Drucker-Prager Elastoplasticity for Sand Animation: Supplementary Technical Document

May 5, 2016

We first present pseudocode to provide further details useful for implementing the method in Section 1. Then in Sections 2-6 we provide details related to the derivation and basic properties of the plastic flow and its discretization.

1 Pseudocode

Pseudocode for our algorithm is given in Algorithm 1, with additional details for the implicit solve in Algorithm 2.

1.1 Derivatives of elasticity and plasticity

As part of an implicit formulation, we encounter the combination

$$\mathbf{Y}(\mathbf{F}) = \frac{\partial \psi}{\partial \mathbf{F}}(\mathbf{Z}(\mathbf{F}, \alpha)) = \mathbf{W}(\mathbf{Z}(\mathbf{F}, \alpha)), \tag{1}$$

where $\mathbf{W}(\mathbf{F}) = \frac{\partial \psi}{\partial \mathbf{F}}(\mathbf{F})$. This corresponds to projecting a deformation gradient for plasticity and then using the result as part of a force computation. This function $\mathbf{Y}$ must be differentiated, resulting in the rank-four tensor

$$\mathbf{M} = \frac{\partial \mathbf{Y}}{\partial \mathbf{F}}(\mathbf{F}). \tag{2}$$

The tensor $\mathbf{M}$ has $3^4 = 81$ entries and no symmetries. Both the construction and application of $\mathbf{M}$ are somewhat expensive, and both can be avoided.

If $\mathbf{F} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, then it turns out that $\mathbf{Z}(\mathbf{F}, \alpha) = \mathbf{U}\hat{\mathbf{Z}}(\mathbf{\Sigma}, \alpha)\mathbf{V}^T$ and $\mathbf{W}(\mathbf{F}) = \mathbf{U}\hat{\mathbf{W}}(\mathbf{\Sigma})\mathbf{V}^T$, where $\hat{\mathbf{Z}}(\mathbf{\Sigma}, \alpha)$ and $\hat{\mathbf{W}}(\mathbf{\Sigma})$ are diagonal matrices. It follows then that $\mathbf{Y}(\mathbf{F}) = \mathbf{U}\hat{\mathbf{Y}}(\mathbf{\Sigma})\mathbf{V}^T$, with $\hat{\mathbf{Y}}(\mathbf{\Sigma}) = \hat{\mathbf{W}}(\hat{\mathbf{Z}}(\mathbf{\Sigma}, \alpha))$, where $\hat{\mathbf{Y}}(\mathbf{\Sigma})$ is also a diagonal matrix. To be able to carry out these steps, it is required of the energy density function ψ, that it depends only on the singular values of $\mathbf{F}$. In essence, we need to be able to define $\hat{\psi}$ such that, $\hat{\psi}(\mathbf{\Sigma}) = \psi(\mathbf{F})$. This allows us to write the definition of $\hat{\mathbf{W}}$ as $\hat{\mathbf{W}}(\mathbf{\Sigma}) = \frac{\partial \hat{\psi}}{\partial \mathbf{\Sigma}}(\mathbf{\Sigma})$.

Note that we have taken advantage of these relationships to avoid computing the singular value decomposition more often than necessary. Indeed, $\hat{\mathbf{W}}$ is implemented by ENERGY_DERIVATIVE, and $\hat{\mathbf{Z}}$ is implemented by PROJECT.

Since these functions are rather simple in *diagonal space*, it might not be too surprising that the derivatives are also simpler there. Let $\hat{\mathbf{M}}$ be the diagonal space version of $\mathbf{M}$, defined by

$$M_{ijkl} = \hat{M}_{rsuv} U_{ir} V_{js} U_{ku} V_{lv}, \tag{3}$$

where index notation is used and summation is implied. In the pseudocode, the operation

$$\mathbf{A} = \hat{\mathbf{M}} : \mathbf{T} \tag{4}$$

Algorithm 1 Simulate sand

procedure TIME_STEP
  TRANSFER_TO_GRID
  if explicit **then**
    EXPLICIT_GRID_STEP
  else
    IMPLICIT_GRID_STEP
  TRANSFER_TO_PARTICLES
  UPDATE_PARTICLE_STATE
  PLASTICITY_HARDENING

procedure TRANSFER_TO_GRID
  for all grid nodes i **do**
    $m_i^n \leftarrow \sum_p w_{ip}^n m_p$
    $\mathbf{v}_i^n \leftarrow \frac{1}{m_i^n} \sum_p w_{ip}^n m_p \big(\mathbf{v}_p^n + \frac{3}{h^2}\mathbf{B}_p^n(\mathbf{x}_i - \mathbf{x}_p^n)\big)$
      ▷ assuming cubic spline

procedure EXPLICIT_GRID_STEP
  $\langle \mathbf{v}_i^\star \rangle \leftarrow \langle \mathbf{v}_i^n \rangle + \text{FORCE\_INCREMENT}(\langle \mathbf{F}_p^{E,n} \rangle, 0)$
  $\langle \overline{\mathbf{v}}_i^{n+1} \rangle \leftarrow \text{GRID\_COLLISIONS}(\langle \mathbf{v}_i^\star \rangle)$
  $\langle \tilde{\mathbf{v}}_i^{n+1} \rangle \leftarrow \text{FRICTION}(\langle \overline{\mathbf{v}}_i^{n+1} \rangle, \langle \overline{\mathbf{v}}_i^{n+1} - \mathbf{v}_i^\star \rangle)$

