1$ and thus cannot match the linear slope. The last equations for K_n give the value of K_n for new n to match the amount of hardening that occurs up to any specified α between the $n = 1$ and n laws.

The numerical solution uses the following iterative equations

$$\boldsymbol{\sigma}^{(k)} = \boldsymbol{\sigma}^{trial} - \lambda^{(k)} \mathbf{C} d\boldsymbol{f}(\lambda^{(k)}) \tag{2.195}$$

$$\boldsymbol{h}^{(k)} = -\sqrt{\frac{2}{3}\left(d\boldsymbol{f}_{xx}^2 + d\boldsymbol{f}_{yy}^2 + d\boldsymbol{f}_{zz}^2 + \frac{1}{2} d\boldsymbol{f}_{yz}^2 + \frac{1}{2} d\boldsymbol{f}_{xz}^2 + \frac{1}{2} d\boldsymbol{f}_{xy}^2 \right)} \tag{2.196}$$

$$f^{(k)} = f(\boldsymbol{\sigma}^{(k)}, \boldsymbol{\alpha}^{(k)}) \tag{2.197}$$

$$\frac{df^{(k)}}{d\lambda} = -\left(d\boldsymbol{f}(\boldsymbol{\sigma}^{(k)}) \cdot \mathbf{C} d\boldsymbol{f}(\boldsymbol{\sigma}^{(k)}) + d\boldsymbol{f}^\alpha \cdot \boldsymbol{h}^{(k)} \right) \tag{2.198}$$

$$\lambda^{(k+1)} = \lambda^{(k)} - \frac{f^{(k)}}{df^{(k)}/d\lambda} \tag{2.199}$$

$$\boldsymbol{\alpha}^{(k+1)} = \boldsymbol{\alpha}^0 - \lambda^{(k+1)} \boldsymbol{h}^{(k)} \tag{2.200}$$

2.14 More General Plasticity Methods

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

$$0 = \Delta\boldsymbol{\sigma} - \mathsf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_p) = \Delta\boldsymbol{\sigma} - \mathsf{C}d\boldsymbol{\varepsilon} + \lambda\mathsf{C}\nabla f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) \tag{2.201}$$

$$0 = f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + d\alpha) = f\left(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}, \alpha + \sqrt{\frac{3}{2}}\lambda\,\|\nabla f\|\right) \tag{2.202}$$

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:

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)} - \boldsymbol{x}^{(n)}\right) = -F(\boldsymbol{x}^{(n)}) \tag{2.203}$$

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

$$J(\boldsymbol{x}^{(n)})\left(\boldsymbol{x}^{(n+1)} - \boldsymbol{x}^{(n)}\right) = \begin{bmatrix} \mathsf{I} + \lambda\mathsf{C}\frac{d\nabla f}{d\Delta\boldsymbol{\sigma}} & \mathsf{C}\nabla f \\ \nabla f & \frac{df}{d\alpha}\frac{d\alpha}{d\lambda} \end{bmatrix}^{(n)} \begin{bmatrix} \delta\boldsymbol{\sigma}^{(n)} \\ \delta\lambda^{(n)} \end{bmatrix} = -\begin{bmatrix} \boldsymbol{p}^{(n)} \\ q^{(n)} \end{bmatrix} \tag{2.204}$$

where

$$\boldsymbol{p}^{(n)} = \Delta\boldsymbol{\sigma}^{(n)} - \mathsf{C}d\boldsymbol{\varepsilon} + \lambda^{(n)}\mathsf{C}\nabla f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}^{(n)}, \alpha + d\alpha^{(n)}) \tag{2.205}$$

$$q^{(n)} = f\left(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}^{(n)}, \alpha + d\alpha^{(n)}\right) \tag{2.206}$$

$$d\alpha^{(n)} = \sqrt{\frac{3}{2}}\lambda\left\|\nabla f(\boldsymbol{\sigma} + \Delta\boldsymbol{\sigma}^{(n)}, \alpha + d\alpha^{(n)})\right\| \tag{2.207}$$

The next iteration for stress and λ are

$$\Delta\boldsymbol{\sigma}^{(n+1)} = \Delta\boldsymbol{\sigma}^{(n)} + \delta\boldsymbol{\sigma}^{(n)} \tag{2.208}$$

$$\delta\lambda^{(n+1)} = \lambda^{(n)} + \delta\lambda^{(n)} \tag{2.209}$$

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:

$$\delta\boldsymbol{\sigma}^{(n)} = -\boldsymbol{p}^{(n)} - \delta\lambda^{(n)}\mathsf{C}\nabla f \qquad \text{and} \qquad \delta\lambda^{(n)} = -\frac{q^{(n)} - \nabla f \cdot \boldsymbol{p}^{(n)}}{\nabla f \cdot \mathsf{C}\nabla f - \frac{df}{d\alpha}\frac{d\alpha}{d\lambda}} \tag{2.210}$$

For next increment:

$$\boldsymbol{p}^{(n+1)} = \Delta\boldsymbol{\sigma}^{(n+1)} - \mathsf{C}d\boldsymbol{\varepsilon} + \lambda^{(n+1)}\mathsf{C}\nabla f \tag{2.211}$$

$$= \Delta\boldsymbol{\sigma}^{(n)} - \boldsymbol{p}^{(n)} - \delta\lambda^{(n)}\mathsf{C}\nabla f - \mathsf{C}d\boldsymbol{\varepsilon} + (\lambda^{(n)} + \delta\lambda^{(n)})\mathsf{C}\nabla f \tag{2.212}$$

$$= 0 \tag{2.213}$$

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:

$$\Delta\boldsymbol{\sigma}^{(n)} = -\sum_{i=0}^{n}\delta\lambda^{(i)}\mathsf{C}\nabla f = -\lambda^{(n)}\mathsf{C}\nabla f \tag{2.214}$$

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

$$0 = f\left(\boldsymbol{\sigma} + \mathsf{C}d\boldsymbol{\varepsilon} - \lambda^{(n)}\mathsf{C}\nabla f, \alpha + d\alpha^{(n)}\right) = f_{trial} - \lambda^{(n)}\left(\nabla f \cdot \mathsf{C}\nabla - \frac{df}{d\alpha}\frac{d\alpha}{d\lambda}\right) \tag{2.215}$$

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

$$\delta\lambda^{(n)} = -\frac{q^{(n)}}{\nabla f \cdot \mathsf{C}\nabla f - \frac{df}{d\alpha}\frac{d\alpha}{d\lambda}} \tag{2.216}$$

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. After performing the constitutive law (in material axes), the result are rotated to the current analysis coordinates. The default mode is a "small rotation" mode which is the default mode and similar to before, but has be updated to track deformation gradient 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 matrix rather the find it by polar decomposition. The small rotation mode is therefore more efficient and mauy be very close to the large rotation mode for many problems. 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 to deformation gradient.

3.2 Analysis in Current Configuration

For isotropic materials, any axis system can be considered as material axis systems and therefore, for efficiency (maybe), the small strains increment is found in the current analysis axis system. The same approach can be used for anisotropic materials, provided the material properties are rotated as well. The deformation gradients after step $n-1$ and n can be decomposed into

$$\mathbf{F}_n = \mathbf{V}_n\mathbf{R}_n, \qquad \mathbf{F}_{n-1} = \mathbf{V}_{n-1}\mathbf{R}_{n-1}, \qquad \text{leading to} \qquad \mathbf{dR} = \mathbf{R}_n\mathbf{R}_{n-1}^T \tag{3.1}$$

where $\mathbf{dR}$ is increment rotation due to incremental deformation gradient $\mathbf{dF}$ (or $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$) and we have not assume dR is same matrix as decomposition of $\mathbf{dF}$, but I think they might be same (at least for a small increment). The small strains from previous and current step are:

$$\boldsymbol{\varepsilon}_n = \mathbf{V}_n - \mathbf{I} \qquad \text{and} \qquad \boldsymbol{\varepsilon}_{n-1} = \mathbf{V}_{n-1} - \mathbf{I} \tag{3.2}$$

This the strain increment in current coordinates is found by rotating previous strain by dR and subtracting from new strain:

$$d\varepsilon = \mathbf{V}_n - \mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T \tag{3.3}$$

The incremental stress is

$$d\boldsymbol{\sigma} = \mathbf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res}) \tag{3.4}$$

where $d\boldsymbol{\varepsilon}_{res}$ is the incremental residual strain. The stress update rotates previous stress to new axes and adds this stress:

$$\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + d\boldsymbol{\sigma} \tag{3.5}$$

where **dR** found from above and not by polar decomposition of **dF** (although it could be found approximately that way).

The algorithm is

1. Decompose current $\mathbf{F}_{n-1} = \mathbf{V}_{n-1}\mathbf{R}_{n-1}$ to get $\mathbf{V}_{n-1}$ and $\mathbf{R}_{n-1}$. Note that if the particle tracks its rotation matrix, this polar decomposition can be skipped and just retrieve $\mathbf{R}_{n-1}$
2. Calculate $\mathbf{dF} = \exp(\nabla v \Delta t)$, find $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$ and decompose to get $\mathbf{F}_{n-1} = \mathbf{V}_{n-1}\mathbf{R}_{n-1}$ and find $\mathbf{dR} = \mathbf{R}_n\mathbf{R}_{n-1}^T$.
3. Find incremental strain from $d\boldsymbol{\varepsilon} = \mathbf{V}_n - \mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T$.
4. Update stress to $\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + \mathbf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res})$. For anisotropic materials, **C** and $d\boldsymbol{\varepsilon}_{res}$ need to be rotated into the current configuration.

Compared to Hypoelastic correction method (see next section), this algorithm adds two polar decompositions. One of them can be eliminated by tracking **R** as well. For plasticity materials, the plastic strain must be rotated like the stress ($\boldsymbol{\varepsilon}_{p,n} = \mathbf{dR}\boldsymbol{\varepsilon}_{p,n-1}\mathbf{dR}^T + d\boldsymbol{\varepsilon}_p$). It is tracked as plastic strain in the analysis coordinates.

3.2.1 Hypoelastic Version

Assuming small incremental strain and rotation, the algorithm can be approximated as a hypoelastic material using:

1. Calculate $\mathbf{dF} = \mathbf{I} + \nabla v \Delta t$ and decompose to get $\mathbf{dV} = \mathbf{I} + d\boldsymbol{\varepsilon}$ and $\mathbf{dR} = \mathbf{I} + d\boldsymbol{\omega}$
2. Previous $\mathbf{F}_{n-1}$ in small strain decomposes to $\mathbf{V}_{n-1} = \mathbf{I} + \varepsilon_{n-1}$ and $\mathbf{R}_{n-1} = \mathbf{I} + \boldsymbol{\omega}_{n-1}$.
3. Total deformation is $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$, which in small strain is $(\mathbf{I} + d\boldsymbol{\varepsilon} + d\boldsymbol{\omega})(\mathbf{I} + \varepsilon_{n-1} + \boldsymbol{\omega}_{n-1})$ which decompose to $\mathbf{V}_n = \mathbf{I} + d\boldsymbol{\varepsilon} + \varepsilon_{n-1}$ and $\mathbf{R}_n = \mathbf{I} + d\boldsymbol{\omega} + \boldsymbol{\omega}_{n-1}$.
4. The strain increment can come for $d\boldsymbol{\varepsilon} = \mathbf{V}_n - \mathbf{V}_{n-1} = \mathbf{dV} - \mathbf{I}$.
5. Update deformation gradient to $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$. Note that full matrix method is needed otherwise large rotations will deteriorate the solution.
6. The incremental stress is $d\boldsymbol{\sigma} = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T - \boldsymbol{\sigma}_{n-1} + \mathbf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res})$, which expands to

$$\begin{aligned} d\boldsymbol{\sigma} &\approx d\boldsymbol{\omega}\boldsymbol{\sigma}_{n-1} + \boldsymbol{\sigma}_{n-1}d\boldsymbol{\omega}^T + d\boldsymbol{\omega}\boldsymbol{\sigma}_{n-1}d\boldsymbol{\omega}^T + \mathbf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res}) &(3.6)\\ &= d\boldsymbol{\omega}\boldsymbol{\sigma}_{n-1} + (d\boldsymbol{\omega}\boldsymbol{\sigma}_{n-1})^T + d\boldsymbol{\omega}\boldsymbol{\sigma}_{n-1}d\boldsymbol{\omega}^T + \mathbf{C}(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_{res}) &(3.7)\end{aligned}$$

For 2D calculations, an expansion to second order of the **dR** decomposition results in

$$d\boldsymbol{\omega} = \mathbf{dR} - \mathbf{I} = \begin{pmatrix} -\frac{d\omega_{xy}^2}{8} & -\left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right)\frac{d\omega_{xy}}{2} \\ \left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right)\frac{d\omega_{xy}}{2} & -\frac{d\omega_{xy}^2}{8} \end{pmatrix} \tag{3.8}$$

where $d\omega_{xy}$ is engineering rotational strain tracked in the code and equal to $2\Omega_{yx}$ where $2\Omega = \nabla \boldsymbol{u} - \nabla \boldsymbol{u}^T$. Substituting into above expression and truncating at second order gives stress update of

$$\begin{pmatrix} d\sigma_{xx} \\ d\sigma_{yy} \\ d\tau_{xy} \end{pmatrix} = \begin{pmatrix} d\sigma^{(0)}_{xx} - \left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}\tau_{xy} - \frac{d\omega^2_{xy}}{4}(\sigma_{xx} - \sigma_{yy}) \\ d\sigma^{(0)}_{yy} + \left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}\tau_{xy} + \frac{d\omega^2_{xy}}{4}(\sigma_{xx} - \sigma_{yy}) \\ d\tau^{(0)}_{xy} + \frac{1}{2}\left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}(\sigma_{xx} - \sigma_{yy}) - \frac{d\omega^2_{xy}}{2}\tau_{xy} \end{pmatrix} \tag{3.9}$$

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

$$\begin{pmatrix} d\varepsilon_{xx,p} \\ d\varepsilon_{yy,p} \\ d\gamma_{xy,p} \end{pmatrix} = \begin{pmatrix} d\varepsilon^{(0)}_{xx,p} - \frac{1}{2}\left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}\gamma_{xy,p} - \frac{d\omega^2_{xy}}{4}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) \\ d\varepsilon^{(0)}_{yy,p} + \frac{1}{2}\left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}\gamma_{xy,p} + \frac{d\omega^2_{xy}}{4}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) \\ d\gamma^{(0)}_{xy,p} + \left(1 - \frac{d\varepsilon_{xx}+d\varepsilon_{yy}}{2}\right) d\omega_{xy}(\varepsilon_{xx,p} - \varepsilon_{yy,p}) - \frac{d\omega^2_{xy}}{2}\gamma_{xy,p} \end{pmatrix} \tag{3.10}$$

where $d\varepsilon^{(0)}_{ij,p}$ on calculated plastic strain increments (and may be zero when deformation is elastic). Most published implementation of hypoelasticity truncate at the first order term. In 2D, it is easy to add the second order term.

For 3D calculations, it appears difficult to do a second order expansion of **dR**. Instead, a first order expansion is used:

$$d\boldsymbol{\omega} = \mathbf{dR} - \mathbf{I} = \begin{pmatrix} 0 & -\frac{d\omega_{xy}}{2} & -\frac{d\omega_{xz}}{2} \\ \frac{d\omega_{xy}}{2} & 0 & -\frac{d\omega_{yz}}{2} \\ \frac{d\omega_{xz}}{2} & \frac{d\omega_{yz}}{2} & 0 \end{pmatrix} \tag{3.11}$$

The first order update becomes:

$$\begin{pmatrix} d\sigma_{xx,p} \\ d\sigma_{yy,p} \\ d\sigma_{zz,p} \\ d\tau_{yz,p} \\ d\tau_{xz,p} \\ d\tau_{xy,p} \end{pmatrix} = \begin{pmatrix} d\sigma^{(0)}_{xx,p} - d\omega_{xy}\tau_{xy,p} - d\omega_{xz}\tau_{xz,p} \\ d\sigma^{(0)}_{yy,p} + d\omega_{xy}\tau_{xy,p} - d\omega_{yz}\tau_{yz,p} \\ d\sigma^{(0)}_{zz,p} + d\omega_{xz}\tau_{xz,p} + d\omega_{yz}\tau_{yz,p} \\ d\tau^{(0)}_{yz,p} + \frac{d\omega_{yz}}{2}(\sigma_{yy,p} - \sigma_{zz,p}) + \frac{d\omega_{xz}\tau_{xz}}{2} + \frac{d\omega_{xy}\tau_{xy}}{2} \\ d\tau^{(0)}_{xz,p} + \frac{d\omega_{xz}}{2}(\sigma_{xx,p} - \sigma_{zz,p}) + \frac{d\omega_{yz}\tau_{yz}}{2} - \frac{d\omega_{xy}\tau_{xy}}{2} \\ d\tau^{(0)}_{xy,p} + \frac{d\omega_{xy}}{2}(\sigma_{xx,p} - \sigma_{yy,p}) - \frac{d\omega_{xz}\tau_{xz}}{2} - \frac{d\omega_{yz}\tau_{yz}}{2} \end{pmatrix} \tag{3.12}$$

The same update can be used to account for rotations of plastic strain (being sure to account for tracking of engineering plastic shear strain) as:

$$\begin{pmatrix} d\varepsilon_{xx,p} \\ d\varepsilon_{yy,p} \\ d\varepsilon_{zz,p} \\ d\gamma_{yz,p} \\ d\gamma_{xz,p} \\ d\gamma_{xy,p} \end{pmatrix} = \begin{pmatrix} d\varepsilon^{(0)}_{xx,p} - \frac{d\omega_{xy}\gamma_{xy,p}}{2} - \frac{d\omega_{xz}\gamma_{xz,p}}{2} \\ d\varepsilon^{(0)}_{yy,p} + \frac{d\omega_{xy}\gamma_{xy,p}}{2} - \frac{d\omega_{yz}\gamma_{yz,p}}{2} \\ d\varepsilon^{(0)}_{zz,p} + \frac{d\omega_{xz}\gamma_{xz,p}}{2} + \frac{d\omega_{yz}\gamma_{yz,p}}{2} \\ d\gamma^{(0)}_{yz,p} + d\omega_{yz}(\sigma_{yy,p} - \sigma_{zz,p}) + \frac{d\omega_{xz}\gamma_{xz}}{2} + \frac{d\omega_{xy}\gamma_{xy}}{2} \\ d\gamma^{(0)}_{xz,p} + d\omega_{xz}(\sigma_{xx,p} - \sigma_{zz,p}) + \frac{d\omega_{yz}\gamma_{yz}}{2} - \frac{d\omega_{xy}\gamma_{xy}}{2} \\ d\gamma^{(0)}_{xy,p} + d\omega_{xy}(\sigma_{xx,p} - \sigma_{yy,p}) - \frac{d\omega_{xz}\gamma_{xz}}{2} - \frac{d\omega_{yz}\gamma_{yz}}{2} \end{pmatrix} \tag{3.13}$$

These equations appear with published hypoelasticity equation, but the derivation explicitly from polar decomposition is usually not give along with the equations.

3.3 Analysis in Current Configuration - OLD METHOD

For isotropic materials, any axis system can be considered as material axis systems and therefore, for efficiency, the small strains increment is found in the current analysis axis system. The same approach can be used for anisotropic materials, provided the material properties are rotated as well. The deformation gradient after step n can be decomposed into

$$\mathbf{F}_n = \mathbf{V}_n\mathbf{R}_n = \mathbf{dV}\mathbf{V}_{n-1}^{(R)}\mathbf{dR}\mathbf{R}_{n-1} \tag{3.14}$$

where $\mathbf{V}$ is the left stretch and $\mathbf{R}$ is the rotation matrix., $\mathbf{dV}$ is incremental stretch this time step, and $\mathbf{V}_{n-1}^{(R)}$ is the left stretch from previous time step rotated to current time step. If $\mathbf{dR}$ is the incremental rotation this time step then

$$\mathbf{V}_{n-1}^{(R)} = \mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T \tag{3.15}$$

then

$$\mathbf{F}_n = \mathbf{dV}\mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T\mathbf{dR}\mathbf{R}_{n-1} = (\mathbf{dV}\mathbf{dR})(\mathbf{V}_{n-1}\mathbf{R}_{n-1}) = \mathbf{dF}\mathbf{F}_{n-1} \tag{3.16}$$

where $\mathbf{dF}$ is the incremental deformation this time step.

The small strain in the analysis axis system is $\varepsilon = \mathbf{V} - \mathbf{I}$. The incremental strain (in current axes) is

$$\begin{aligned} d\varepsilon &= (\mathbf{V}-\mathbf{I}) - (\mathbf{V}_{n-1}^{(R)} - \mathbf{I}) = \mathbf{V} - \mathbf{V}_{n-1}^{(R)} && (3.17)\\ &= \mathbf{dV}\mathbf{V}_{n-1}^{(R)} - \mathbf{V}_{n-1}^{(R)} = (\mathbf{dV}-\mathbf{I})\mathbf{V}_{n-1}^{(R)} && (3.18)\\ &= (\mathbf{dV}-\mathbf{I})\mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T && (3.19)\end{aligned}$$

The incremental stress is

$$d\boldsymbol{\sigma} = \mathbf{C}(d\varepsilon - d\varepsilon_{res}) \tag{3.20}$$

where $d\varepsilon_{res}$ is the incremental residual strain. The stress update rotated previous stress to new axes and adds this stress:

$$\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + d\boldsymbol{\sigma} \tag{3.21}$$

The algorithm is

1. Decompose current $\mathbf{F}_{n-1} = \mathbf{V}_{n-1}\mathbf{R}_{n-1}$ to get $\mathbf{V}_{n-1}$ and $\mathbf{R}_{n-1}$. Note that if the particle tracks its rotation matrix, this polar decomposition can be skipped and just retrieve $\mathbf{R}_{n-1}$
2. Calculate $\mathbf{dF} = \exp(\nabla v \Delta t)$ and decompose to get $\mathbf{dV}$ and $\mathbf{dR}$ and calculate $\mathbf{R}_n = \mathbf{dR}\mathbf{R}_{n-1}$.
3. Find incremental strain from

   $$d\varepsilon = (\mathbf{dV}-\mathbf{I})\mathbf{dR}\mathbf{V}_{n-1}\mathbf{dR}^T = (\mathbf{dV}-\mathbf{I})\mathbf{dR}\mathbf{F}_{n-1}\mathbf{R}_{n-1}^T\mathbf{dR}^T = (\mathbf{dV}-\mathbf{I})\mathbf{dR}\mathbf{F}_{n-1}\mathbf{R}_n^T \tag{3.22}$$

   Use first is decomposition found $\mathbf{V}_{n-1}$ or use last if rotation matrix is tracked
4. Update deformation gradient to $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$
5. Update stress to $\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + \mathbf{C}(d\varepsilon - d\varepsilon_{res})$. For anisotropic materials, $\mathbf{C}$ and $d\varepsilon_{res}$ need to be rotated into the current configuration.

Compared to Hypoelastic correction method (see next section), this algorithm adds two polar decompositions. One of them can be eliminated by tracking $\mathbf{R}$ as well. For plasticity materials, the plastic strain must be rotated like the stress ($\boldsymbol{\varepsilon}_{p,n} = \mathbf{dR}\boldsymbol{\varepsilon}_{p,n-1}\mathbf{dR}^T + d\boldsymbol{\varepsilon}_p$). It is tracked as plastic strain in the analysis coordinates.

3.4 Analysis in Material Axis System

An alternative is to do calculations in the material axis system. This approach is only used for anisotropic materials when using large rotation method with polar decompositions. For anisotropic materials, the system has to be rotated into the material axes and those axes may not line up with the initial analysis axes. Accounting for arbitrary initial orientation, the total deformation gradient from the material axes is

$$\mathbf{F}_n^{(tot)} = \mathbf{F}_n\mathbf{F}_0 = \mathbf{F}_n\mathbf{R}_0 \tag{3.23}$$

where $\mathbf{F}_n$ is deformation from the analysis axes (and the $\mathbf{F}$ tracked in calculations) and $\mathbf{F}_0 = \mathbf{R}_0$ is initial deformation (which is only a rotation) from material axes to the initial analyses axes. We decompose total deformation into:

$$\mathbf{F}_n^{(tot)} = \mathbf{R}_n\mathbf{U}_n\mathbf{R}_0 \tag{3.24}$$

where $\mathbf{R}_n$ is rotation from initial analysis axes to the current configuration and $\mathbf{U}_n$ is the right stretch in the initial analysis axes.

Next imagine incremental deformation $\mathbf{dF}$. Then

$$\mathbf{F}_n^{(tot)} = \mathbf{dF}\mathbf{F}_{n-1}\mathbf{R}_0 \tag{3.25}$$

and decompose previous deformation

$$\mathbf{F}_{n-1}^{(tot)} = \mathbf{F}_{n-1}\mathbf{R}_0 = \mathbf{R}_{n-1}\mathbf{U}_{n-1}\mathbf{R}_0 \tag{3.26}$$

Defining strain in initial axes from the right stretch (*i.e.*, $\varepsilon = \mathbf{U} - \mathbf{I}$), the strain in the material axes is found by rotating from initial axes to the material axes

$$\varepsilon = \mathbf{R}_0^T(\mathbf{U}_n - \mathbf{I})\mathbf{R}_0 \tag{3.27}$$

The incremental strain in the material axes becomes

$$d\varepsilon = \varepsilon_n - \varepsilon_{n-1} = \mathbf{R}_0^T(\mathbf{U}_n - \mathbf{U}_{n-1})\mathbf{R}_0 \tag{3.28}$$

Although above analysis is correct, the incremental strain is found by subtracting two non-incremental terms, which might be cause for concern. We can derive an alternate approach that appears to be more stable numerically. We can decompose $\mathbf{F}_n$ using incremental terms

$$\mathbf{F}_n = \mathbf{dRdUR}_{n-1}\mathbf{U}_{n-1} = \mathbf{dRR}_{n-1}\mathbf{R}_{n-1}^T\mathbf{dUR}_{n-1}\mathbf{U}_{n-1} \approx \mathbf{R}_n\mathbf{U}_n \tag{3.29}$$

where $\mathbf{dR}$ and $\mathbf{dU}$ are from polar decomposition of $\mathbf{dF}$. From the last result we can associate:

$$\mathbf{R}_n \approx \mathbf{dRR}_{n-1} \qquad \text{and} \qquad \mathbf{U}_n \approx \mathbf{R}_{n-1}^T\mathbf{dUR}_{n-1}\mathbf{U}_{n-1} \tag{3.30}$$

The are not exact in large deformation theory, but they are exact (to strain increment squared) in small strain theory. The strain increment becomes

$$d\varepsilon = \mathbf{R}_0^T\big[(\,\mathbf{R}_{n-1}^T\mathbf{dUR}_{n-1} - \mathbf{I})\mathbf{U}_{n-1}\big]\mathbf{R}_0 \tag{3.31}$$

which no longer subtracts two non increment strains. Instead, an incremental strain, $(\mathbf{R}_{n-1}^T\mathbf{dUR}_{n-1} - \mathbf{I})$, is multiplied by non-incremental stretch, $\mathbf{U}_{n-1}$, and then rotated.

The algorithm is

1. Decompose current $\mathbf{F}_{n-1}$ to get $\mathbf{U}_{n-1}$ and $\mathbf{R}_{n-1}$.

2. Calculate $\mathbf{dF} = \exp(\nabla v t)$, decompose it to get $\mathbf{dR}$ and $\mathbf{dU}$, and update deformation gradient to $\mathbf{F}_n = \mathbf{dF}\mathbf{F}_{n-1}$.

3. Find incremental strain from

$$d\varepsilon = \mathbf{R}_0^T\big[(\ \mathbf{R}_{n-1}^T\mathbf{dU}\mathbf{R}_{n-1} - \mathbf{I})\mathbf{U}_{n-1}\big]\mathbf{R}_0 \tag{3.32}$$

4. Find incremental stress from $d\boldsymbol{\sigma} = \mathbf{C}(d\varepsilon - d\varepsilon_{res})$.

5. Rotate previous stress and incremental stress to analysis axes using

$$\boldsymbol{\sigma}_n = \mathbf{dR}\boldsymbol{\sigma}_{n-1}\mathbf{dR}^T + \mathbf{R}^{(tot)}d\boldsymbol{\sigma}\mathbf{R}^{(tot)^T} \tag{3.33}$$

   The first term rotates prior stress into new configuration and the second rotates incremental stress from material axes to new configuration. The total rotation matrix is $R^{(tot)} = \mathbf{dR}\mathbf{R}_{n-1}\mathbf{R}_0$.

Compared to prior versions of the code, which used Hypoelastic correction to stress that worked OK but did not track strains well, this algorithm adds two polar decompositions and a need to rotate increments into current axes, but avoids prior need to rotate the stiffness tensor into current configuration. For plasticity materials, the plastic strain must be rotated like the stress. It is tracked as plastic strain in the analysis coordinates.

Note that tracking rotation matrix can improve efficiency and eliminate need for one of the polar decompositions. It appears to provide no efficiency in 2D. Some test in 3D would be worthwhile, but it also takes more memory (each particle needs to store rotation matrix). It replaces polar decomposition with a matrix multiplication (to find $\mathbf{U}_{n-1}$).

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 boundary conditions may cause heat flow that models general conditions of the problem. Example 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 separate 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. 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.

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`,`$\mathtt{dT}_{dS=0}$`,`$\mathtt{d}\Phi$`)` where `mptr` is pointer to the material point, dT in temperature increment this time step (not used in these updates), $\mathtt{dT}_{dS=0}$ 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).

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.

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.

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

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

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

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

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

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

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).

Chapter 5

Hyperelastic Materials

5.1 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:

$$\mathbf{F} = \begin{pmatrix} 1+\varepsilon_{xx} & \frac{1}{2}(\gamma_{xy}-\omega_{xy}) & \frac{1}{2}(\gamma_{xz}-\omega_{xz}) \\ \frac{1}{2}(\gamma_{xy}+\omega_{xy}) & 1+\varepsilon_{yy} & \frac{1}{2}(\gamma_{yz}-\omega_{yz}) \\ \frac{1}{2}(\gamma_{xz}+\omega_{xz}) & \frac{1}{2}(\gamma_{yz}+\omega_{yz}) & 1+\varepsilon_{zz} \end{pmatrix} \tag{5.1}$$

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

$$\frac{\boldsymbol{\sigma}}{\rho} = \frac{\boldsymbol{\sigma} J}{\rho_0} = \frac{\boldsymbol{\tau}}{\rho_0} \tag{5.2}$$

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.

5.2 Incremental Deformation Gradient

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

$$\frac{d\mathbf{F}}{dt} = \nabla \boldsymbol{v} \mathbf{F} \tag{5.3}$$

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

$$\mathbf{F}(t+\Delta t) = \exp(\Delta t \nabla \boldsymbol{v})\mathbf{F}(t) = \mathbf{dF}\,\mathbf{F}(t) \tag{5.4}$$

where

$$\mathbf{dF} = \exp(\Delta t \nabla \boldsymbol{v}) = \mathbf{F}(t+\Delta t)\mathbf{F}(t)^{-1} \tag{5.5}$$

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

$$\exp(\Delta t \nabla \boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \sum_{k=2}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{5.6}$$

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

$$\nabla u = \begin{pmatrix} \begin{bmatrix} du_{xx} & du_{xy} \\ du_{yx} & du_{yy} \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz} \end{pmatrix} \tag{5.7}$$

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

$$(\nabla u)^k = \begin{pmatrix} \mathsf{A}^k & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & du_{zz}^k \end{pmatrix} \tag{5.8}$$

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

$$c(z) = \det(z\mathbf{I} - \mathsf{A}) = z^n - \sum_{k=0}^{n-1} c_k z^k \tag{5.9}$$

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

$$\mathsf{A}^n = \sum_{k=0}^{n-1} c_k \mathsf{A}^k \tag{5.10}$$

For $n = 2$, these reduce to

$$c_0 = -\det(\mathsf{A}), \qquad c_1 = \mathrm{Tr}(\mathsf{A}), \qquad \text{and} \qquad \mathsf{A}^2 = c_0\mathbf{I} + c_1\mathsf{A} \tag{5.11}$$

Higher powers of A can be found by recursion to be

$$\mathsf{A}^k = \beta_{k,0}\mathbf{I} + \beta_{k,1}\mathsf{A} \tag{5.12}$$

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

$$\mathbf{dF}(k_{max}) = \begin{pmatrix} [\alpha_0\mathbf{I} + \alpha_1\mathsf{A}] & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & 0 \end{matrix} & 1 + du_{zz} + \sum_{k=2}^{k_{max}} \frac{du_{zz}^k}{k!} \end{pmatrix} \tag{5.13}$$

where

$$\alpha_0 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,0}}{k!} \qquad \text{and} \qquad \alpha_1 = 1 + \sum_{k=2}^{k_{max}} \frac{\beta_{k,1}}{k!} \tag{5.14}$$

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

$$\exp(\Delta t\nabla\boldsymbol{v}) = \sum_{k=0}^{k_{max}} \frac{(\nabla u)^k}{k!} = \mathbf{I} + \nabla u + \frac{1}{2}(\nabla u)^2 + \sum_{k=3}^{k_{max}} \frac{(\nabla u)^k}{k!} \tag{5.15}$$

which can be reduced to

$$\exp(\Delta t\nabla\boldsymbol{v}) = \alpha_0\mathbf{I} + \alpha_1\nabla u + \alpha_2(\nabla u)^2 \tag{5.16}$$

$$\alpha_0 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,0}}{k!}, \qquad \alpha_1 = 1 + \sum_{k=3}^{k_{max}} \frac{\beta_{k,1}}{k!}, \quad \text{and} \quad \alpha_2 = \frac{1}{2} + \sum_{k=3}^{k_{max}} \frac{\beta_{k,2}}{k!} \tag{5.17}$$

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

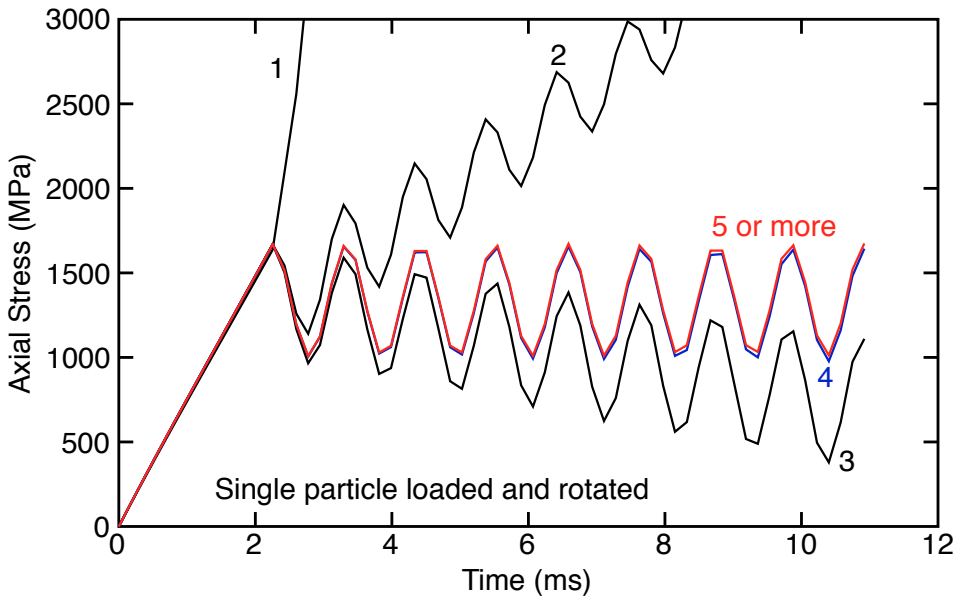

Figure 5.1: Calculation for a single particle loaded in tension, held, and then rotated. The different curves show k_{max} or the number of terms used to expand the matrix exponential in the incremental deformation gradient.