procedure IMPLICIT_GRID_STEP
  COUPLED_SOLVE
  $\langle \mathbf{v}_i^\star \rangle \leftarrow \langle \mathbf{v}_i^n \rangle + \text{FORCE\_INCREMENT\_VEL}(\langle \overline{\mathbf{v}}_i^{n+1} \rangle)$
  $\langle \Delta \mathbf{v}_i \rangle \leftarrow \text{GRID\_COLLISIONS}(\langle \mathbf{v}_i^\star \rangle) - \langle \mathbf{v}_i^\star \rangle$
  $\langle \tilde{\mathbf{v}}_i^{n+1} \rangle \leftarrow \text{FRICTION}(\langle \overline{\mathbf{v}}_i^{n+1} \rangle, \langle \Delta \mathbf{v}_i \rangle)$

procedure TRANSFER_TO_PARTICLES
  for all particles p **do**
    $\mathbf{v}_p^{n+1} \leftarrow \sum_i w_{ip}^n \tilde{\mathbf{v}}_i^{n+1}$
    $\mathbf{B}_p^{n+1} \leftarrow \sum_i w_{ip}^n \tilde{\mathbf{v}}_i^{n+1} (\mathbf{x}_i - \mathbf{x}_p^n)^T$

procedure UPDATE_PARTICLE_STATE
  for all particles p **do**
    $\mathbf{x}_p^{n+1} \leftarrow \sum_i w_{ip}^n (\mathbf{x}_i^n + \Delta t w_{ip}^n \overline{\mathbf{v}}_i^{n+1})$
    $\mathbf{T} \leftarrow \sum_i \overline{\mathbf{v}}_i^{n+1} (\nabla w_{ip}^n)^T$
    $\hat{\mathbf{F}}_p^{E,n+1} \leftarrow (\mathbf{I} + \Delta t \mathbf{T}) \mathbf{F}_p^{E,n}$
    $\hat{\mathbf{F}}_p^{P,n+1} \leftarrow \mathbf{F}_p^{P,n}$

procedure PLASTICITY_HARDENING
  for all particles p **do**
    $(\mathbf{U}, \mathbf{\Sigma}, \mathbf{V}) \leftarrow \text{SVD}(\hat{\mathbf{F}}_p^{E,n+1})$
    $(\mathbf{T}, \delta q) \leftarrow \text{PROJECT}(\mathbf{\Sigma}, \alpha_p^n)$
    $\mathbf{F}_p^{E,n+1} \leftarrow \mathbf{U}\mathbf{T}\mathbf{V}^T$
    $\mathbf{F}_p^{P,n+1} \leftarrow \mathbf{V}\mathbf{T}^{-1}\mathbf{\Sigma}\mathbf{V}^T \hat{\mathbf{F}}_p^{P,n+1}$
    $q_p^{n+1} \leftarrow q_p^n + \delta q$
    $\phi_F \leftarrow h_0 + (h_1 q_p^{n+1} - h_3) e^{-h_2 q_p^{n+1}}$
    $\alpha_p^{n+1} \leftarrow \sqrt{\frac{2}{3}} \frac{2 \sin \phi_F}{3 - \sin \phi_F}$

function FRICTION($\langle \mathbf{v}_i \rangle, \langle \Delta \mathbf{v}_i \rangle$)
  for all recorded collisions $(b, i, \cdot, \mathbf{n}, \cdot)$ **do**
    $\mathbf{v}_t \leftarrow \overline{\mathbf{v}}_i^{n+1} - \mathbf{n}(\mathbf{n} \cdot \mathbf{v}_i)$
    $\mathbf{t} \leftarrow \frac{\mathbf{v}_t}{\|\mathbf{v}_t\|}$
    $\mathbf{v}_i \leftarrow \mathbf{v}_i - \min(\|\mathbf{v}_t\|, \mu_b \|\Delta \mathbf{v}_i\|)\mathbf{t}$
  return $\langle \mathbf{v}_i \rangle$

function GRID_COLLISIONS($\langle \mathbf{v}_i \rangle$)
  FORGET_RECORDED_ITEMS
  $\langle \hat{\mathbf{v}}_i \rangle \leftarrow \langle \mathbf{v}_i \rangle$;
  for all collision bodies b **do**
    $\hat{\mathbf{x}}_i \leftarrow \mathbf{x}_i^n + \Delta t \hat{\mathbf{v}}_i$
    if IS_STICKY(b) **and** $\phi_b(\mathbf{x}_i^n) < 0$ **then**
      RECORD_STICKY(b, i)
      $\hat{\mathbf{v}}_i \leftarrow \mathbf{v}_b(\hat{\mathbf{x}}_i)$
    else
      $\hat{\phi} \leftarrow \phi_b(\hat{\mathbf{x}}_i) - \min(\phi_b(\mathbf{x}_i^n), 0)$
      if (IS_SEPARATING(b) **and** $\hat{\phi} < 0$) **or**
          (IS_SLIPPING(b) **and** $\phi_b(\mathbf{x}_i^n) < 0$) **then**
        RECORD_COLLISION($b, i, \nabla \phi_b(\hat{\mathbf{x}}_i)$)
        $\hat{\mathbf{v}}_i \leftarrow \hat{\mathbf{v}}_i - \hat{\phi} \nabla \phi_b(\hat{\mathbf{x}}_i) / \Delta t$
  return $\langle \hat{\mathbf{v}}_i \rangle$

function PROJECT($\mathbf{\Sigma}, \alpha$)
  $\boldsymbol{\epsilon} \leftarrow \ln \mathbf{\Sigma}$
  $\hat{\boldsymbol{\epsilon}} \leftarrow \boldsymbol{\epsilon} - \frac{\text{tr}(\boldsymbol{\epsilon})}{d}\mathbf{I}$
  if $\hat{\boldsymbol{\epsilon}} = \mathbf{0}$ **or** $\text{tr}(\boldsymbol{\epsilon}) > 0$ **then** ▷ Case II
    return $(\mathbf{I}, \|\boldsymbol{\epsilon}\|_F)$
  $\delta\gamma \leftarrow \|\hat{\boldsymbol{\epsilon}}\|_F + \frac{d\lambda + 2\mu}{2\mu} \text{tr}(\boldsymbol{\epsilon}) \alpha$
  if $\delta\gamma \leq 0$ **then** ▷ Case I
    return $(\mathbf{\Sigma}, 0)$
  $\mathbf{H} \leftarrow \boldsymbol{\epsilon} - \delta\gamma \frac{\hat{\boldsymbol{\epsilon}}}{\|\hat{\boldsymbol{\epsilon}}\|_F}$ ▷ Case III
  return $(\exp(\mathbf{H}), \delta\gamma)$

function ENERGY_DERIVATIVE($\mathbf{F}$)
  return $2\mu \mathbf{\Sigma}^{-1} \ln \mathbf{\Sigma} + \lambda \text{tr}(\ln \mathbf{\Sigma}) \mathbf{\Sigma}^{-1}$

function FORCE_INCREMENT($\langle \mathbf{F}_p \rangle, b$)
  for all particles p **do**
    $(\mathbf{U}, \mathbf{\Sigma}, \mathbf{V}) \leftarrow \text{SVD}(\mathbf{F}_p)$
    if $b \neq 0$ **then**
      $(\mathbf{\Sigma}, \cdot) \leftarrow \text{PROJECT}(\mathbf{\Sigma}, \alpha_p^n)$ ▷ ignore hardening
    $\mathbf{T} \leftarrow \text{ENERGY\_DERIVATIVE}(\mathbf{\Sigma})$
    $\mathbf{A}_p \leftarrow V_p^0 \mathbf{U}\mathbf{T}\mathbf{V}^T (\mathbf{F}_p^n)^T$
  for all grid nodes i **do**
    $\mathbf{f}_i \leftarrow -\frac{\Delta t}{m_i^n} \sum_p \mathbf{A}_p \nabla w_{ip}^n$
  return $\langle \mathbf{f}_i \rangle$

function FORCE_INCREMENT_VEL($\langle \mathbf{v}_i \rangle$)
  for all particles p **do**
    $\mathbf{T} \leftarrow \sum_i \mathbf{v}_i (\nabla w_{ip}^n)^T$
    $\mathbf{A}_p \leftarrow (\mathbf{I} + \Delta t \mathbf{T}) \mathbf{F}_p^{E,n}$
  return FORCE_INCREMENT($\langle \mathbf{A}_p \rangle, 1$)

Algorithm 2 Implicit solve

procedure COUPLED_SOLVE
  $\langle \hat{\mathbf{v}}_i \rangle \leftarrow \langle \mathbf{v}_i^n \rangle +$ FORCE_INCREMENT_VEL$(\langle \mathbf{v}_i^n \rangle)$
  return CONSTRAINED_NEWTON$(\langle \hat{\mathbf{v}}_i \rangle)$

function CONSTRAINED_NEWTON$(\langle \mathbf{z}_i \rangle)$
  $\langle \mathbf{z}_i \rangle \leftarrow$ GRID_COLLISIONS$(\langle \mathbf{z}_i \rangle)$
  while not too many iterations **do**
    $\langle \mathbf{y}_i \rangle \leftarrow$ NONLINEAR_FUNCTION$(\langle \mathbf{z}_i \rangle)$
    $a \leftarrow \sqrt{\sum_i m_i \mathbf{y}_i \cdot \mathbf{y}_i}$
    if $a < \tau \Delta t$ **and** not first iteration **then**
      return $\langle \mathbf{z}_i \rangle$
    Find $\langle \Delta \mathbf{z}_i \rangle$ so TIMES_DIFF$(\langle \Delta \mathbf{z}_i \rangle) = -\langle \mathbf{y}_i \rangle$
      ▷ Solve using GMRES
    $\langle \mathbf{z}_i \rangle \leftarrow \langle \mathbf{z}_i \rangle + \langle \Delta \mathbf{z}_i \rangle$
    $\langle \mathbf{z}_i \rangle \leftarrow$ GRID_COLLISIONS$(\langle \mathbf{z}_i \rangle)$
  return $\langle \mathbf{z}_i \rangle$

function NONLINEAR_FUNCTION$(\langle \mathbf{v}_i \rangle)$
  $\langle \hat{\mathbf{v}}_i \rangle \leftarrow$ GRID_COLLISIONS$(\langle \mathbf{v}_i \rangle)$
  $\langle \overline{\mathbf{v}}_i \rangle \leftarrow \langle \hat{\mathbf{v}}_i \rangle - \langle \mathbf{v}_i^n \rangle -$ FORCE_INCREMENT_VEL$(\langle \hat{\mathbf{v}}_i \rangle)$
  return PRUNE_COLLISIONS$(\langle \overline{\mathbf{v}}_i \rangle)$

function PRUNE_COLLISIONS$(\langle \mathbf{v}_i \rangle)$
  $\langle \hat{\mathbf{v}}_i \rangle \leftarrow \langle \mathbf{v}_i \rangle$
  for all recorded sticky $(\cdot, i)$ **do**
    $\hat{\mathbf{v}}_i \leftarrow \mathbf{0}$
  for all recorded collisions $(b, i, \mathbf{n})$ **do**
    if IS_SEPARATING(b) **and** $\hat{\mathbf{v}}_i \cdot \mathbf{n} < 0$ **then**
      FORGET_COLLISION$(\cdot, i)$
    else
      $\hat{\mathbf{v}}_i \leftarrow \hat{\mathbf{v}}_i - (\hat{\mathbf{v}}_i \cdot \mathbf{n})\mathbf{n}$