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. 5.1. 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.

5.3 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:

$$\mathbf{F} = \begin{pmatrix} \lambda_1\cos\theta & \lambda_2\sin\theta & 0 \\ -\lambda_1\sin\theta & \lambda_2\cos\theta & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \mathsf{R}[\lambda] \tag{5.18}$$

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:

$$\boldsymbol{m} = (\mathbf{dF}_{11}\mathsf{F}_{11} + \mathbf{dF}_{12}\mathsf{F}_{21}, \mathbf{dF}_{21}\mathsf{F}_{11} + \mathbf{dF}_{22}\mathsf{F}_{21}) \tag{5.19}$$

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:

$$\mathbf{F} = \begin{pmatrix} m_x & -\frac{\lambda_2}{\lambda_1}m_y & 0 \\ m_y & \frac{\lambda_2}{\lambda_1}m_x & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \tag{5.20}$$

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:

$$\boldsymbol{\tau} = \mathsf{R}\boldsymbol{\tau}\mathsf{R}^T = \mathsf{R}[\lambda]\big([\lambda]^{-1}\boldsymbol{\sigma}[\lambda]^{-T}\big)[\lambda]^T\mathsf{R}^T = \mathbf{F}\mathsf{S}\mathbf{F}^T \tag{5.21}$$

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:

$$dw = \tau_{11}du_{11} \qquad \text{and} \qquad dw_{res} = \tau_{11}du_{11}^{res} + \tau_{33}du_{33}^{res} \tag{5.22}$$

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:

$$\mathbf{dF}_m = \exp(\nabla\boldsymbol{u}) = \begin{pmatrix} \frac{\lambda_1}{\lambda_1^{(n-1)}} & 0 & 0 \\ 0 & \frac{\lambda_2}{\lambda_2^{(n-1)}} & 0 \\ 0 & 0 & \frac{\lambda_2}{\lambda_2^{(n-1)}} \end{pmatrix} \quad \text{or} \quad du_{11} = \ln\frac{\lambda_1}{\lambda_1^{(n-1)}} \tag{5.23}$$

where $\lambda_1^{(n-1)}$ are the stretches at the start of the time step.

5.4 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:

$$\mathbf{F} = \mathsf{R}\begin{pmatrix} \lambda_1 & \lambda_2\cos\omega & 0 \\ 0 & \lambda_2\sin\omega & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} = \mathsf{R}[\lambda\omega] \tag{5.24}$$

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:

$$\lambda_1 = ||\boldsymbol{m_1}||, \quad \lambda_2 = ||\boldsymbol{m_2}||, \quad \cos\omega = \frac{\boldsymbol{m_1}\cdot\boldsymbol{m_2}}{\lambda_1\lambda_2}, \quad \text{and} \quad \sin\omega = \frac{||\boldsymbol{m_1}\times\boldsymbol{m_2}||}{\lambda_1\lambda_2} \tag{5.25}$$

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:

$$\boldsymbol{\tau}\ (\text{MPM}) = \mathsf{R}\boldsymbol{\tau}\mathsf{R}^T = \mathsf{R}[\lambda\omega]\big([\lambda\omega]^{-1}\boldsymbol{\tau}[\lambda\omega]^{-T}\big)[\lambda\omega]^T\mathsf{R}^T = \mathbf{F}\mathsf{S}\mathbf{F}^T \tag{5.26}$$

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:

$$\mathsf{S} = \begin{pmatrix} \frac{1}{\lambda_1} & -\frac{\cot\omega}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix}\begin{pmatrix} \tau_{11} & \tau_{12} & 0 \\ \tau_{12} & \tau_{y22} & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \frac{1}{\lambda_1} & 0 & 0 \\ -\frac{\cot\omega}{\lambda_1} & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix} \tag{5.27}$$

The result is

$$\mathsf{S} = \begin{pmatrix} \frac{1}{\lambda_1} & -\frac{\cot\omega}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & \frac{1}{\lambda_3} \end{pmatrix}\begin{pmatrix} \frac{\tau_{11}}{\lambda_1} - \frac{\tau_{12}\cot\omega}{\lambda_1} & \frac{\tau_{12}}{\lambda_2\sin\omega} & 0 \\ \frac{\tau_{12}}{\lambda_1} - \frac{\tau_{22}\cot\omega}{\lambda_1} & \frac{\tau_{22}}{\lambda_2\sin\omega} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.28}$$

which simplifies to

$$S_{11} = \frac{1}{\lambda_1^2}\left(\tau_{11} - 2\tau_{12}\cot\omega + \tau_{22}\cot^2\omega\right) \tag{5.29}$$

$$S_{22} = \frac{\tau_{22}}{\lambda_2^2\sin^2\omega} \tag{5.30}$$

$$S_{12} = \frac{(\tau_{12} - \tau_{22}\cot\omega)}{\lambda_1\lambda_2\sin\omega} \tag{5.31}$$

These can be inverted to

$$\tau_{11} = S_{11}\lambda_1^2 + 2S_{12}\lambda_1\lambda_2\cos\omega + S_{22}\lambda_2^2\cos^2\omega \tag{5.32}$$
$$\tau_{22} = S_{22}\lambda_2^2\sin^2\omega \tag{5.33}$$
$$\tau_{12} = S_{12}\lambda_1\lambda_2\sin\omega + S_{22}\lambda_2^2\cos\omega\sin\omega \tag{5.34}$$

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:

$$dw = \tau_{11}du_{11} + \tau_{12}(du_{12} + du_{21}) + \tau_{22}du_{22} \tag{5.35}$$
$$dw_{res} = \tau_{11}du_{11}^{res} + \tau_{12}(du_{12}^{res} + (du_{12}^{res}) + \tau_{22}du_{22}^{res} \tag{5.36}$$

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

$$\mathbf{dF}_m = \exp(\nabla\boldsymbol{u}) = [\lambda\omega][\lambda\omega]_{n-1}^{-1} = \begin{pmatrix} \lambda_1 & \lambda_2\cos\omega & 0 \\ 0 & \lambda_2\sin\omega & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}\begin{pmatrix} \frac{1}{M_{11}} & -\frac{M_{12}}{M_{11}M_{22}} & 0 \\ 0 & \frac{1}{M_{22}} & 0 \\ 0 & 0 & \frac{1}{M_{33}} \end{pmatrix} \tag{5.37}$$
$$= \begin{pmatrix} \frac{\lambda_1}{M_{11}} & \frac{\lambda_2\cos\omega}{M_{22}} - \frac{M_{12}\lambda_1}{M_{11}M_{22}} & 0 \\ 0 & \frac{\lambda_2\sin\omega}{M_{22}} & 0 \\ 0 & 0 & \frac{\lambda_3}{M_{33}} \end{pmatrix} \tag{5.38}$$

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:

$$\exp(\nabla\boldsymbol{u}) = \begin{pmatrix} e^{du_{11}} & \frac{du_{12}}{du_{11}}\left(e^{du_{22}} - e^{du_{11}}\right) & 0 \\ 0 & e^{du_{22}} & 0 \\ 0 & 0 & e^{du_{33}} \end{pmatrix} \tag{5.39}$$

From which

$$du_{11} = \ln\frac{\lambda_1}{M_{11}} \tag{5.40}$$
$$du_{22} = \ln\frac{\lambda_2\sin\omega}{M_{22}} \tag{5.41}$$
$$du_{33} = \ln\frac{\lambda_3}{M_{33}} \tag{5.42}$$
$$du_{12} = \ln\frac{\lambda_1}{M_{11}}\frac{\frac{\lambda_2\cos\omega}{M_{22}} - \frac{M_{12}\lambda_1}{M_{11}M_{22}}}{\frac{\lambda_2\sin\omega}{M_{22}} - \frac{\lambda_1}{M_{11}}} \tag{5.43}$$

Alternatively, the incremental work can be written as

$$dw = \mathbf{S}\cdot\dot{\mathbf{E}}\,dt = \frac{1}{2}\mathbf{S}\cdot\dot{\mathbf{C}}\,dt \tag{5.44}$$

where $\mathbf{E}$ is Green-Lagrange strain. Evaluating $\dot{\mathbf{C}}$ and using $\dot{\mathbf{F}} = \nabla v\mathbf{F}$ gives

$$\dot{\mathbf{C}} = \dot{\mathbf{F}}^T\mathbf{F} + \mathbf{F}^T\dot{\mathbf{F}} = \mathbf{F}^T\left(\nabla v^T + \nabla v\right)\mathbf{F} \tag{5.45}$$

The energy increment (using tensors in the membrane coordinates) becomes

$$dw = \mathbf{S} \cdot [\lambda\omega]^T \left(\frac{1}{2}\left(\nabla u^T + \nabla u\right) \right) [\lambda\omega] \tag{5.46}$$

Expansion of this expression is identical to Eq. (5.35) (as it must be).

5.5 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 **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

$$\mathbf{B} = \mathbf{F}\mathbf{F}^T = \begin{pmatrix} \lambda_1^2 + \lambda_2^2\cos^2\omega & \lambda_2^2 \sin\omega\cos\omega & 0 \\ \lambda_2^2 \sin\omega\cos\omega & \lambda_2^2\sin^2\omega & 0 \\ 0 & 0 & \lambda_3^2 \end{pmatrix} \tag{5.47}$$

and the right Cauchy-Green deformation tensor in the membrane coordinates is

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} = \begin{pmatrix} \lambda_1^2 & \lambda_1\lambda_2\cos\omega & 0 \\ \lambda_1\lambda_2\cos\omega & \lambda_2^2 & 0 \\ 0 & 0 & \lambda_3^2 \end{pmatrix} \tag{5.48}$$

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.

5.6 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:

$$I_1 = \text{Tr}(\mathbf{B}) = B_{11} + B_{22} + B_{33} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \tag{5.49}$$

$$I_2 = \frac{1}{2}\left(I_1^2 - \mathbf{B}\cdot\mathbf{B}\right) = \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_1^2\lambda_3^2 \tag{5.50}$$

$$I_3 = \det(\mathbf{B}) = (\det(\mathbf{F}))^2 = J^2 = \lambda_1^2\lambda_2^2\lambda_3^2 \tag{5.51}$$

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

$$\sigma_{ij} = \frac{1}{J}\sum_k F_{ik}\frac{\partial W}{\partial F_{jk}} \tag{5.52}$$

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

$$B_{ij} = \sum_k F_{ik}F_{jk}, \quad \frac{\partial B_{kl}}{\partial F_{ij}} = \delta_{ki}F_{lj} + \delta_{li}F_{kj} \tag{5.53}$$

$$I_1 = \sum_k\sum_l F_{kl}^2 = ||\mathbf{F}||_F^2, \quad I_2 = \frac{1}{2}\left(I_1^2 - \sum_k\sum_l B_{kl}^2\right) \tag{5.54}$$

$$\frac{\partial I_1}{\partial F_{ij}} = 2F_{ij}, \quad \frac{\partial I_2}{\partial F_{ij}} = 2\left(I_1F_{ij} - \sum_k B_{ik}F_{kj}\right), \quad \frac{\partial J}{\partial F_{ij}} = J(F_{ji})^{-1}, \quad \frac{\partial I_3}{\partial F_{ij}} = 2I_3(F_{ji})^{-1} \tag{5.55}$$

$$\frac{\partial \overline{I_1}}{\partial F_{ij}} = \frac{2}{J^{2/3}}\left(F_{ij} - \frac{I_1(F_{ij})^{-1}}{3}\right) = \frac{2F_{ij}}{J^{2/3}} - \frac{2\overline{I_1}(F_{ij})^{-1}}{3} \tag{5.56}$$

$$\frac{\partial \overline{I_2}}{\partial F_{ij}} = \frac{2\overline{I_1}F_{ij}}{J^{2/3}} - \frac{2\sum_k B_{ik}F_{kj}}{J^{4/3}} - \frac{4\overline{I_2}(F_{ij})^{-1}}{3} \tag{5.57}$$

the Cauchy stress can be found from

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\mathbf{B} + \frac{\partial W}{\partial I_2}\left(I_1\mathbf{B} - \mathbf{B}^2\right)\right] \tag{5.58}$$

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + 2\left[\frac{1}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{1}{J^{7/3}}\frac{\partial W}{\partial \overline{I_2}}\left(I_1\mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right)\right] \tag{5.59}$$

$$\boldsymbol{\sigma} = \sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k}\boldsymbol{b}_k \otimes \boldsymbol{b}_k \tag{5.60}$$

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

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial J}\mathbf{I} + 2\left[\frac{1}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\mathrm{dev}(\mathbf{B}) + \frac{1}{J^{7/3}}\frac{\partial W}{\partial \overline{I_2}}\mathrm{dev}(I_1\mathbf{B}-\mathbf{B}^2)\right] \tag{5.61}$$

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

$$\begin{aligned} P &= -\frac{\partial W}{\partial J} - \frac{2}{3J}\left[\frac{\partial W}{\partial I_1}I_1 + \frac{\partial W}{\partial I_2}2I_2\right] && (5.62)\\ P &= -\frac{\partial W}{\partial J} && (5.63)\\ P &= -\frac{1}{3}\sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k} && (5.64)\end{aligned}$$

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

$$\begin{aligned} \mathbf{s} &= \frac{2}{J}\left[\frac{\partial W}{\partial I_1}\mathrm{dev}(\mathbf{B}) + \frac{\partial W}{\partial I_2}\mathrm{dev}\left(I_1\mathbf{B}-\mathbf{B}^2\right)\right] && (5.65)\\ \mathbf{s} &= \frac{2}{J}\left[\frac{1}{J^{2/3}}\frac{\partial W}{\partial \overline{I_1}}\mathrm{dev}(\mathbf{B}) + \frac{1}{J^{4/3}}\frac{\partial W}{\partial \overline{I_2}}\mathrm{dev}(I_1\mathbf{B}-\mathbf{B}^2)\right] && (5.66)\\ \mathbf{s} &= \sum_k \frac{\lambda_k}{J}\frac{\partial W}{\partial \lambda_k}\mathrm{dev}(\boldsymbol{b}_k\otimes\boldsymbol{b}_k) && (5.67)\end{aligned}$$