function TIMES_DIFF$(\langle \mathbf{v}_i \rangle)$
  $\langle \hat{\mathbf{v}}_i \rangle \leftarrow \langle \mathbf{v}_i \rangle$
  for all recorded sticky $(\cdot, i)$ **do**
    $\hat{\mathbf{v}}_i \leftarrow \mathbf{0}$
  for all recorded collisions $(\cdot, i, \mathbf{n})$ **do**
    $\hat{\mathbf{v}}_i \leftarrow \hat{\mathbf{v}}_i - (\hat{\mathbf{v}}_i \cdot \mathbf{n})\mathbf{n}$
  $\langle \overline{\mathbf{v}}_i \rangle \leftarrow$ HESSIAN_TIMES$(\langle \hat{\mathbf{v}}_i \rangle)$
  for all grid nodes i **do**
    $\overline{\mathbf{v}}_i \leftarrow \hat{\mathbf{v}}_i + \frac{\Delta t^2}{m_i^n} \overline{\mathbf{v}}_i$
  for all recorded sticky $(\cdot, i)$ **do**
    $\overline{\mathbf{v}}_i \leftarrow \mathbf{0}$
  for all recorded collisions $(\cdot, i, \mathbf{n})$ **do**
    $\overline{\mathbf{v}}_i \leftarrow \overline{\mathbf{v}}_i - (\overline{\mathbf{v}}_i \cdot \mathbf{n})\mathbf{n}$
  return $\langle \mathbf{z}_i \rangle$

function HESSIAN_TIMES$(\langle \mathbf{z}_i \rangle)$
  for all particles p **do**
    LOAD$(\mathbf{U}_p, \mathbf{Q}_p, \hat{\mathbf{M}})$
    $\mathbf{T}_1 \leftarrow \sum_i \mathbf{z}_i (\nabla w_{ip}^n)^T$
    $\mathbf{T}_2 \leftarrow \mathbf{U}_p^T \mathbf{T}_1 \mathbf{Q}_p$
    $\mathbf{T}_3 \leftarrow \hat{\mathbf{M}} : \mathbf{T}_2$ ▷ See (§1.1)
    $\mathbf{A}_p = V_p^0 \mathbf{U}_p \mathbf{T}_3 \mathbf{Q}_p^T$
  for all grid nodes i **do**
    $\mathbf{y}_i \leftarrow \sum_p \mathbf{A}_p \nabla w_{ip}^n$
  return $\langle \mathbf{y}_i \rangle$

procedure PRECOMPUTE$(\langle \mathbf{v}_i \rangle)$
  for all particles p **do**
    $\mathbf{T} \leftarrow \sum_i \mathbf{z}_i (\nabla w_{ip}^n)^T$
    $\mathbf{F}_p \leftarrow (\mathbf{I} + \Delta t \mathbf{T}) \mathbf{F}_p^{E,n}$
    $(\mathbf{U}_p, \mathbf{\Sigma}, \mathbf{V}) \leftarrow \mathrm{SVD}(\mathbf{F}_p)$
    $\mathbf{Q}_p \leftarrow \mathbf{F}_p^{E,n} \mathbf{V}$
    Construct $\hat{\mathbf{M}}$ ▷ See (§1.1)
    STORE$(\mathbf{U}_p, \mathbf{Q}_p, \hat{\mathbf{M}})$

is requested. This is equivalent to $A_{ij} = \hat{M}_{ijkl} T_{kl}$. What remains is to determine the structure of $\hat{\mathbf{M}}$. The way that this is done follows from the approach taken in [5], but we summarize the result here.

Introducing the auxiliary variables $\overline{Y}_{ij}, D_{ij}, S_{ij}$, the nonzero entries of $\hat{\mathbf{M}}$ are (with no summation implied)

$$\hat{M}_{iijj} = \overline{Y}_{ij} = \frac{\partial \hat{Y}_{ii}}{\partial \Sigma_{jj}} \tag{5}$$

$$\hat{M}_{ijij} = \frac{D_{ij} + S_{ij}}{2} \qquad i \neq j \tag{6}$$

$$\hat{M}_{ijji} = \frac{D_{ij} - S_{ij}}{2} \qquad i \neq j \tag{7}$$

$$D_{ij} = \frac{\hat{Y}_{ii} - \hat{Y}_{jj}}{\Sigma_{ii} - \Sigma_{jj}} \tag{8}$$

$$S_{ij} = \frac{\hat{Y}_{ii} + \hat{Y}_{jj}}{\Sigma_{ii} + \Sigma_{jj}} \tag{9}$$

Note that $D_{ij} = D_{ji}$ and $S_{ij} = S_{ji}$, so that $\hat{M}_{ijij} = \hat{M}_{jiji}$ and $\hat{M}_{ijji} = \hat{M}_{jiij}$. Thus, there are only $9 + 3 + 3 = 15$ distinct nonzero entries to compute, and $9 + 6 + 6 = 21$ multiplications (plus 12 additions) are required to apply the tensor. Of the computations required, $\overline{Y}_{ij}$ and D_{ij} merit further attention. S_{ij} can be computed directly, since division by zero is not a concern there.