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

$$\tau_{kl} = \sum_j F_{kj}\frac{\partial W}{\partial F_{lj}} \tag{5.68}$$

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

$$\frac{\partial W}{\partial F_{lj}} = \frac{\partial W}{\partial J}J(F_{jl})^{-1} + 2\frac{\partial W}{\partial I_1}F_{lj} + 2\frac{\partial W}{\partial I_2}\left(I_1F_{lj} - \sum_m B_{lm}F_{mj}\right) \tag{5.69}$$

$$\tau_{kl} = \sum_j F_{kj}\frac{\partial W}{\partial F_{lj}} = J\frac{\partial W}{\partial J}\delta_{kl} + 2\left[\frac{\partial W}{\partial I_1}B_{kl} + \frac{\partial W}{\partial I_2}\left(I_1B_{kl} - \sum_m B_{km}B_{ml}\right)\right] \tag{5.70}$$

Differentiation again gives:

$$\begin{aligned} \frac{\partial \tau_{kl}}{\partial F_{ij}} &= J(F_{ij})^{-1}\frac{\partial W}{\partial J}\delta_{kl} + J\frac{\partial^2 W}{\partial F_{ij}\partial J}\delta_{kl} + 2\frac{\partial^2 W}{\partial F_{ij}\partial I_1}B_{kl} + 2\frac{\partial W}{\partial I_1}(\delta_{ki}F_{lj} + \delta_{li}F_{kj})\\ &\quad + 2\frac{\partial^2 W}{\partial F_{ij}\partial I_2}I_1B_{kl} + 2\frac{\partial W}{\partial I_2}\frac{\partial I_1}{\partial F_{ij}}B_{kl} + 2\frac{\partial W}{\partial I_2}I_1(\delta_{ki}F_{lj} + \delta_{li}F_{kj})\\ &\quad - \sum_n 2\frac{\partial^2 W}{\partial F_{ij}\partial I_2}B_{ln}F_{nm} - 2\frac{\partial W}{\partial I_2}\delta_{li}C_{mj} - 2\frac{\partial W}{\partial I_2}F_{lj}F_{im} - 2\frac{\partial W}{\partial I_2}B_{li}\delta_{mj} \end{aligned} \tag{5.71}$$

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

$$\frac{\partial^2 W}{\partial J \partial F_{ij}} = \frac{\partial}{\partial J}\left[\frac{\partial W}{\partial J} J (F_{ji})^{-1} + 2\frac{\partial W}{\partial I_1} F_{ij}\right] \tag{5.72}$$

$$= \frac{\partial^2 W}{\partial J^2} J (F_{ji})^{-1} + \frac{\partial W}{\partial J}(F_{ji})^{-1} + \frac{\partial W}{\partial J} J \frac{\partial (F_{ji})^{-1}}{\partial J} + 2\frac{\partial^2 W}{\partial J \partial I_1} F_{ij} + 2\frac{\partial W}{\partial I_1}\frac{\partial F_{ij}}{\partial J} \tag{5.73}$$

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

$$\frac{\partial P}{\partial J} = -\frac{\partial^2 W}{\partial J^2} \tag{5.74}$$

$$\frac{\partial s_{kl}}{\partial B_{ij}} = \frac{\partial}{\partial B_{ij}}\left[\frac{2}{J^{5/3}}\frac{\partial W}{\partial \overline{I_1}}\left(B_{kl} - \frac{1}{3} I_1 \delta_{kl}\right)\right] \tag{5.75}$$

$$= \frac{2}{J^{5/3}}\left[\left(\frac{\partial^2 W}{\partial B_{ij} \partial \overline{I_1}} - \frac{5}{3J}\frac{\partial J}{\partial B_{ij}}\frac{\partial W}{\partial \overline{I_1}}\right)\left(B_{kl} - \frac{1}{3} I_1 \delta_{kl}\right) + \frac{\partial W}{\partial \overline{I_1}}\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\frac{\partial I_1}{\partial B_{ij}}\delta_{kl}\right)\right] \tag{5.76}$$

5.7 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

$$W(\overline{I_1}, \overline{I_2}, J) = \frac{G_1}{2}\left(\overline{I_1} - 3\right) + \frac{G_2}{2}\left(\overline{I_2} - 3\right) + \frac{K}{2}(J-1)^2 \tag{5.77}$$

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 $K \to \infty$; 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

$$\boldsymbol{\sigma} = \frac{G_1}{J^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) + \frac{G_2}{J^{7/3}}\left(I_1 \mathbf{B} - \mathbf{B}^2 - \frac{2I_2}{3}\mathbf{I}\right) + K(J-1)\mathbf{I} \tag{5.78}$$

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

evaluate to:

$$P = -K(J-1) \tag{5.79}$$

$$s_{xx} = G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}} + G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2-B_{xz}^2+2B_{yz}^2}{3J^{7/3}} \tag{5.80}$$

$$s_{yy} = G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}} + G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2+2B_{xz}^2-B_{yz}^2}{3J^{7/3}} \tag{5.81}$$

$$s_{zz} = G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}} + G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2-B_{xz}^2-B_{yz}^2}{3J^{7/3}} \tag{5.82}$$

$$s_{xy} = G_1\frac{B_{xy}}{J^{5/3}} + G_2\frac{B_{zz}B_{xy}-B_{xz}B_{yz}}{J^{7/3}} \tag{5.83}$$

$$s_{xz} = G_1\frac{B_{xz}}{J^{5/3}} + G_2\frac{B_{yy}B_{xz}-B_{xy}B_{yz}}{J^{7/3}} \tag{5.84}$$

$$s_{yz} = G_1\frac{B_{yz}}{J^{5/3}} + G_2\frac{B_{xx}B_{yz}-B_{xy}B_{xz}}{J^{7/3}} \tag{5.85}$$

5.7.1 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

$$s_{xx} = G_1\frac{2B_{xx}-B_{yy}-B_{zz}}{3J^{5/3}} + G_2\frac{B_{xx}(B_{yy}+B_{zz})-2B_{yy}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{5.86}$$

$$s_{yy} = G_1\frac{2B_{yy}-B_{xx}-B_{zz}}{3J^{5/3}} + G_2\frac{B_{yy}(B_{xx}+B_{zz})-2B_{xx}B_{zz}-B_{xy}^2}{3J^{7/3}} \tag{5.87}$$

$$s_{zz} = G_1\frac{2B_{zz}-B_{xx}-B_{yy}}{3J^{5/3}} + G_2\frac{B_{zz}(B_{xx}+B_{yy})-2B_{xx}B_{yy}+2B_{xy}^2}{3J^{7/3}} \tag{5.88}$$

$$s_{xy} = G_1\frac{B_{xy}}{J^{5/3}} + G_2\frac{B_{zz}B_{xy}}{J^{7/3}} \tag{5.89}$$

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

$$f = -3J_{res}J_{eff}^2P(J_{eff}) + G_1J^{1/3}(2B_{zz}-\alpha_1) + \frac{G_2}{J^{1/3}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{5.90}$$

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

$$f = -3J_{res}J_{eff}^2P(J_{eff}) + G_1B_{zz}^{1/6}\alpha_2^{1/6}(2B_{zz}-\alpha_1) + \frac{G_2}{B_{zz}^{1/6}\alpha_2^{1/6}}\left(B_{zz}\alpha_1 - 2\alpha_2\right) \tag{5.91}$$

For more efficient Newton's method, we need

$$\frac{df}{dB_{zz}} = -3J_{res}\frac{d\left(J_{eff}^2P(J_{eff})\right)}{dJ_{eff}}\frac{dJ_{eff}}{dB_{zz}} + \frac{G_1J^{1/3}(14B_{zz}-\alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1B_{zz}+2\alpha_2)}{6B_{zz}J^{1/3}} \tag{5.92}$$

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:

$$\frac{df}{dB_{zz}} = -\frac{3J}{2B_{zz}}\frac{d\left(J_{eff}^2 P(J_{eff})\right)}{dJ_{eff}} + \frac{G_1 J^{1/3}(14B_{zz}-\alpha_1)}{6B_{zz}} + \frac{G_2(5\alpha_1 B_{zz}+2\alpha_2)}{6B_{zz}J^{1/3}} \tag{5.93}$$

For the pressure term above

$$-\frac{3J}{2B_{zz}}\frac{d\left(J_{eff}^2 P(J_{eff})\right)}{dJ_{eff}} = \frac{3J}{2B_{zz}}KJ_{eff}(3J_{eff}-2) \tag{5.94}$$

Other pressure models are given below.

5.7.2 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

$$\mathbf{F} = \mathbf{F}^*\mathbf{F}^{res} = \mathbf{F}^*\lambda_{res}\mathbf{I} \tag{5.95}$$

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

$$\lambda_{res} = \exp(\alpha\Delta T + \beta\Delta c) \approx 1 + \alpha\Delta T + \beta\Delta c \tag{5.96}$$

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:

$$\boldsymbol{\sigma} = \frac{J_{res}G_1}{J^{5/3}}\left(\mathbf{B}-\frac{I_1}{3}\mathbf{I}\right) + \frac{J_{res}G_2}{J^{7/3}}\left(I_1\mathbf{B}-\mathbf{B}^2-\frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{5.97}$$

$$\boldsymbol{\sigma} = \frac{G_1}{J_{eff}J^{2/3}}\left(\mathbf{B}-\frac{I_1}{3}\mathbf{I}\right) + \frac{G_2}{J_{eff}J^{4/3}}\left(I_1\mathbf{B}-\mathbf{B}^2-\frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{5.98}$$

$$\boldsymbol{\sigma} = \frac{G_1}{J_{res}^{2/3}J_{eff}^{5/3}}\left(\mathbf{B}-\frac{I_1}{3}\mathbf{I}\right) + \frac{G_2}{J_{res}^{4/3}J_{eff}^{7/3}}\left(I_1\mathbf{B}-\mathbf{B}^2-\frac{2I_2}{3}\mathbf{I}\right) - P(J_{eff})\mathbf{I} \tag{5.99}$$

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

$$\mathbf{B} \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad I_1 \approx 3 + 2\mathrm{Tr}(\boldsymbol{\varepsilon}), \quad \mathbf{B}^2 \approx \mathbf{I} + 2\boldsymbol{\varepsilon}, \quad J \approx 1 + \mathrm{Tr}(\boldsymbol{\varepsilon}), \quad \text{and} \quad \frac{1}{J_{res}} \approx 1 - 3\alpha\Delta T \tag{5.100}$$

leading to

$$\boldsymbol{\sigma} = G_1\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + G_2\left(2\boldsymbol{\varepsilon} + \left(I_1\left(1-\frac{I_1}{3}\right) - 1 + \frac{\mathbf{B}\cdot\mathbf{B}}{3}\right)\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} \tag{5.101}$$

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

$$\boldsymbol{\sigma} = (G_1+G_2)\left(2\boldsymbol{\varepsilon} - \frac{2}{3}\mathrm{Tr}(\boldsymbol{\varepsilon})\mathbf{I}\right) + K(\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3\alpha\Delta T)\mathbf{I} \tag{5.102}$$

$$= \left[\left(K - \frac{2}{3}(G_1+G_2)\right)\mathrm{Tr}(\boldsymbol{\varepsilon}) - 3K\alpha\Delta T\right]\mathbf{I} + 2(G_1+G_2)\boldsymbol{\varepsilon} \tag{5.103}$$

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

$$J_{eff,k+1} = \frac{V_{k+1}}{V_{sf,k+1}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}\frac{V_k}{V_{sf,k}} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}}J_{eff,k} = dJ_{eff}J_{eff,k} \tag{5.104}$$

which implies that

$$dJ_{eff} = \frac{V_{k+1}}{V_k}\frac{V_{sf,k}}{V_{sf,k+1}} = dJ/d\lambda_{res}^3 \tag{5.105}$$

where

$$d\lambda_{res} = \exp(\alpha dT + \beta dc) \approx 1 + \alpha dT + \beta dc \tag{5.106}$$

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

5.7.3 Alternate Bulk Modulus Term

Besides the dilation energy term used above of

$$W = \frac{K}{2}(J-1)^2 \qquad \text{with} \qquad P = -K(J-1), \tag{5.107}$$

two alternative compressibility terms are:

$$W = \frac{K}{2}(\ln J)^2 \qquad \text{and} \qquad W = \frac{K}{2}\left(\frac{1}{2}(J^2-1) - \ln J\right) \tag{5.108}$$

which gives normal Cauchy pressure terms of

$$P = -K\frac{\ln J}{J} \qquad \text{and} \qquad P = -\frac{K}{2}\left(J - \frac{1}{J}\right) \tag{5.109}$$

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:

$$\frac{d(J_{eff}^2 P(J_{eff}))}{dJ_{eff}} = -K\frac{d\left(J_{eff}\ln J_{eff}\right)}{dJ_{eff}} = -K(1+\ln J_{eff}) \tag{5.110}$$

$$\frac{d(J_{eff}^2 P(J_{eff}))}{dJ_{eff}} = -\frac{K}{2}\frac{d\left(J_{eff}^3 - J_{eff}\right)}{dJ_{eff}} = -\frac{K}{2}(3J_{eff}^2 - 1) \tag{5.111}$$

5.7.4 Tangent Bulk Modulus

The incremental bulk modulus is

$$\frac{1}{K(P)} = -\frac{d\ln V}{dP} = -\frac{d\ln J_{eff}}{dP} \qquad \text{or} \qquad K = -J_{eff}\frac{dP}{dJ_{eff}} \tag{5.112}$$

The various bulk moduli are:

$$P = -K_0(J_{eff} - 1) \qquad \text{gives} \qquad K = K_0 J_{eff} \tag{5.113}$$

$$P = -K_0 \frac{\ln J_{eff}}{J_{eff}} \qquad \text{gives} \qquad K = K_0 \frac{1 - \ln J_{eff}}{J_{eff}^2} \tag{5.114}$$

$$P = -\frac{K_0}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \qquad \text{gives} \qquad K = \frac{K_0}{2}\left(J_{eff} + \frac{1}{J_{eff}}\right) \tag{5.115}$$

If implementing increment pressure law, the result is:

$$P_n = P_{n-1} - K(J_{eff}) d \ln J_{eff} = P_{n-1} - K(J_{eff}) \ln dJ_{eff} \tag{5.116}$$

5.7.5 Tangent Shear Modulus

Assuming $G_2 = 0$, the deviatoric stress is

$$\mathsf{s} = \frac{J_{res} G_1}{J^{5/3}}\left(\mathbf{B} - \frac{I_1}{3}\mathbf{I}\right) \tag{5.117}$$

and the tangent shear modulus including residual stresses is

$$\frac{\partial s_{kl}}{\partial B_{ij}} = \frac{J_{res} G_1}{J^{5/3}}\left[\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\frac{\partial I_1}{\partial B_{ij}}\delta_{kl}\right) - \frac{5}{3J}\frac{\partial J}{\partial B_{ij}}\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right] \tag{5.118}$$

$$= \frac{J_{res} G_1}{J^{5/3}}\left[\left(\delta_{ki}\delta_{lj} - \frac{1}{3}\delta_{ij}\delta_{kl}\right) - \frac{5}{6}(B_{ij})^{-1}\left(B_{kl} - \frac{1}{3}I_1\delta_{kl}\right)\right] \tag{5.119}$$

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

$$\frac{\partial J^2}{\partial B_{ij}} = J^2 (B_{ij})^{-1} = 2J\frac{\partial J}{B_{ij}} \qquad \text{or} \qquad \frac{\partial J}{\partial B_{ij}} = \frac{J}{2}(B_{ij})^{-1} \tag{5.120}$$

The normal and shear deviatoric stress increments are:

$$\frac{\partial s_{kk}}{\partial B_{ij}} = \frac{J_{res} G_1}{3J^{5/3}}\left[\left(3\delta_{ki}\delta_{kj} - \delta_{ij}\right) - \frac{5}{6}(B_{ij})^{-1}\left(3B_{kk} - I_1\right)\right] \tag{5.121}$$

$$\frac{\partial s_{kl}\ (k \neq l)}{\partial B_{ij}} = \frac{J_{res} G_1}{J^{5/3}}\left[\delta_{ki}\delta_{lj} - \frac{5}{6}(B_{ij})^{-1}\left(B_{kl}\right)\right] \tag{5.122}$$

Explicitly, for example:

$$\frac{3J^{5/3}}{J_{res} G_1}\frac{\partial s_{xx}}{\partial B_{ij}} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} - \frac{5}{6}\mathbf{B}^{-1}(2B_{xx} - B_{yy} - B_{zz}) \tag{5.123}$$

$$\frac{J^{5/3}}{J_{res} G_1}\frac{\partial s_{xy}}{\partial B_{ij}} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{5}{6}\mathbf{B}^{-1}B_{xy} \tag{5.124}$$

5.7.6 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:

$$\sigma_{11} = -P(J_{eff}) + 2J_{res}G_1\frac{\lambda^2 - \frac{J}{\lambda}}{3J^{5/3}} + 2J_{res}G_2\frac{\lambda - \frac{J}{\lambda^2}}{3J^{4/3}} \tag{5.125}$$

$$\sigma_{22} = \sigma_{33} = -P(J_{eff}) + J_{res}G_1\frac{\frac{J}{\lambda} - \lambda^2}{3J^{5/3}} + J_{res}G_2\frac{\frac{J}{\lambda^2} - \lambda}{3J^{4/3}} \tag{5.126}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = J_{res}G_1\frac{\lambda^2 - \frac{J}{\lambda}}{3J^{5/3}} + J_{res}G_2\frac{\lambda - \frac{J}{\lambda^2}}{3J^{4/3}} \tag{5.127}$$

For Newton's method, solve $f = 0$ for J using

$$f = 3J_{res}J_{eff}^2P(J_{eff}) + (J^{1/3}G_1 + J^{2/3}G_2)\left(\lambda^2 - \frac{J}{\lambda}\right) \tag{5.128}$$

$$\frac{df}{dJ} = 3\frac{d(J_{eff}^2P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G_1}{3}\left(\frac{\lambda^2}{J} - \frac{4}{\lambda}\right) + \frac{J^{2/3}G_2}{3}\left(\frac{2\lambda}{J} - \frac{5}{\lambda^2}\right) \tag{5.129}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{J^{2/3}G_2}{\lambda}\right)\left(\lambda^2 - \frac{J}{\lambda}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{5.130}$$

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:

$$\tau_{11} = \left(J_{res}^{1/3}G_1 + \frac{J_{res}^{2/3}G_2}{\lambda}\right)\left(\lambda^2 - \frac{J_{res}}{\lambda}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{5.131}$$

and $\lambda_2 = \lambda_3 = \sqrt{J_{res}/\lambda}$. Note that during free thermal expansion, $J_{res} = \lambda^3$ and all stresses are zero.

5.7.7 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:

$$\sigma_{11} = -P(J_{eff}) + 2J_{res}G\frac{\lambda_n^2 - \frac{J}{\lambda_n}}{3J^{5/3}} \tag{5.132}$$

$$\sigma_{22} = \sigma_{33} = -P(J_{eff}) + J_{res}G\frac{\frac{J}{\lambda_n} - \lambda_n^2}{3J^{5/3}} \tag{5.133}$$

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:

$$\lambda_n^3 + \frac{3J^{2/3}J_{eff}P(J_{eff})}{G}\lambda_n - J = 0 \tag{5.134}$$

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.

5.7.8 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:

$$\sigma_{11} = -P(J_{eff}) + J_{res}G_1\frac{2\lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2} - \lambda_3^2}{3J^{5/3}} + J_{res}G_2\frac{\lambda^2\lambda_3^2 + \frac{J^2}{\lambda_3^2} - 2\frac{J^2}{\lambda^2}}{3J^{7/3}} \tag{5.135}$$

$$\sigma_{22} = -P(J_{eff}) + J_{res}G_1\frac{2\frac{J^2}{\lambda^2\lambda_3^2} - \lambda^2 - \lambda_3^2}{3J^{5/3}} + J_{res}G_2\frac{\frac{J^2}{\lambda_3^2} + \frac{J^2}{\lambda^2} - 2\lambda^2\lambda_3^2}{3J^{7/3}} \tag{5.136}$$

$$\sigma_{33} = -P(J_{eff}) + J_{res}G\frac{2\lambda_3^2 - \lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2}}{3J^{5/3}} + J_{res}G_2\frac{\lambda^2\lambda_3^2 + \frac{J^2}{\lambda^2} - 2\frac{J^2}{\lambda_3^2}}{3J^{7/3}} \tag{5.137}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = J_{res}G_1\frac{\lambda_3^2 + \lambda^2 - 2\frac{J^2}{\lambda^2\lambda_3^2}}{3J^{5/3}} + J_{res}G_2\frac{2\lambda^2\lambda_3^2 - \frac{J^2}{\lambda_3^2} - \frac{J^2}{\lambda^2}}{3J^{7/3}} \tag{5.138}$$

For Newton's method, solve $f = 0$ for J using

$$\begin{aligned} f &= 3J_{res}J_{eff}^2P(J_{eff}) + J^{1/3}G_1\left(\lambda_3^2 + \lambda^2 - 2\frac{J^2}{\lambda^2\lambda_3^2}\right) + \frac{G_2}{J^{1/3}}\left(2\lambda^2\lambda_3^2 - J^2\left(\frac{1}{\lambda_3^2} + \frac{1}{\lambda^2}\right)\right) \\ \frac{df}{dJ} &= 3\frac{d(J_{eff}^2P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G_1}{3}\left(\frac{\lambda_3^2 + \lambda^2}{J} - \frac{14J}{\lambda^2\lambda_3^2}\right) - \frac{G_2}{3J^{1/3}}\left(\frac{2\lambda^2\lambda_3^2}{J} + 5J\left(\frac{1}{\lambda_3^2} + \frac{1}{\lambda^2}\right)\right) \end{aligned} \tag{5.139}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{G_2\lambda_3^2}{J^{1/3}}\right)\left(\lambda^2 - \frac{J^2}{\lambda^2\lambda_3^2}\right) \tag{5.140}$$

$$\tau_{33} = \frac{1}{J_{eff}}\left(J^{1/3}G_1 + \frac{G_2\lambda^2}{J^{1/3}}\right)\left(\lambda_3^2 - \frac{J^2}{\lambda^2\lambda_3^2}\right) \tag{5.141}$$

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:

$$\tau_{11} = \left(J_{res}^{1/3}G_1 + \frac{G_2\lambda_3^2}{J_{res}^{1/3}}\right)\left(\lambda^2 - \frac{J_{res}^2}{\lambda^2\lambda_3^2}\right) \tag{5.142}$$

$$\tau_{33} = \left(J_{res}^{1/3}G_1 + \frac{G_2\lambda^2}{J_{res}^{1/3}}\right)\left(\lambda_3^2 - \frac{J_{res}^2}{\lambda^2\lambda_3^2}\right) \tag{5.143}$$

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.

5.7.9 3D Mooney-Rivlin Membrane

Using the deformation state for 3D membranes, a Mooney-Rivlin material has the normal Cauchy stresses:

$$\begin{aligned}
\sigma_{11} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(2\lambda_1^2 + \lambda_2^2(2\cos^2\omega - \sin^2\omega) - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\
&\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega + \left(\lambda_1^2 + \lambda_2^2\left(\cos^2\omega - 2\sin^2\omega\right)\right)\frac{J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (5.144)
\end{aligned}$$

$$\begin{aligned}
\sigma_{22} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(\lambda_2^2(2\sin^2\omega - \cos^2\omega) - \lambda_1^2 - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \qquad (5.145) \\
&\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega - \left(2\lambda_1^2 + \lambda_2^2\left(2\cos^2\omega - \sin^2\omega\right)\right)\frac{J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (5.146)
\end{aligned}$$

$$\begin{aligned}
\sigma_{33} &= -P(J_{eff}) + \frac{J_{res}G_1}{3J^{5/3}}\left(\frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega} - \lambda_1^2 - \lambda_2^2\right) \qquad (5.147) \\
&\quad + \frac{J_{res}G_2}{3J^{7/3}}\left(\frac{\left(\lambda_1^2 + \lambda_2^2\right)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega} - 2\lambda_1^2\lambda_2^2\sin^2\omega\right) \qquad (5.148)
\end{aligned}$$

$$\sigma_{12} = \frac{J_{res}G_1}{J^{5/3}}\lambda_2^2\sin\omega\cos\omega + \frac{J_{res}G_2}{J^{1/3}}\frac{\cos\omega}{\lambda_1^2\sin\omega} \qquad (5.149)$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{33} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{J_{res}G_1}{3J^{5/3}}\left(\lambda_1^2 + \lambda_2^2 - \frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) + \frac{J_{res}G_2}{3J^{7/3}}\left(2\lambda_1^2\lambda_2^2\sin^2\omega - \frac{\left(\lambda_1^2 + \lambda_2^2\right)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (5.150)$$

For Newton's method, solve $f = 0$ for J using

$$\begin{aligned}
f &= 3J_{res}J_{eff}^2P(J_{eff}) + J^{1/3}G_1\left(\lambda_1^2 + \lambda_2^2 - \frac{2J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\
&\quad + \frac{G_2}{J^{1/3}}\left(2\lambda_1^2\lambda_2^2\sin^2\omega - \frac{\left(\lambda_1^2 + \lambda_2^2\right)J^2}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (5.151) \\
\frac{df}{dJ} &= 3\frac{d(J_{eff}^2P(J_{eff}))}{dJ_{eff}} + \frac{J^{1/3}G}{3}\left(\frac{\lambda_1^2 + \lambda_2^2}{J} - \frac{14J}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \\
&\quad - \frac{G_2}{3J^{1/3}}\left(\frac{2\lambda_1^2\lambda_2^2\sin^2\omega}{J} + \frac{5\left(\lambda_1^2 + \lambda_2^2\right)J}{\lambda_2^2\lambda_1^2\sin^2\omega}\right) \qquad (5.152)
\end{aligned}$$

Given this J, the final results for Kirchhoff stresses are:

$$\tau_{11} = \frac{J^{1/3}G_1}{J_{eff}}\left(\lambda_1^2+\lambda_2^2\cos^2\omega-\frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)+\frac{G_2}{J_{eff}J^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{J^2}{\lambda_1^2}\right) \quad (5.153)$$

$$\tau_{22} = \frac{J^{1/3}G_1}{J_{eff}}\left(\lambda_2^2\sin^2\omega-\frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) + \frac{G_2}{J_{eff}J^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{\left(\lambda_1^2+\lambda_2^2\cos^2\omega\right)J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \quad (5.154)$$

$$\tau_{12} = \frac{J^{1/3}G_1}{J_{eff}}\lambda_2^2\sin\omega\cos\omega+\frac{G_2}{J_{eff}J^{1/3}}\frac{J^2\cos\omega}{\lambda_1^2\sin\omega} \quad (5.155)$$

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:

$$\tau_{11} = J_{res}^{1/3}G_1\left(\lambda_1^2+\lambda_2^2\cos^2\omega-\frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)+\frac{G_2}{J_{res}^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{J_{res}^2}{\lambda_1^2}\right) \quad (5.156)$$

$$\tau_{22} = J_{res}^{1/3}G_1\left(\lambda_2^2\sin^2\omega-\frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) + \frac{G_2}{J_{res}^{1/3}}\left(\lambda_1^2\lambda_2^2\sin^2\omega-\frac{\left(\lambda_1^2+\lambda_2^2\cos^2\omega\right)J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \quad (5.157)$$

$$\tau_{12} = J_{res}^{1/3}G_1\lambda_2^2\sin\omega\cos\omega+\frac{G_2}{J_{res}^{1/3}}\frac{J_{res}^2\cos\omega}{\lambda_1^2\sin\omega} \quad (5.158)$$

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.

5.8 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:

$$W(I_1,I_2,J) = \frac{G}{2}(I_1-3-2\ln J)+\frac{\lambda}{2}(\ln J)^2 \quad (5.159)$$

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

$$\boldsymbol{\sigma} = \frac{\lambda\ln J_{eff}}{J_{eff}}\mathbf{I}+\frac{G}{J_{eff}}\left(\frac{\mathbf{B}}{J_{res}^{2/3}}-\mathbf{I}\right) \quad (5.160)$$

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

$$\boldsymbol{\sigma} = \left(\lambda\mathrm{Tr}(\boldsymbol{\varepsilon})-(3\lambda+2G)\alpha\Delta T\right)\mathbf{I}+2G\boldsymbol{\varepsilon} \qquad \text{low strain} \quad (5.161)$$

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:

$$P = P(J_{eff}) - \frac{G}{J_{eff}}\left(\frac{B_{xx}+B_{yy}+B_{zz}}{3J_{res}^{2/3}} - 1\right) \tag{5.162}$$

$$s_{xx} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{xx} - B_{yy} - B_{zz}\right) \tag{5.163}$$

$$s_{yy} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{yy} - B_{zz} - B_{zz}\right) \tag{5.164}$$

$$s_{zz} = \frac{J_{res}^{1/3}G}{3J}\left(2B_{zz} - B_{xx} - B_{xx}\right) \tag{5.165}$$

$$s_{ij} = \frac{J_{res}^{1/3}G}{J}B_{ij} \qquad \text{for } i \neq j \tag{5.166}$$

where $P(J_{eff})$ uses any pressure above except that K is replaced by λ. When doing plane stress calculations, one task is to solve for $\sigma_{zz} = 0$, which is equivalent to solving numerically for $f = 0$ give

$$f = -J_{res}^{2/3}J_{eff}P(J_{eff}) + G\left(B_{zz} - J_{res}^{2/3}\right) \tag{5.167}$$

$$\frac{df}{dB_{zz}} = G - \frac{J_{res}^{2/3}J_{eff}}{2B_{zz}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} \tag{5.168}$$

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

$$B_{zz} = J_{res}^2\frac{\lambda + 2G}{\lambda\alpha_2 + 2GJ_{res}^{4/3}} \qquad \text{when} \quad J_{eff}P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff}^2 - 1\right) \tag{5.169}$$

and

$$\sqrt{B_{zz}} = J_{res}\frac{\lambda\sqrt{\alpha_2} + \sqrt{\lambda^2\alpha_2 + 4G\left(\lambda\alpha_2 + GJ_{res}^{4/3}\right)}}{2\left(\lambda\alpha_2 + GJ_{res}^{4/3}\right)} \tag{5.170}$$

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

$$f = G\left(B_{zz} - J_{res}^{2/3}\right) + \lambda J_{res}^{2/3}\ln J_{eff} \tag{5.171}$$

$$\frac{df}{dB_{zz}} = G + \frac{\lambda J_{res}^{2/3}}{2B_{zz}} \tag{5.172}$$

5.8.1 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}):

$$P(J_{eff}) = -\lambda(J-1) \qquad \text{gives} \qquad K = \lambda J + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{5.173}$$

$$P(J_{eff}) = -\lambda\frac{\ln J}{J} \qquad \text{gives} \qquad K = \lambda\frac{1-\ln J}{J^2} + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{5.174}$$

$$P(J_{eff}) = -\frac{\lambda}{2}\left(J - \frac{1}{J}\right) \qquad \text{gives} \qquad K = \frac{\lambda}{2}\left(J + \frac{1}{J}\right) + G\left(1 - \frac{I_1}{3} + \frac{1}{3}\frac{dI_1}{dJ}\right) \tag{5.175}$$

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

$$G\left(1 - J^{2/3} + \frac{2}{3J^{1/3}}\right) \tag{5.176}$$

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

5.8.2 Plane Stress Neo-Hookean Membrane

Using the deformation state for plane stress membrane, a neo-Hookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_1^2}{J_{res}^{2/3}} - 1\right) \tag{5.177}$$

$$\sigma_{22} = \sigma_{33} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{J}{\lambda_1 J_{res}^{2/3}} - 1\right) \tag{5.178}$$

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:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1 - \frac{J}{\lambda_1 J_{res}^{2/3}}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G} - \frac{J_{res}^{1/3}J_{eff}}{\lambda_1} + 1 = 0 \tag{5.179}$$

For two models, this can be solved analytically:

$$J_{eff} = -\frac{J_{res}^{1/3}G}{\lambda\lambda_1} + \sqrt{1 + \frac{2G}{\lambda} + \left(\frac{J_{res}^{1/3}G}{\lambda\lambda_1}\right)^2} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \tag{5.180}$$

$$J_{eff} = \frac{1}{2}\left(1 - \frac{J_{res}^{1/3}G}{\lambda\lambda_1} + \sqrt{\frac{4G}{\lambda} + \left(1 - \frac{J_{res}^{1/3}G}{\lambda\lambda_1}\right)^2}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff} - 1\right) \tag{5.181}$$

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:

$$f = \lambda_1 J_{res}^{2/3} J_{eff} P(J_{eff}) + G\left(\lambda_1 J_{res}^{2/3} - J\right) = -\lambda\lambda_1 J_{res}^{2/3} \ln J_{eff} + G\left(\lambda_1 J_{res}^{2/3} - J\right) \tag{5.182}$$

$$\frac{df}{dJ} = \frac{\lambda_1}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - G = -\frac{\lambda\lambda_1 J_{res}^{2/3}}{J} - G \tag{5.183}$$

Given this J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 - \frac{J}{\lambda_1}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{5.184}$$

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:

$$\tau_{11} = \frac{G}{J_{res}^{2/3}}\left(\lambda_1^2 - \frac{J_{res}}{\lambda_1}\right) \quad \text{and} \quad \tau_{33} = 0 \tag{5.185}$$

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.