First we describe the computation of $\overline{\mathbf{Y}}$. Since $\hat{\mathbf{Y}}$ is the composition of two functions, $\overline{\mathbf{Y}}$ is computed using the chain rule. Note that both $\hat{\mathbf{W}}$ and $\overline{\mathbf{W}}$ are evaluated at $\hat{\mathbf{Z}} = \hat{\mathbf{Z}}(\mathbf{\Sigma}, \alpha)$.

$$\overline{Y}_{ij} = \frac{\partial \hat{Y}_{ii}}{\partial \Sigma_{jj}} = \sum_k \frac{\partial \hat{W}_{ii}}{\partial \Sigma_{kk}} \frac{\partial \hat{Z}_{kk}}{\partial \Sigma_{jj}} = \sum_k \overline{W}_{ik} \overline{Z}_{kj}, \tag{10}$$

where the matrices $\overline{\mathbf{Y}}$, $\overline{\mathbf{W}}$, and $\overline{\mathbf{Z}}$ represent the derivatives of the functions $\hat{\mathbf{Y}}$, $\hat{\mathbf{W}}$, and $\hat{\mathbf{Z}}$ when diagonal matrices are treated as functions taking vector and returning a vector. Differentiating $\hat{\mathbf{W}}$ gives

$$\overline{\mathbf{W}} = \hat{\mathbf{Z}}^{-1}(2\mu\mathbf{I} - 2\mu \ln(\hat{\mathbf{Z}}) + \lambda \mathbf{o}\mathbf{o}^T - \lambda \mathrm{tr}(\ln(\hat{\mathbf{Z}}))\mathbf{I})\hat{\mathbf{Z}}^{-1}, \tag{11}$$

where $\mathbf{o}$ is the all-ones vector.

Next, we need to differentiate the projection to get $\overline{\mathbf{Z}}$. There are three cases to consider. In Case I, $\overline{\mathbf{Z}} = \mathbf{I}$. In Case II, $\overline{\mathbf{Z}} = \mathbf{0}$. This leaves only Case III, in which case

$$\boldsymbol{\epsilon} = \mathrm{diag}(\ln \mathbf{\Sigma}) \qquad \mathbf{w} = \mathrm{diag}(\mathbf{\Sigma}^{-1}) \qquad k = \mathrm{tr}(\ln \mathbf{\Sigma}) \qquad \mathbf{s} = \boldsymbol{\epsilon} - \frac{k}{d}\mathbf{o} \qquad \hat{\mathbf{s}} = \frac{\mathbf{s}}{\|\mathbf{s}\|} \qquad p = \frac{\alpha k (d\lambda + 2\mu)}{2\mu \|\mathbf{s}\|} \tag{12}$$

$$\overline{\mathbf{Z}} = \hat{\mathbf{Z}}\left(\left(\frac{1+2p}{d}\mathbf{o} - \frac{p}{k}\boldsymbol{\epsilon}\right)\mathbf{w}^T - p\big(\mathbf{I} - \hat{\mathbf{s}}\hat{\mathbf{s}}^T\big)\mathbf{\Sigma}^{-1}\right). \tag{13}$$

With this, $\overline{\mathbf{Y}}$ can be readily computed as $\overline{\mathbf{Y}} = \overline{\mathbf{W}}\,\overline{\mathbf{Z}}$ by Equation (10).

Finally, for D_{ij}, we can avoid potential numerical problems in the case where $\Sigma_{ii} \approx \Sigma_{jj}$ by writing

$$D_{ij} = \frac{\hat{Y}_{ii} - \hat{Y}_{jj}}{\Sigma_{ii} - \Sigma_{jj}} = \left(\frac{\hat{Y}_{ii} - \hat{Y}_{jj}}{\hat{Z}_{ii} - \hat{Z}_{jj}}\right)\left(\frac{\hat{Z}_{ii} - \hat{Z}_{jj}}{\Sigma_{ii} - \Sigma_{jj}}\right). \tag{14}$$

This works as long as both factors can be robustly computed. Consider the first term.

$$\hat{Y}_{ii} = \frac{2\mu \ln \hat{Z}_{ii}}{\hat{Z}_{ii}} + \frac{\lambda \mathrm{tr}(\ln \hat{\mathbf{Z}})}{\hat{Z}_{ii}} \tag{15}$$

$$\hat{Y}_{ii} - \hat{Y}_{jj} = \frac{2\mu(\ln(\hat{Z}_{ii}) - \ln(\hat{Z}_{jj}))}{\hat{Z}_{ii}} - \frac{\lambda \mathrm{tr}(\ln \hat{\mathbf{Z}}) + 2\mu \ln \hat{Z}_{jj}}{\hat{Z}_{ii}\hat{Z}_{jj}}(\hat{Z}_{ii} - \hat{Z}_{jj}) \tag{16}$$

$$\frac{\hat{Y}_{ii} - \hat{Y}_{jj}}{\hat{Z}_{ii} - \hat{Z}_{jj}} = \frac{2\mu}{\hat{Z}_{ii}} \frac{\ln(\hat{Z}_{ii}) - \ln(\hat{Z}_{jj})}{\hat{Z}_{ii} - \hat{Z}_{jj}} - \frac{\lambda \mathrm{tr}(\ln \hat{\mathbf{Z}}) + 2\mu \ln \hat{Z}_{jj}}{\hat{Z}_{ii}\hat{Z}_{jj}} \tag{17}$$

The only term that presents further difficulties is the divided difference on the natural log. This can be computed by noting

$$\frac{\ln(x) - \ln(y)}{x - y} = \frac{1}{y} \frac{\ln(w+1)}{w} \qquad x = (w+1)y \tag{18}$$

$$= \frac{1}{y} \begin{cases} 1 & |w| < \epsilon \\ \mathrm{log1p}(w)/w & |w| \geq \epsilon \end{cases} \tag{19}$$

Here we have made use of the log1p library routine, which is designed to be robust in this case.