5.8.3 Plane Strain and Axisymmetric Neohookean Membrane

Using the deformation state for plane strain or axiymmetric membranes, a Neohookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_1^2}{J_{res}^{2/3}} - 1\right) \tag{5.186}$$

$$\sigma_{22} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_3^2} - 1\right) \tag{5.187}$$

$$\sigma_{33} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_3^2}{J_{res}^{2/3}} - 1\right) \tag{5.188}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by numerically solving $\sigma_{22} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1 - \frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_3^2}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G} - \frac{J_{res}^{4/3}J_{eff}^2}{\lambda_1^2\lambda_3^2} + 1 = 0 \tag{5.189}$$

For two models, this can be solved analytically:

$$J_{eff} = \sqrt{\frac{\lambda + 2G}{\lambda + 2G\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_3^2}}} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \tag{5.190}$$

$$J_{eff} = \frac{1}{2}\left(\frac{1 + \sqrt{1 + \frac{4G}{\lambda}\left(1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^1\lambda_3^2}\right)}}{1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^1\lambda_3^2}}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff} - 1\right) \tag{5.191}$$

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:

$$f = \lambda_1^2\lambda_3^2 J_{res}^{2/3} J_{eff}P(J_{eff}) + G\left(\lambda_1^2\lambda_3^2 J_{res}^{2/3} - J^2\right) \tag{5.192}$$

$$= -\lambda\lambda_1^2\lambda_3^2 J_{res}^{2/3}\ln J_{eff} + G\left(\lambda_1^2\lambda_3^2 J_{res}^{2/3} - J^2\right) \tag{5.193}$$

$$\frac{df}{dJ} = \frac{\lambda_1^2\lambda_3^2}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - 2GJ = -\frac{\lambda\lambda_1^2\lambda_3^2 J_{res}^{2/3}}{J} - 2GJ \tag{5.194}$$

Given the solved J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 - \frac{J^2}{\lambda_1^2\lambda_3^2}\right) \quad \text{and} \quad \tau_{33} = J_{res}^{1/3}G\left(\lambda_3^2 - \frac{J^2}{\lambda_1^2\lambda_3^2}\right) \tag{5.195}$$

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:

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 - \frac{J_{res}^2}{\lambda_1^2\lambda_3^2}\right) \quad \text{and} \quad \tau_{33} = J_{res}^{1/3}G\left(\lambda_3^2 - \frac{J_{res}^2}{\lambda_1^2\lambda_3^2}\right) \tag{5.196}$$

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.

5.8.4 3D Neo-Hookean Membrane

Using the deformation state for 3D membranes, a Neohookean material has the normal Cauchy stresses:

$$\sigma_{11} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_1^2 + \lambda_2^2\cos^2\omega}{J_{res}^{2/3}} - 1\right) \tag{5.197}$$

$$\sigma_{22} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{\lambda_2^2\sin^2\omega}{J_{res}^{2/3}} - 1\right) \tag{5.198}$$

$$\sigma_{33} = -P(J_{eff}) + \frac{G}{J_{eff}}\left(\frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega} - 1\right) \tag{5.199}$$

$$\sigma_{12} = \frac{G}{J_{eff}}\frac{\lambda_2^2\sin\omega\cos\omega}{J_{res}^{2/3}} \tag{5.200}$$

where the $P(J_{eff})$ is the pressure model. The stress state is found by solving $\sigma_{33} = 0$ for J or solving:

$$-P(J_{eff}) = \frac{G}{J_{eff}}\left(1 - \frac{J^2}{J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega}\right) \quad \text{or} \quad \frac{J_{eff}P(J_{eff})}{G} - \frac{J_{res}^{4/3}J_{eff}^2}{\lambda_1^2\lambda_2^2\sin^2\omega} + 1 = 0 \tag{5.201}$$

For two models, this can be solved analytically:

$$J_{eff} = \sqrt{\frac{\lambda + 2G}{\lambda + 2G\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}}} \quad \text{for } P(J_{eff}) = -\frac{\lambda}{2}\left(J_{eff} - \frac{1}{J_{eff}}\right) \tag{5.202}$$

$$J_{eff} = \frac{1}{2}\left(\frac{1 + \sqrt{1 + \frac{4G}{\lambda}\left(1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}\right)}}{1 + \frac{G}{\lambda}\frac{J_{res}^{4/3}}{\lambda_1^2\lambda_2^2\sin^2\omega}}\right) \quad \text{for } P(J_{eff}) = -\lambda\left(J_{eff} - 1\right) \tag{5.203}$$

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:

$$f = J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega(J_{eff}P(J_{eff})) + G\left(J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega - J^2\right) \tag{5.204}$$

$$= -\lambda J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega(\ln J_{eff}) + G\left(J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega - J^2\right) \tag{5.205}$$

$$\frac{df}{dJ} = \frac{\lambda_1^2\lambda_2^2\sin^2\omega}{J_{res}^{1/3}}\frac{d(J_{eff}P(J_{eff}))}{dJ_{eff}} - 2GJ = -\frac{\lambda J_{res}^{2/3}\lambda_1^2\lambda_2^2\sin^2\omega}{J} - 2GJ \tag{5.206}$$

Given the solved J, the final Kirchhoff stress results are

$$\tau_{11} = J_{res}^{1/3}G\left(\lambda_1^2 + \lambda_2^2\cos^2\omega - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{5.207}$$

$$\tau_{22} = J_{res}^{1/3}G\left(\lambda_2^2\sin^2\omega - \frac{J^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{5.208}$$

$$\tau_{12} = J_{res}^{1/3}G\lambda_2^2\sin\omega\cos\omega \tag{5.209}$$

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:

$$\tau_{11} = J_{res}^{1/3} G\left(\lambda_1^2 + \lambda_2^2\cos^2\omega - \frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{5.210}$$

$$\tau_{22} = J_{res}^{1/3} G\left(\lambda_2^2\sin^2\omega - \frac{J_{res}^2}{\lambda_1^2\lambda_2^2\sin^2\omega}\right) \tag{5.211}$$

$$\tau_{12} = J_{res}^{1/3} G\lambda_2^2 \sin\omega\cos\omega \tag{5.212}$$

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.

5.9 Mie-Grüniesen Equation of State

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

$$P = \frac{\rho_0 C_0^2 \eta\left(1 - \frac{1}{2}\gamma_0\eta\right)}{(1 - S_1\eta - S_2\eta^2 - S_3\eta^3)^2} + \rho_0\gamma_0 U \tag{5.213}$$

where η is fraction compression and given by

$$\eta = 1 - \frac{\rho_0}{\rho} = 1 - \frac{V}{V_0} = 1 - J \tag{5.214}$$

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:

$$P = -\rho_0 C_0^2 (J_{eff} - 1) \tag{5.215}$$

The Kirchhoff pressure needed by MPM is

$$\frac{\tau}{\rho_0} = \frac{JP}{\rho_0} \tag{5.216}$$

This material model also causes a temperature change of

$$dT = -T\gamma_0 \frac{\rho_0}{\rho} \frac{V(t+\Delta t) - V(t)}{V} + \frac{dq}{C_v} \tag{5.217}$$

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

$$dT_{dq=0} = -JT\gamma_0 \frac{V(t+\Delta t) - V(t)}{V} \tag{5.218}$$

The volume change relative to current volume can be found from

$$\frac{V(t+\Delta t) - V(t)}{V(t+\Delta t)} = 1 - \frac{1}{|dF|} \tag{5.219}$$

The temperature rise here, which is

$$dT_{dq=0} = -JT\gamma_0 \frac{\Delta V}{V} \qquad vs. \qquad dT_{dq=0} = -JT\frac{K}{K_0}\gamma_0 \frac{\Delta V}{V} \tag{5.220}$$

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. (5.275) for comparable results in an ideal gas.

Noticing that

$$\frac{dT_{dq=0}}{T} = \gamma_0 d\eta \tag{5.221}$$

The temperature due to isoentropic heating alone can be integrated to

$$T = T_0 \exp(\gamma_0 \eta) \tag{5.222}$$

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

$$dT = T_0(\exp(\gamma_0 \eta) - 1)\big) + \frac{\Phi}{C_v} \tag{5.223}$$

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

$$\eta = 1/1.24 = 0.806 \tag{5.224}$$

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.

5.9.1 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:

$$3\alpha = \frac{\rho_0 \gamma_0 C_v}{K_0} \qquad \text{or} \qquad \gamma_0 = \frac{3K_0\alpha}{\rho_0 C_v} \tag{5.225}$$

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

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

$$P = -K_0 \frac{\Delta V}{V_0} + 3K_0 \alpha \Delta T \tag{5.226}$$

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

$$\frac{\Delta V}{V_0} = 3\alpha \Delta T \tag{5.227}$$

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

5.10 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

$$P = JP(J_{eff}) \tag{5.228}$$

$$s_{xx}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{xx}^{trial} - B_{yy}^{trial} - B_{zz}^{trial}\right) \tag{5.229}$$

$$s_{yy}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{yy}^{trial} - B_{xx}^{trial} - B_{zz}^{trial}\right) \tag{5.230}$$

$$s_{zz}^{trial} = \frac{J_{res}G_1}{3J^{2/3}}\left(2B_{zz}^{trial} - B_{xx}^{trial} - B_{yy}^{trial}\right) \tag{5.231}$$

$$s_{ij}^{trial} = \frac{J_{res}G_1}{J^{2/3}}B_{ij}^{trial} \qquad \text{for } i \neq j \tag{5.232}$$

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:

$$\mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{5.233}$$

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

$$\mathbf{s} = J_{res}G_1 \mathrm{dev}\,\overline{\mathbf{B}} \tag{5.234}$$

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

$$f_{trial} = \|\mathbf{s}\| - \sqrt{\frac{2}{3}}K(\alpha) \tag{5.235}$$

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:

$$\mathbf{B} = \mathbf{B}^{trial} - \frac{2}{3}\lambda\overline{I_1}\mathbf{n} \tag{5.236}$$

$$\mathbf{s} = \mathbf{s}^{trial} - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right)\mathbf{n} \tag{5.237}$$

$$\|\mathbf{s}\| = \|\mathbf{s}^{trial}\| - 2\lambda\left(\frac{J_{res}G\overline{I_1}}{3}\right) \tag{5.238}$$

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

$$\overline{I_1} = \frac{B_{xx} + B_{yy} + B_{zz}}{J^{2/3}} \tag{5.239}$$

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

$$\overline{\mu} = \frac{J_{res} G \overline{I_1}}{3} \tag{5.240}$$

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. (5.234) 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.

5.11 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

$$PV = nRT \tag{5.241}$$

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:

$$\rho_0 = \frac{P_0}{T_0}\frac{M}{R} \tag{5.242}$$

We can now eliminate n and R to derive

$$P = P_0 \frac{V_0}{V}\frac{T}{T_0} = P_0 \frac{T}{T_0}\frac{1}{J} \tag{5.243}$$

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:

$$\boldsymbol{\sigma} = -P_0 \frac{T}{T_0}\frac{1}{J}\mathbf{I} = \frac{dU(J)}{dJ}\mathbf{I} \qquad \text{or} \qquad U(J) = -P_i \ln J \tag{5.244}$$

where $P_i = P_0 T/T_0$ 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:

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\, dV = -\frac{P_0 T}{T_0}\int_{V_0}^{V}\frac{1}{V}\, dV = -P_i \ln\frac{V}{V_0} = -P_i \ln J \tag{5.245}$$

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

$$\boldsymbol{\tau}^{(s)} = -\frac{PJ}{\rho_0}\mathbf{I} = -\frac{P_0}{\rho_0}\frac{T}{T_0}\mathbf{I} \tag{5.246}$$

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

$$\tau_{n+1}^{(s)} = -\frac{P_0}{\rho_0}\frac{T_{n+1}}{T_0} = -\frac{P_0}{\rho_0}\frac{T_n}{T_0}\frac{T_{n+1}}{T_n} = \tau_n^{(s)}\frac{T_{n+1}}{T_n} \tag{5.247}$$

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

$$\frac{dU}{\rho_0 V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1} - V_n}{V_0} = -\frac{1}{2}\frac{P_n + P_{n+1}}{\rho_0}\frac{V_{n+1}}{V_0}\left(1 - \frac{V_n}{V_{n+1}}\right) \tag{5.248}$$

Let deformation gradient for step $n+1$ be

$$\mathbf{F}_{n+1} = \mathbf{f} \cdot \mathbf{F}_n \quad \text{where} \quad \mathbf{f} = \exp(\Delta t \nabla \boldsymbol{v}) \quad \text{and} \quad J_{n+1} = \det \mathbf{f} J_n \tag{5.249}$$

which leads to

$$\frac{dU}{\rho_0 V_0} = -\frac{J_{n+1}}{2}\frac{P_n + P_{n+1}}{\rho_0}\left(1 - \frac{1}{\det f}\right) = -\frac{1}{2}\left(\frac{P_n}{\rho_n}\det f + \frac{P_{n+1}}{\rho_{n+1}}\right)\left(1 - \frac{1}{\det f}\right) \tag{5.250}$$

But, P/ρ is $-\tau^{(s)}$ leading to

$$\frac{dU}{\rho_0 V_0} = \frac{1}{2}\left(\tau_n^{(s)}\det f + \tau_{n+1}^{(s)}\right)\left(1 - \frac{1}{\det f}\right) \tag{5.251}$$

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

$$\tau_i^{(s)} = -\frac{P_i}{\rho_0} = -\frac{P_0}{\rho_0}\frac{T}{T_0} \tag{5.252}$$

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

$$C_v = \frac{3}{2}\frac{P_0}{\rho_0 T_0} \tag{5.253}$$

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

$$K = -\frac{\frac{V}{V_0}}{\frac{d(V/V_0)}{dP}} = \gamma P = \frac{\gamma \rho R T}{M} \tag{5.254}$$

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

$$C = \sqrt{\frac{K}{\rho}} = \sqrt{\frac{5\rho_0 P_0 T}{3T_0}} \tag{5.255}$$

where T is particle temperature.

5.11.1 Verification Examples

A simple gas problem is to confine all sides by rigid particles and move one wall for compression or expansion. If the movable wall is in the x direction, the volume will be $V = V_0(1+\varepsilon_{xx})$. For isothermal compression and expansion:

$$P = \frac{P_i}{1+\varepsilon_{xx}} \tag{5.256}$$
$$U = 0 \tag{5.257}$$
$$w = -P_i V_0 \ln(1+\varepsilon_{xx}) \tag{5.258}$$
$$q = -w \tag{5.259}$$
$$S = nR\ln(1+\varepsilon_{xx}) = \frac{P_0 V_0}{T_0}\ln(1+\varepsilon_{xx}) \tag{5.260}$$

For adiabatic compression and expansion

$$P = \frac{P_i}{(1+\varepsilon_{xx})^{\gamma}} \tag{5.261}$$
$$T = \frac{T_i}{(1+\varepsilon_{xx})^{\gamma-1}} \tag{5.262}$$
$$U = C_v(T-T_i) = \frac{3P_0V_0}{2T_0}T_i\left(\frac{1}{(1+\varepsilon_{xx})^{\gamma-1}}-1\right) \tag{5.263}$$
$$w = U \tag{5.264}$$
$$q = 0 \tag{5.265}$$
$$S = -(\gamma-1)C_v\ln(1+\varepsilon_{xx}) + \frac{P_0V_0}{T_0}\ln(1+\varepsilon_{xx}) = 0 \tag{5.266}$$

where $\gamma = C_P/C_v = 5/3$ for monotonic gas or $\gamma = 7/5$ for diatomic. An undocumented custom task in `NairnMPM` can subject an ideal gas to a Carnot cycle and recover an efficiency close to the theoretical maximum of:

$$\eta = 1 - \frac{T_2}{T_1} \tag{5.267}$$

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

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

Equation (5.243) can be rewritten as an increment in pressure from initial pressure P_0 at temperature T_0:

$$P - P_0 = \kappa_0\left[\left(\frac{J_{res}}{J}\right)-1\right] \tag{5.268}$$

where κ_0 is the bulk modulus at P_0:

$$\frac{1}{\kappa_0} = -\frac{1}{V_0}\left(\frac{\partial V_0}{\partial P}\right)_T = \frac{1}{P_0} \tag{5.269}$$

and

$$J = \frac{V(P,T)}{V(P_0,T_0)} = \frac{V}{V_0} \qquad \text{and} \qquad J_{res} = \frac{V(P_0,T)}{V(P_0.T_0)} = \frac{T}{T_0} \tag{5.270}$$

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:

$$T = \frac{T_0}{J^{\gamma-1}} \qquad \text{and} \qquad J_{res} = \frac{1}{J^{\gamma-1}} \tag{5.271}$$

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

$$P - P_0 = \kappa_0 \left[\left(\frac{1}{J} \right) - 1 \right] \qquad \text{isothermal} \tag{5.272}$$

$$P - P_0 = \kappa_0 \left[\left(\frac{1}{J} \right)^{\gamma} - 1 \right] \qquad \text{adiabatic} \tag{5.273}$$

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

$$dT = -\frac{P dV}{C_v} = -\frac{nRT}{C_v}\frac{dV}{V} = -\frac{nRT}{C_v}\frac{\rho}{\rho_0}\frac{dV}{V_0} \tag{5.274}$$

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

$$\frac{dT}{T} = \frac{nR}{C_v}\frac{1}{J} d\eta = \frac{\gamma_0}{J} d\eta = -\gamma_0 \frac{dJ}{J} \qquad \text{where} \qquad \eta = 1 - \frac{\rho_0}{\rho} = 1 - J \tag{5.275}$$

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. (5.220) by using $K = P$, $3\alpha = 1/T$ and $C_v = (3/2)nR/(\rho V)$ (or $5/2$ for diatomic gas).