The next term that must be considered is the divided difference on $\hat{\mathbf{Z}}$. Following the same general procedure yields

$$\frac{\hat{Z}_{ii} - \hat{Z}_{jj}}{\Sigma_{ii} - \Sigma_{jj}} = \left(1 - \frac{\delta\gamma}{\|\hat{\boldsymbol{\epsilon}}\|_F}\right) \left(\frac{\exp(H_{ii}) - \exp(H_{jj})}{H_{ii} - H_{jj}}\right) \left(\frac{\ln(\Sigma_{ii}) - \ln(\Sigma_{jj})}{\Sigma_{ii} - \Sigma_{jj}}\right). \tag{20}$$

The first term is not a problem, and we have already seen how to handle the last term. For the middle term,

$$\frac{e^x - e^y}{x - y} = e^y \frac{e^w - 1}{w} \qquad x = y + w \tag{21}$$

$$= e^y \begin{cases} 1 & |w| < \epsilon \\ \mathrm{expm1}(w)/w & |w| \geq \epsilon \end{cases} \tag{22}$$

where in this case we have made use of the expm1 library function.

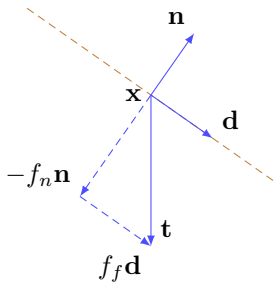
2 Yield surface and plastic flow

In the continuum conception of sand, mechanical interactions are expressed through elasticity, modified with plasticity to model the effects of frictional contact. We use the Drucker-Prager plasticity model, which is built to enforce that shear stresses do not exceed a coefficient times normal stresses in magnitude. In Section 2.1 we detail the connection between Coulomb friction, and the Drucker-Prager stress condition.

The stress condition defines a notion of admissibility for states of stress. In stress space, this is a region whose boundary is often referred to as the yield surface. This places a constraint on the constitutive model defining the mechanical response of the body. The multiplicative decomposition of the deformation gradient into elastic and plastic parts is a means for designing a constitutive model that meets these constraints. For states of stress in the interior of the feasible region, there is no plastic flow since the elastic constitutive model suffices. However, as a state on the boundary of the region (yield surface) is approached, plastic flow will be defined as means of modifying the constitutive model to satisfy the constraints. In Section 3 we derive the plastic flow as a means of satisfying the Drucker-Prager stress constraint.

2.1 Drucker-Prager yield surface derivation

Consider a Coulomb friction interaction between two grains in contact. If $\tilde{\alpha}$ is the coefficient of friction, then the frictional force f_f can only be as large as the coefficient of friction times the normal force f_n: $f_f \leq \tilde{\alpha} f_n$. The Drucker-Prager model generalizes this to a continuum. At any point in the continuum body, the Cauchy stress $\boldsymbol{\sigma}$ expresses the local mechanical interactions in the material. Specifically, at point $\mathbf{x}$, $\boldsymbol{\sigma}(\mathbf{x})$ relates the force per area (or traction) $\mathbf{t}$ that material on one side of an imaginary plane with normal $\mathbf{n}$ exerts on material on the other side, as $\mathbf{t} = \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}$. If we consider this interaction to be from friction, we can use the Coulomb model to relate the frictional force (per area) $f_f = \mathbf{d}^T\mathbf{t}$ to the normal force (per area) $f_n = -\mathbf{n}^T\mathbf{t}$ as $\mathbf{d}^T\mathbf{t} \leq -\tilde{\alpha}\mathbf{n}^T\mathbf{t}$. Here, $\mathbf{d}$ is the normalized projection of the traction $\mathbf{t}$ into the plane orthogonal to $\mathbf{n}$. In terms of $\boldsymbol{\sigma}$, this is expressed as $\mathbf{d}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n} \leq -\tilde{\alpha}\mathbf{n}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n}$.



The frictional force (per area) $f_f = \mathbf{d}^T\mathbf{t}$ is often referred to as the shear stress (at $\mathbf{x}$, in direction $\mathbf{n}$) and the normal force (per area) is often referred to as the normal stress (at $\mathbf{x}$, in direction $\mathbf{n}$). If we consider all shear stresses to arise from friction, then we get a notion of states of stress consistent with the Coulomb model of frictional interaction. That is, we consider the stress field $\boldsymbol{\sigma}(\mathbf{x})$ as admissible (or consistent with the Coulomb model) if

$$\mathbf{d}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n} \leq -\tilde{\alpha}\mathbf{n}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n} \tag{23}$$

for all $\mathbf{x}$ in the material and for arbitrary directions $\mathbf{d}$ and $\mathbf{n}$ with $\mathbf{d}^T\mathbf{n} = 0$.

When the normal stress $\mathbf{n}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n}$ is positive, the material on one side of the imaginary plane is pulling on the material on the other side. This does not arise from a contact/frictional interaction and is a cohesive interaction. Note that Equation (23) implies that in the presence of a positive normal stress, the shear stress would have to be zero. In fact, it can be shown that it is not possible to be consistent with Equation (23) (for all $\mathbf{d}$ and $\mathbf{n}$) with a positive normal stress, and thus cohesion is not possible with this model.

2.1.1 Reformulation of stress admissibility

Consider the two dimensional case and states of stress consistent with Inequality (23). In this case, given normal $\mathbf{n}$, there are only two directions $\mathbf{d}$ orthogonal to it, namely $\mathbf{d} = \pm\mathbf{R}\mathbf{n}$ where

$$\mathbf{R} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{24}$$

In this case, satisfaction of Inequality (23) is achieved when

$$\pm\mathbf{n}^T\mathbf{R}\boldsymbol{\sigma}(\mathbf{x})\mathbf{n} + \tilde{\alpha}\mathbf{n}^T\boldsymbol{\sigma}(\mathbf{x})\mathbf{n} \leq 0 \tag{25}$$

for all directions $\mathbf{n}$. Since the Cauchy stress must be symmetric (by conservation of angular momentum), it has an eigen decomposition

$$\boldsymbol{\sigma} = \mathbf{Q}\mathbf{D}\mathbf{Q}^T = \mathbf{Q}\begin{pmatrix} s_1 & \\ & s_2 \end{pmatrix}\mathbf{Q}^T \tag{26}$$

where $\mathbf{Q}$ is a rotation matrix. Rewriting Inequality (25) in terms of the eigen decomposition gives

$$\pm\mathbf{n}^T\mathbf{R}\mathbf{Q}\mathbf{D}\mathbf{Q}^T\mathbf{n} + \tilde{\alpha}\mathbf{n}^T\mathbf{Q}\mathbf{D}\mathbf{Q}^T\mathbf{n} \leq 0 \tag{27}$$

and since $\mathbf{R}$ and $\mathbf{Q}$ commute (2D rotations commute), satisfaction of Inequality (25) is the same as

$$\tilde{\mathbf{n}}^T\left(\pm\mathbf{R}\mathbf{D} + \tilde{\alpha}\mathbf{D}\right)\tilde{\mathbf{n}} \leq 0 \tag{28}$$

where $\tilde{\mathbf{n}} = \mathbf{Q}\mathbf{n}$ and

$$\mathbf{R}\mathbf{D} = \begin{pmatrix} & -s_2 \\ s_1 & \end{pmatrix}. \tag{29}$$

Since Inequality (28) must be true for all $\tilde{\mathbf{n}}$ and choice of sign, it is equivalent to require that the maximum of

$$F(\tilde{\mathbf{n}}, h) = \tilde{\mathbf{n}}^T \left(h\mathbf{R}\mathbf{D} + \tilde{\alpha}\mathbf{D}\right) \tilde{\mathbf{n}} \tag{30}$$

subject to $\|\tilde{\mathbf{n}}\|^2 = 1$ and $h^2 = 1$, is less than 0. Using the method of Lagrange multipliers it can be shown that this maximum is given by

$$\frac{s_1 + s_2}{2}\tilde{\alpha} + \frac{|s_1 - s_2|}{2}\sqrt{1 + \tilde{\alpha}^2}. \tag{31}$$

Dividing by $\frac{\sqrt{1+\tilde{\alpha}^2}}{\sqrt{2}}$ we obtain that

$$\begin{aligned}(s_1 + s_2)\frac{\tilde{\alpha}}{\sqrt{2}\sqrt{1+\tilde{\alpha}^2}} + \frac{|s_1 - s_2|}{\sqrt{2}} &\leq 0 \\ \operatorname{tr}(\boldsymbol{\sigma}(\mathbf{x}))\alpha + \left\|\boldsymbol{\sigma}(\mathbf{x}) - \frac{\operatorname{tr}(\boldsymbol{\sigma}(\mathbf{x}))}{2}\mathbf{I}\right\|_F &\leq 0\end{aligned} \tag{32}$$

Where $\|\cdot\|_F$ is the Frobenius norm and $\alpha = \frac{\tilde{\alpha}}{\sqrt{2}\sqrt{1+\tilde{\alpha}^2}}$.

If we solve the analogous maximization problem in three dimensions we obtain the Mohr-Coulomb yield surface [3]. However, there is a simple generalization of Inequality (32) that works for both two and three dimensions given by

$$\operatorname{tr}(\boldsymbol{\sigma}(\mathbf{x}))\alpha + \left\|\boldsymbol{\sigma}(\mathbf{x}) - \frac{\operatorname{tr}(\boldsymbol{\sigma}(\mathbf{x}))}{d}\mathbf{I}\right\|_F \leq 0. \tag{33}$$

where d is the number of space dimensions. The Drucker-Prager model uses Inequality (33) in both two and three dimensions, because it is easier to work with than the Mohr-Coulomb model in 3D and it is a decent approximation of Mohr-Coulomb in that case.

In summary, the Drucker-Prager model for the stress field $\boldsymbol{\sigma}$ requires that

$$y(\boldsymbol{\sigma}(\mathbf{x})) \leq 0 \tag{34}$$

for all points $\mathbf{x}$ in the domain occupied by the material, where $y(\boldsymbol{\sigma}) = \operatorname{tr}(\boldsymbol{\sigma})\alpha + \|\boldsymbol{\sigma} - \frac{\operatorname{tr}(\boldsymbol{\sigma})}{d}\mathbf{I}\|_F$ and d is the number of space dimensions. Note that this function is actually defined in terms of the eigenvalues of $\boldsymbol{\sigma}$ as $y(\boldsymbol{\sigma}) = \operatorname{tr}(\mathbf{D})\alpha + \|\mathbf{D} - \frac{\operatorname{tr}(\mathbf{D})}{d}\mathbf{I}\|_F$.

2.2 Kirchhoff stress

The Kirchhoff stress $\boldsymbol{\tau}$ is related to the Cauchy stress $\boldsymbol{\sigma}$ as $\boldsymbol{\tau} = J\boldsymbol{\sigma}$ where $J = \det(\mathbf{F})$ is the determinant of the deformation gradient $\mathbf{F}$. It is often mathematically convenient to express the Drucker-Prager stress condition in terms of this stress measure. We will find this useful when deriving and analyzing properties of the plastic flow. Expressing the Drucker-Prager condition in terms of $\boldsymbol{\tau}$ is simply the requirement that $y(\boldsymbol{\tau}(\mathbf{x})) \leq 0$ for all $\mathbf{x}$ in the domain.