5.11.3 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

$$\left(P - \frac{an^2}{V^2} \right) \left(\frac{V}{n} - b \right) = RT \tag{5.276}$$

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

$$P = \left(P_0 - a' \right) \left(\frac{1 - b'}{J - b'} \right) \frac{T}{T_0} + \frac{a'}{J^2} \tag{5.277}$$

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

$$U(J) = -\left[\left(P_i - a' \right) \left(1 - b' \right) \ln(J - b') - \frac{a'}{J} \right] \tag{5.278}$$

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

$$P_i = \left(P_0 - a'\right)\frac{T}{T_0} + a' \tag{5.279}$$

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

$$U(J) = -\frac{1}{V_0}\int_{V_0}^{V} P\,dV = -\int_1^J \left(\left(P_i - a'\right)\left(\frac{1-b'}{J-b'}\right) + \frac{a'}{J^2}\right) dJ \tag{5.280}$$

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

$$U = C_v(T - T_0) - \frac{a'}{\rho_0 J} \tag{5.281}$$

In hyperelastic code, an incremental form is

$$dU = C_v dT + \frac{a'}{\rho_0 J^2} dJ \tag{5.282}$$

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

$$\frac{ab}{V_0^2}n^3 - \frac{a}{V_0}n^2 - (P_0 b + RT_0)n + P_0 V_0 = 0 \tag{5.283}$$

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

5.12 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

$$W = G(J_P)||\mathbf{F}_E - \mathsf{R}_E||_F^2 + \frac{\lambda(J_p)}{2}(J_E - 1)^2 \tag{5.284}$$

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

$$G(J_P) = G_0 e^{\xi(1-J_P)} \qquad \text{and} \qquad \lambda(\mathrm{J_P}) = \lambda_0 \mathrm{e}^{\xi(1-\mathrm{J_P})} \tag{5.285}$$

where ξ is a hardening parameter and μ_0 and λ_0 are the initial Lamé coefficients. Note the plastic stretch ($J_P > 1$) causing 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

$$\begin{aligned} ||\mathbf{F} - \mathsf{R}||_F^2 &= \mathrm{Tr}\big((\mathbf{F} - \mathsf{R})^T(\mathbf{F} - \mathsf{R})\big) = \mathrm{Tr}\big((\mathsf{U} - \mathbf{I})^T R^T R(\mathsf{U} - \mathbf{I})\big) = ||\mathsf{U} - \mathbf{I}||_F^2 & (5.286)\\ &= ||\mathsf{Q}^T(\Lambda - \mathbf{I})\mathsf{Q}||_F^2 = ||\Lambda - \mathbf{I}||_F^2 = (\lambda_1 - 1)^2 + (\lambda_2 - 1)^2 + (\lambda_3 - 1)^2 & (5.287)\end{aligned}$$

The energy function is more practically written as

$$W(\lambda_1,\lambda_2,\lambda_3) = G(J_P)\sum_i(\lambda_i-1)^2 + \frac{\lambda(J_p)}{2}(\lambda_1\lambda_2\lambda_3-1)^2 \tag{5.288}$$

where λ_i are the stretches of the elastic part of the deformation. The Cauchy stress and pressure are

$$\boldsymbol{\sigma} = \sum_k\left(\frac{2G(J_P)}{J_E}\lambda_k(\lambda_k-1)+\lambda(J_p)(J_E-1)\right)\boldsymbol{b}_k\otimes\boldsymbol{b}_k \tag{5.289}$$

$$P = -\lambda(J_p)(J_E-1)-\frac{2G(J_P)}{3J_E}\left(\lambda_1^2+\lambda_2^2+\lambda_3^2-\lambda_1-\lambda_2-\lambda_3\right) \tag{5.290}$$

To account for residual stress, replace J_E by J_E/J_{res} and λ_k by λ_k/λ_{res}.

This 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 $\mathbf{B}$:

$$\mathbf{F}_{n+1} = d\mathbf{F}\,\mathbf{F}_n, \qquad J_{n+1} = |d\mathbf{F}|J_n, \qquad \text{and} \qquad \mathbf{B}_{n+1}^{trial} = \mathbf{dF}\mathbf{B}_n\mathbf{dF}^T \tag{5.291}$$

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).

5.12.1 Deformation Examples

This 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:

$$P = -\left[\lambda(J_p)\left(1+\varepsilon+\frac{1}{3}\varepsilon^2\right)-\frac{2G(J_P)}{3(1+\varepsilon)^2}\right]3\varepsilon \tag{5.292}$$

For small ε, this result reduces to

$$P = -\left(\lambda(J_p)+\frac{2G(J_P)}{3}\right)3\varepsilon = -K\frac{\Delta V}{V} \tag{5.293}$$

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

$$\sigma_{xx} = \big(\lambda(J_p) + 2G(J_P)\big)\,\varepsilon \qquad \text{and} \qquad \sigma_{yy} = \sigma_{zz} = \lambda(J_p)\varepsilon \tag{5.294}$$

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

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

$$\lambda_1^2 = \frac{1}{2}\left(2+\gamma^2+\gamma\sqrt{4+\gamma^2}\right) \tag{5.295}$$

$$\lambda_2^2 = \frac{1}{2}\left(2+\gamma^2-\gamma\sqrt{4+\gamma^2}\right) \tag{5.296}$$

$$\lambda_3^2 = 1 \tag{5.297}$$

$$\boldsymbol{b}_1 = \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4+\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma+\sqrt{4+\gamma^2}\right),1,0\right) \tag{5.298}$$

$$\boldsymbol{b}_2 = \frac{1}{\sqrt{1+\frac{1}{4}\left(\gamma+\sqrt{4-\gamma^2}\right)^2}}\left(\frac{1}{2}\left(\gamma-\sqrt{4+\gamma^2}\right),1,0\right) \tag{5.299}$$

$$\boldsymbol{b}_3 = (0,0,1) \tag{5.300}$$

The Cauchy stress reduces to

$$\boldsymbol{\sigma} = 2G(J_P)\left(\lambda_1(\lambda_1-1)\boldsymbol{b}_1\otimes\boldsymbol{b}_1 + \lambda_2(\lambda_2-1)\boldsymbol{b}_2\otimes\boldsymbol{b}_2\right) \tag{5.301}$$

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

$$\sigma_{xx} = G(J_P)\left(2(1+\gamma^2) + \frac{k_1(\gamma-\sqrt{4+\gamma^2}) - k_2(\gamma+\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{5.302}$$

$$\sigma_{yy} = G(J_P)\left(2 - \frac{k_1(\gamma+\sqrt{4+\gamma^2}) - k_2(\gamma-\sqrt{4+\gamma^2})}{\sqrt{8+2\gamma^2}}\right) \tag{5.303}$$

$$\tau_{xy} = 2G(J_P)\left(\gamma + \frac{k_1-k_2}{\sqrt{8+2\gamma^2}}\right) \tag{5.304}$$

$$\sigma_{zz} = 0 \tag{5.305}$$

where

$$k_1 = \sqrt{2+\gamma^2-\gamma\sqrt{4+\gamma^2}} \qquad \text{and} \qquad k_2 = \sqrt{2+\gamma^2+\gamma\sqrt{4+\gamma^2}} \tag{5.306}$$

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

5.13 Tait Liquid

The Tait liquid uses the Tait equation for the pressure response and assumes the shear term follows Newtonian viscosity. The Tait equation for volume of a liquid at any temperature and pressure is:

$$V(P,T) = V(0,T)\left[1 - C\ln\left(1+\frac{P}{B(T)}\right)\right] \tag{5.307}$$

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

$$V(0,T) = A_0 + A_1 T + A_2 T^2 + \cdots \tag{5.308}$$
$$V(0,T) = V(0,T_0) e^{\beta(T-T_0)} \tag{5.309}$$

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

$$B(T) = B_0 e^{-B_1 T} \tag{5.310}$$

Note that bulk modulus from the Tait equation is

$$\frac{1}{K(P,T)} = -\frac{1}{V}\left(\frac{dV}{dP}\right)_T = \frac{C}{P+B(T)} \frac{1}{\left[1 - C\ln\left(1+\frac{P}{B(T)}\right)\right]} = \frac{C}{P+B(T)} \frac{V(P,T)}{V(0,T)} \tag{5.311}$$

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

$$B(T) = CK(0,T) \tag{5.312}$$

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

$$\beta(P,T) = \frac{1}{V}\left(\frac{dV}{dT}\right)_P = \beta(0,T) - \frac{PB_1}{K(P,T)} \tag{5.313}$$

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

$$J = \frac{V(P,T)}{V(0,T_0)} \qquad \text{and} \qquad J_{res} = \frac{V(0,T)}{V(0,T_0)} = e^{\beta_0(T-T_0)} \tag{5.314}$$

as relative volumes. The constitutive law is rewritten as

$$\frac{J}{J_{res}} = 1 - C\ln\left(1 + \frac{P}{CK_0}\right) \tag{5.315}$$

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

$$P = CK_0\left[\exp\left(\frac{1-J^*}{C}\right) - 1\right] \tag{5.316}$$

where $J^* = J/J_{res}$. This material is equivalent to a hyperelastic material with volumetric strain energy function of

$$U(J^*) = CK_0\left[C\exp\left(\frac{1-J^*}{C}\right) + J^*\right] \tag{5.317}$$

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:

$$\tau = \eta\left(\nabla\mathbf{v} + \nabla\mathbf{v}^T - \frac{2}{3}\mathrm{Tr}(\nabla\mathbf{v})\mathbf{I}\right) \tag{5.318}$$

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

$$K(P,T) = \frac{P + CK_0}{C} J^* = K_0 \exp\left(\frac{1-J^*}{C}\right) J^* \tag{5.319}$$

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

$$dP = -K_0 \exp\left(\frac{1-J^*}{C}\right) dJ^* = -K(P,T) d\ln J^* = -K(P,T) \ln dJ^* \tag{5.320}$$

Chapter 6

Viscoelastic Materials

6.1 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

$$P = -K(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} - 3\varepsilon^{(res)}) \tag{6.1}$$

$$s_{ij} = \int_0^t 2G(t-\tau)\frac{de_{xy}}{d\tau}d\tau \tag{6.2}$$

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

$$G(t) = G_0 + \sum_{k=1}^{n} G_k e^{-t/\tau_k} \tag{6.3}$$

Each element of deviatoric stress (with $e(0) = 0$) becomes:

$$s = 2G_0 e(t) + \sum_{k=1}^{n} 2G_k \int_0^t e^{-(t-\tau)/\tau_k}\frac{de(\tau)}{d\tau}d\tau \tag{6.4}$$

where subscripts ij on s and e have been dropped for simplicity,

6.2 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

$$\frac{d\alpha_k}{dt} + \frac{\alpha_k}{\tau_k} = \frac{e(t)}{\tau_k} \tag{6.5}$$

This first order differential equations (with $\alpha_k(0) = 0$) can be solved and integrated by parts to get

$$\alpha_k = \int_0^t e^{-(t-\tau)/\tau_k}\frac{e(\tau)}{\tau_k}d\tau = e(t) - \int_0^t e^{-(t-\tau)/\tau_k}\frac{de(\tau)}{d\tau}d\tau \tag{6.6}$$

Substitution into stress give

$$\frac{s(t)}{2} = G_0 e(t) + \sum_{k=1}^{n} G_k (e(t) - \alpha_k) = G_e e(t) - \sum_{k=1}^{n} G_k \alpha_k \tag{6.7}$$

where

$$G_e = \sum_{k=0}^{n} G_k \tag{6.8}$$

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

$$d\alpha_k = e^{-\Delta t/\tau_k} \int_0^{t+\Delta t} e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau - \int_0^t e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau \tag{6.9}$$

$$= \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + e^{-\Delta t/\tau_k} \int_t^{t+\Delta t} e^{-(t-\tau)/\tau_k} \frac{e(\tau)}{\tau_k} d\tau \tag{6.10}$$

Evaluating the second term by midpoint rule gives

$$d\alpha_k = \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + \frac{\Delta t}{2\tau_k} \left(e(t + \Delta t) + e^{-\Delta t/\tau_k} e(t)\right) \tag{6.11}$$

$$= \left(e^{-\Delta t/\tau_k} - 1\right) \alpha_k(t) + \frac{\Delta t}{2\tau_k} \left(\left(e^{-\Delta t/\tau_k} + 1\right) e(t) + de\right) \tag{6.12}$$

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 $G(t)$.

6.3 Final, Small Strain, Incremental Results

The pressure change is

$$dP = -K(d\varepsilon_{xx} + d\varepsilon_{yy} + d\varepsilon_{zz} - 3d\varepsilon^{(res)}) \tag{6.13}$$

The deviatoric stress updates using

$$ds_{ij} = 2\left(G_e de_{ij} - \sum_{k=1}^{n} G_k d\alpha_{ij,k}\right) \tag{6.14}$$

where $d\alpha_{ij,k}$ is the ij^{th} element of $d\alpha_k$. The dissipated energy (by midpoint rule) is

$$\Phi = \sum_{ij} \sum_{k=1}^{n} 2G_k (e_{ij}(t) - \alpha_{ij,k}) d\alpha_{ij,k} = \sum_{ij} \sum_{k=1}^{n} 2G_k \left(e_{ij} + \frac{de_{ij}}{2} - \alpha_{ij,k} + \frac{d\alpha_{ij,k}}{2}\right) d\alpha_{ij,k} \tag{6.15}$$

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.

6.4 Alternate Internal Variables

Physically, the sum of exponential relaxation elements corresponds to a collection of Maxwell elements (spring 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 the stresses in each Maxwell element, s_k (with implied subscript ij for each component of stress), and then total stress is sum of those stresses:

$$s = s_0 + \sum_{k=1}^{n} s_k \tag{6.16}$$

Comparing to Eq. (6.7), the s_k variables are equivalent to α_k and they are related by:

$$s_k = 2G_k(e(t) - \alpha_k) \qquad \text{and} \qquad \alpha_k = e(t) - \frac{s_k}{2G_k} \tag{6.17}$$

This approach is the one described by Zerelli and Armstrong and the one used in Unintah MPM code.

The evolution equation for Maxwell stresses is the standard differential equation for a single Maxwell element:

$$\frac{1}{2G_k}\frac{ds_k}{dt} + \frac{s_k}{\eta_k} = \frac{de(t)}{dt} \tag{6.18}$$

Substitution of α_k correctly reduces to the evolution equations for α_k variables. The resulting stress update is

$$ds = 2G_0 de(t) + \sum_{k=1}^{n} ds_k \tag{6.19}$$

Using $ds_k = 2G_k de(t) - s_k/\tau_k$, this result reduces to

$$ds = 2G_e de(t) - \sum_{k=1}^{n} \frac{s_k}{\tau_k} \tag{6.20}$$

Replacing α_k in the energy dissipation equation leads to

$$\Phi = \sum_{k=1}^{n} 2G_k(e(t) - \alpha_k)d\alpha_k = \sum_{k=1}^{n} s_k d\alpha_k = \sum_{k=1}^{n} \frac{s_k^2}{2G_k\tau_k} \tag{6.21}$$

Chapter 7

Manufactured Solutions

7.1 Introduction

Brannon (and several coworkers) have proposed manufactured solutions as a method to valid 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 manufacture solutions used in testing `NairnMPM` and easily adapted to testing new material models.

7.2 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

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\frac{t}{t_f} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.1}$$

Here Λ is the final extension, which is reached at $t = t_f$. The initial particle velocities are $\boldsymbol{v} = \big((\Lambda-1)X/t_f, 0, 0\big)$, where X is the initial particle position. 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 large deformation mapping and its inverse are

$$\chi(X,t) = x = X + v(X)t = X\left(1+(\Lambda-1)\frac{t}{t_f}\right) \qquad \text{and} \qquad \chi^{-1}(x,t) = X = \frac{x}{1+(\Lambda-1)\frac{t}{t_f}} \tag{7.2}$$

The x-components of material and spatial descriptions of velocity are

$$V(X,t) = \frac{d\chi(X,t)}{dt} = (\Lambda-1)\frac{X}{t_f} \qquad \text{and} \qquad v(x,t) = V(\chi^{-1}(x,t),t) = \frac{(\Lambda-1)\frac{x}{t_f}}{1+(\Lambda-1)\frac{t}{t_f}} \tag{7.3}$$

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

$$A(X,t) = \frac{d^2\chi(X,t)}{dt^2} = 0 \tag{7.4}$$

To get this same result for spatial velocity requires the material derivative

$$\frac{Dv(x,t)}{Dt} = \frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{(\Lambda-1)^2\frac{x}{t_f^f}}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)^2} + \frac{(\Lambda-1)^2\frac{x}{t_f^2}}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)^2} = 0 \tag{7.5}$$

The material velocity gradient is

$$\dot{\mathsf{F}} = \frac{dV(X,t)}{dX} \qquad \text{giving} \qquad F_{11} = \frac{(\Lambda-1)}{t_f} \tag{7.6}$$

The spatial velocity gradient comes from change of coordinates:

$$\dot{\mathsf{F}} = \frac{dV(X,t)}{dX} = \frac{dv(x,t)}{dx}\frac{dx(X,t)}{dX} = \frac{dv(x,t)}{dx}\mathsf{F} \qquad \text{giving} \qquad F_{11} = \frac{(\Lambda-1)}{t_f} \tag{7.7}$$

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 it the same constant value (to extrapolate the constant to the particles). The spatial velocity gradient is the $\ell = dv(x,t)/dx$ term, which in this example has:

$$l_{11} = \frac{\frac{(\Lambda-1)}{t_f}}{1+(\Lambda-1)\frac{t}{t_f}} \tag{7.8}$$

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 $d\mathsf{F} = \exp(\boldsymbol{\ell}\Delta t) = \mathsf{F}(t+\Delta t)\mathsf{F}^{-1}(t)$ (see section 5.2). In this example:

$$\exp\left(\frac{(\Lambda-1)\frac{\Delta t}{t_f}}{1+(\Lambda-1)\frac{t}{t_f}}\right) = \frac{1+(\Lambda-1)\frac{(t+\Delta t)}{t_f}}{1+(\Lambda-1)\frac{t}{t_f}} = 1 + \frac{(\Lambda-1)\frac{\Delta t}{t_f}}{1+(\Lambda-1)\frac{t}{t_f}} \tag{7.9}$$

which is correct for small Δt.

7.2.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F})-3\big)\mathbf{I} + G(\mathbf{F}+\mathbf{F}^T-2\mathbf{I}) \tag{7.10}$$

where $\lambda = \nu E/((1+\nu)(1-2\nu))$ is the Lamé constant for the material. For constrained uniaxial tension, the stress is

$$\sigma_{ij} = (\lambda+2G\delta_{i1})(\Lambda-1)\frac{t}{t_f}\delta_{ij} \tag{7.11}$$

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:

$$T_x = \pm(\lambda+2G)(\Lambda-1)\frac{t}{t_f} \tag{7.12}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda(\Lambda-1)\frac{t}{t_f} \qquad \text{or} \qquad v_y = v_z = 0 \tag{7.13}$$

7.2.2 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

$$\boldsymbol{\sigma} = \frac{K}{2}\left(J - \frac{1}{J}\right)\mathbf{I} + \frac{G_1}{J^{5/3}}\text{dev}(\mathbf{F}\mathbf{F}^T) \tag{7.14}$$

where $\text{dev}(\mathbf{F}\mathbf{F}^T)$ is the deviatoric part of the left Cauchy-Green tensor with diagonal elements $(1/3)(2(J^2-1), 1-J^2, 1-J^2)$. Under constrained uniaxial deformation:

$$\sigma_{xx} = \left(\frac{K}{2\left(1+(\Lambda-1)\frac{t}{t_f}\right)} + \frac{2G_1}{3\left(1+(\Lambda-1)\frac{t}{t_f}\right)^{5/3}}\right)\left(2+(\Lambda-1)\frac{t}{t_f}\right)\frac{(\Lambda-1)t}{t_f} \tag{7.15}$$

$$\sigma_{yy} = \left(\frac{K}{2\left(1+(\Lambda-1)\frac{t}{t_f}\right)} - \frac{G_1}{3\left(1+(\Lambda-1)\frac{t}{t_f}\right)^{5/3}}\right)\left(2+(\Lambda-1)\frac{t}{t_f}\right)\frac{(\Lambda-1)t}{t_f} \tag{7.16}$$

$$\sigma_{zz} = \sigma_{yy} \tag{7.17}$$

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 $T_z = \pm\sigma_{yy}$.

7.2.3 Neo-Hookean Material

For an alternate neo-Hookean material with default pressure term (`UJOption=0`) and no residual stresses, the Cauchy stress is

$$\boldsymbol{\sigma} = \frac{\lambda}{2}\left(J - \frac{1}{J}\right)\mathbf{I} + \frac{G}{J}\left(\mathbf{F}\mathbf{F}^T - \mathbf{I}\right) \tag{7.18}$$

where $(\mathbf{F}\mathbf{F}^T) = J^2\mathbf{I}$ for constrained uniaxial deformation:

$$\mathbf{F}\mathbf{F}^T = \begin{pmatrix} J^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.19}$$

The stresses become:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{\lambda+2G}{2\left(1+(\Lambda-1)\frac{t}{t_f}\right)}\left(2+(\Lambda-1)\frac{t}{t_f}\right)\frac{(\Lambda-1)t}{t_f} \tag{7.20}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda}{2\left(1+(\Lambda-1)\frac{t}{t_f}\right)}\left(2+(\Lambda-1)\frac{t}{t_f}\right)\frac{(\Lambda-1)t}{t_f} \tag{7.21}$$

$$\sigma_{zz} = \sigma_{yy} \tag{7.22}$$

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, the Cauchy stress is

$$\boldsymbol{\sigma} = \lambda\frac{\ln J}{J}\mathbf{I} + \frac{G}{J}\left(\mathbf{F}\mathbf{F}^T - \mathbf{I}\right) \tag{7.23}$$

The stresses become:

$$\sigma_{xx} = \frac{\lambda \ln\left(1+(\Lambda-1)\frac{t}{t_f}\right) + G\left(2+(\Lambda-1)\frac{t}{t_f}\right)\frac{(\Lambda-1)t}{t_f}}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)} \tag{7.24}$$

$$\sigma_{zz} = \sigma_{yy} = \frac{\lambda \ln\left(1+(\Lambda-1)\frac{t}{t_f}\right)}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)} \tag{7.25}$$

7.2.4 Disney Snow Model

For the neo-Hookean material in the elastic part of the Disney snow model, the eigenvalues of $\mathbf{B}$ are $1+(\Lambda-1)t/t_f$, 1, and 1 with eigenvectors $\hat{x}$, $\hat{y}$, and $\hat{z}$. The Cauchy stress is

$$\sigma_{xx} = \big(\lambda(J_p)+2G(J_p)\big)(\Lambda-1)\frac{t}{t_f} \tag{7.26}$$

$$\sigma_{yy} = \lambda(J_p)(\Lambda-1)\frac{t}{t_f} \tag{7.27}$$

$$\sigma_{zz} = \sigma_{yy} \tag{7.28}$$

This result is identical to a low-strain, isotropic material, although these two models are not identical in all deformation states.

7.3 Constrained Uniaxial Tension with Thermal Ramp

In addition to linear variation in elongation, we add linear variation in $\lambda_{res} = 1+(\Lambda_{res}-1)t/t_f$, which corresponds to a temperature of

$$\Delta T = \frac{1}{\alpha}\ln\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right) \tag{7.29}$$

For plane strain, the full deformation matrix is

$$\mathbf{F} = \begin{pmatrix} \left(1+(\Lambda-1)\frac{t}{t_f}\right)\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right) & 0 & 0 \\ 0 & 1+(\Lambda_{res}-1)\frac{t}{t_f} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.30}$$

The acceleration will be

$$\boldsymbol{a} = \left(\frac{2X}{t_f^2}(\Lambda-1)(\Lambda_{res}-1), 0, 0\right) \tag{7.31}$$

The initial velocities will be

$$\boldsymbol{v}(t=0) = \left((\Lambda-1)\frac{X}{t_f} + (\Lambda_{res}-1)\frac{X}{t_f}, (\Lambda_{res}-1)\frac{Y}{t_f}, 0\right) \tag{7.32}$$

7.3.1 Neo-Hookean Material

For an alternate neo-Hookean material with the default pressure term and including residual stresses, the Cauchy stress is

$$\boldsymbol{\sigma} = \frac{\lambda}{2}\left(\frac{J}{J_{res}} - \frac{J_{res}}{J}\right)\mathbf{I} + \frac{G}{J}\left(J_{res}^{1/3}\mathbf{F}\mathbf{F}^T - J_{res}\mathbf{I}\right) \tag{7.33}$$

The stresses, which are independent of position (and hence have zero divergence) are:

$$\sigma_{xx} = \left[\frac{\frac{\lambda}{2}(\Lambda-\Lambda_{res})\left(2+(\Lambda+\Lambda_{res}-2)\frac{t}{t_f}\right) + G(\Lambda-1)\left(2+(\Lambda-1)\frac{t}{t_f}\right)\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right)^2}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right)}\right]\frac{t}{t_f} \tag{7.34}$$

$$\sigma_{yy} = \frac{\lambda}{2}\frac{(\Lambda-\Lambda_{res})\left(2+(\Lambda+\Lambda_{res}-2)\frac{t}{t_f}\right)}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right)}\frac{t}{t_f} \tag{7.35}$$

$$\sigma_{zz} = \left[\frac{\frac{\lambda}{2}(\Lambda-\Lambda_{res})\left(2+(\Lambda+\Lambda_{res}-2)\frac{t}{t_f}\right) - G(\Lambda_{res}-1)\left(2+(\Lambda_{res}-1)\frac{t}{t_f}\right)}{\left(1+(\Lambda-1)\frac{t}{t_f}\right)\left(1+(\Lambda_{res}-1)\frac{t}{t_f}\right)}\right]\frac{t}{t_f} \tag{7.36}$$

To be able to implement this in `NairnMPM` need:

1. A method to have a non-linear thermal ramp for the ΔT term

7.4 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

$$\mathbf{F} = \begin{pmatrix} 1 & \Gamma\frac{t}{t_f} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{B} = \begin{pmatrix} 1+\Gamma^2\frac{t^2}{t_f^2} & \Gamma\frac{t}{t_f} & 0 \\ \Gamma\frac{t}{t_f} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.37}$$

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:

$$\boldsymbol{T} = \left(\tau_{xy}, \sigma_{yy}, 0\right) \quad \text{on } \pm y \tag{7.38}$$

$$\boldsymbol{T} = (0, 0, \sigma_{zz}) \quad \text{on } \pm z \tag{7.39}$$

$$\tag{7.40}$$

On the initially $\pm x$ surface, the normal rotates to be

$$\hat{\boldsymbol{n}} = \left(\frac{1}{\sqrt{1+\gamma^2}}, \frac{-\gamma}{\sqrt{1+\gamma^2}}, 0\right) \tag{7.41}$$

where $\gamma = \Gamma t/t_f$. But since $\gamma = \tan\theta$, where θ is the current shear angle, this normal vector is also

$$\hat{\boldsymbol{n}} = (\cos\theta, -\sin\theta, 0) \tag{7.42}$$

For general stress state (but with $\sigma_{xz} = \sigma_{yz} = 0$), the traction will be

$$\boldsymbol{T} = \left(\sigma_{xx}\cos\theta - \sigma_{xy}\sin\theta, \sigma_{xy}\cos\theta - \sigma_{yy}\sin\theta, 0\right) \tag{7.43}$$

This traction can be divided into traction normal and tangential to the current surface:

$$T_n = \boldsymbol{T}\cdot\hat{\boldsymbol{n}} = \sigma_{xx}\cos^2\theta - 2\sigma_{xy}\cos\theta\sin\theta + \sigma_{yy}\sin^2\theta = \frac{\sigma_{xx} - 2\gamma\sigma_{xx} + \gamma^2\sigma_{yy}}{1+\gamma^2} \tag{7.44}$$

$$T_t = \boldsymbol{T}\cdot\hat{\boldsymbol{t}} = (\sigma_{xx} - \sigma_{yy})\cos\theta\sin\theta + \sigma_{xy}(\cos^2\theta - \sin^2\theta) \tag{7.45}$$

$$= \frac{\gamma(\sigma_{xx} - \sigma_{yy}) + \sigma_{xy}(1-\gamma^2)}{1+\gamma^2} \tag{7.46}$$

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

$$\boldsymbol{v} = \left(\Gamma\frac{Y}{t_f}, 0, 0\right) \tag{7.47}$$

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.

7.4.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material for shear sliding can be written as

$$\boldsymbol{\sigma} = G(\mathbf{F} + \mathbf{F}^T - 2\mathbf{I}) \tag{7.48}$$

The only non-zero stress is the shear stress:

$$\sigma_{xy} = G\gamma = G\Gamma\frac{t}{t_f} \tag{7.49}$$

7.4.2 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

$$\sigma_{xx} = \frac{J_{res}\gamma^2}{3}(2G_1 + G_2) \tag{7.50}$$

$$\sigma_{yy} = -\frac{J_{res}\gamma^2}{3}(G_1 + 2G_2) \tag{7.51}$$

$$\sigma_{zz} = \frac{J_{res}\gamma^2}{3}(-G_1 + G_2) \tag{7.52}$$

$$\tau_{xy} = J_{res}\gamma(G_1 + G_2) \tag{7.53}$$

where J_{res} is set to one to generate a solution with no residual stresses.

7.4.3 Neo-Hookean Material

For an alternate Neo-Hookean material with no residual stresses, the Cauchy stress under sliding shear is found from elements of **B**. In addition $J = 1$, which means pressure terms are zero (and result is independent of the `UJoption` setting). The final stresses are

$$\sigma_{xx} = G\gamma^2 \tag{7.54}$$
$$\sigma_{yy} = \sigma_{zz} = 0 \tag{7.55}$$
$$\tau_{xy} = G\gamma \tag{7.56}$$

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:

$$T_n = -\frac{G\gamma^2}{1+\gamma^2} \tag{7.57}$$
$$T_t = \frac{G\gamma}{1+\gamma^2} \tag{7.58}$$

or with tractions along x and y. Both work, but x and y tractions are more stable

7.4.4 Disney Snow Model

For the neo-Hookean material in the elastic part of the Disney snow model, the eigenvalues and eigenvectors of **B**:

$$\lambda_1^2 = 1 + \frac{1}{2}\gamma^2 + \gamma\sqrt{1+\frac{1}{4}\gamma^2} \tag{7.59}$$
$$\lambda_2^2 = 1 + \frac{1}{2}\gamma^2 - \gamma\sqrt{1+\frac{1}{4}\gamma^2} \tag{7.60}$$
$$\lambda_3^2 = 1 \tag{7.61}$$
$$\tag{7.62}$$

7.5 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

$$\mathbf{F} = \begin{pmatrix} 1+(\Lambda-1)\frac{t^2}{t_f^2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{7.63}$$

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:

$$\boldsymbol{b} = \left(\frac{2(\Lambda-1)\frac{x}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{7.64}$$

To apply velocity boundary conditions, the applied velocity (in spatial nodal coordinates) should be

$$\boldsymbol{v} = \left(\frac{2(\Lambda-1)\frac{xt}{t_f^2}}{1+(\Lambda-1)\frac{t^2}{t_f^2}}, 0, 0 \right) \tag{7.65}$$

7.5.1 Low-Strain, Isotropic Material

In terms of $\mathbf{F}$, the stress in a low-strain, isotropic material can be written as

$$\boldsymbol{\sigma} = \lambda\big(\mathrm{Tr}(\mathbf{F})-3\big)\mathbf{I} + G(\mathbf{F}+\mathbf{F}^T-2\mathbf{I}) \tag{7.66}$$

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

$$\sigma_{ij} = (\lambda + 2G\delta_{i1})(\Lambda-1)\frac{t^2}{t_f^2}\delta_{ij} \tag{7.67}$$

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:

$$T_x = \pm(\lambda+2G)(\Lambda-1)\frac{t^2}{t_f^2} \tag{7.68}$$

On the $\pm y$ and $\pm z$ surface, the traction condition should be:

$$T_y = \pm\lambda(\Lambda-1)\frac{t^2}{t_f^2} \qquad \text{or} \qquad v_y = v_z = 0 \tag{7.69}$$

7.5.2 Neo-Hookean Material

For an alternate neo-Hookean material under constrained uniaxial deformation:

$$\sigma_{xx} = \frac{\lambda+2G}{2J}(J^2-1) = \frac{\lambda+2G}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{7.70}$$

$$\sigma_{yy} = \frac{\lambda}{2J}(J^2-1) = \frac{\lambda}{2\left(1+(\Lambda-1)\frac{t^2}{t_f^2}\right)}\left(2+(\Lambda-1)\frac{t^2}{t_f^2}\right)\frac{(\Lambda-1)t^2}{t_f^2} \tag{7.71}$$

$$\sigma_{zz} = \sigma_{yy} \tag{7.72}$$

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 $T_z = \pm\sigma_{yy}$.