2.3 Yield surface

We can think of the condition $y(\boldsymbol{\tau}) = \operatorname{tr}(\boldsymbol{\tau})\alpha + \|\boldsymbol{\tau} - \frac{\operatorname{tr}(\boldsymbol{\tau})}{d}\mathbf{I}\|_F \leq 0$ as defining a feasible region in stress space. Since the constraint can be evaluated as a function of the principal stresses, we can visualize it as the cone $(\tau_1+\tau_2)\alpha + \frac{|\tau_1-\tau_2|}{\sqrt{2}} \leq 0$ for 2D problems, or the cone $(\tau_1+\tau_2+\tau_3)\alpha + \sqrt{\sum_{j=1}^{3}\left(\tau_j - \sum_{i=1}^{3}\frac{\tau_i}{3}\right)^2} \leq 0$ for 3D problems. The plastic flow will be chosen as a means of satisfying this constraint. When the stress is in the feasible region, there is no plastic flow. However, when the stress reaches the boundary of this region, the plastic flow will be chosen in a manner that prevents the stress from leaving the feasible region. For this reason, the boundary of the feasible region is called the yield surface, since plastic "yield" occurs when the state of stress reaches it.

3 Plastic flow

The plastic flow is characterized by the multiplicative decomposition of the deformation gradient $\mathbf{F} = \mathbf{F}^E\mathbf{F}^P$, however it is convenient for analysis and constitutive modeling to consider evolution of the left elastic Cauchy-Green strain $\mathbf{B}^E = \mathbf{F}^E\mathbf{F}^{E^T} = \mathbf{F}\mathbf{C}^{P^{-1}}\mathbf{F}^T$ where $\mathbf{C}^P = \mathbf{F}^{P^T}\mathbf{F}^P$ is the right plastic Cauchy-Green strain. We will use $\mathbf{l} = \nabla\mathbf{v}$ for brevity throughout. Recalling that the deformation then evolves as $\frac{D\mathbf{F}}{Dt} = \mathbf{l}\mathbf{F}$, $\frac{D\mathbf{B}^E}{Dt} = \mathbf{l}\mathbf{B}^E + \mathbf{B}^E\mathbf{l}^T + \mathbf{F}\frac{D\mathbf{C}^{P^{-1}}}{Dt}\mathbf{F}^T$. The term $\mathbf{F}\frac{D\mathbf{C}^{P^{-1}}}{Dt}\mathbf{F}^T$ is the Lie derivative of the of $\mathbf{B}^E$ with respect to $\mathbf{v}$ so we denote it as $\mathcal{L}_\mathbf{v}\mathbf{B}^E$. The Lie derivative of $\mathbf{B}^E$ is its rate of change independent of deformation in the flow, and it will be determined to define the plastic flow as a means of satisfying the stress feasibility condition in Inequality (34). For example, when the stress is inside the feasible region, $\mathcal{L}_\mathbf{v}\mathbf{B}^E = \mathbf{0}$. However, when the stress is on the yield surface, it will be chosen to guarantee that $\dot{y}(t) \leq 0$, thus preventing any future elastic stresses attaining values outside the feasible region. This can be done in infinitely many ways, however care must be taken to avoid artifacts associated with non-volume preserving plastic flows, as well as to guarantee that the plastic flow increases entropy (or decreases the total energy). To illustrate the different choices of $\mathcal{L}_\mathbf{v}\mathbf{B}^E$ in satisfying stress feasibility, we denote it as $\mathcal{L}_\mathbf{v}\mathbf{B}^E = -\gamma\mathbf{L}$ where $\mathbf{L}$ is an arbitrary matrix. With this view, $\mathbf{L}$ is the direction of the Lie derivative and γ is its magnitude. Given any direction $\mathbf{L}$, we can choose magnitude γ to guarantee that $\dot{y}(t) \leq 0$.

3.1 Effect of plastic flow on stress criteria

Consider how the stress criteria function $y(\boldsymbol{\tau})$ varies with the elastic state as a function of time: $y(\boldsymbol{\tau}(\mathbf{B}^E(t)))$. The plastic flow will effect this evolution via

$$\begin{aligned}\dot{y}(t) &= \frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \frac{D\mathbf{B}^E}{Dt}(t) \\ &= \frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \left(\mathbf{l}\mathbf{B}^E + \mathbf{B}^E\mathbf{l}^T + \mathcal{L}_\mathbf{v}\mathbf{B}^E\right)\end{aligned} \tag{35}$$

Here, the : operator denotes a generalized dot product to express the chain rule when differentiating the composition of scalar and matrix valued functions of matrix argument. The material derivative $\frac{D}{Dt}$ appears in the chain rule because we are considering how y evolves with time for one particle of the continuum. Defining β as the rate of change of y in the absence of plasticity ($\mathcal{L}_\mathbf{v}\mathbf{B}^E = \mathbf{0}$) gives

$$\beta = \frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \left(\mathbf{l}\mathbf{B}^E + \mathbf{B}^E\mathbf{l}^T\right) \tag{36}$$

and using the convention that $\mathcal{L}_\mathbf{v}\mathbf{B}^E = -\gamma\mathbf{L}$ gives

$$\dot{y}(t) = \beta - \gamma\frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \mathbf{L}. \tag{37}$$

When the stress criteria is satisfied, we have $y(\boldsymbol{\tau}(\mathbf{B}^E(t))) < 0$ and there is no plastic flow, ($\mathcal{L}_\mathbf{v}\mathbf{B}^E = \mathbf{0}$). However, when we reach the boundary of the feasible region in stress space, $y(\boldsymbol{\tau}(\mathbf{B}^E(t))) = 0$, then we will leave the region if $\beta > 0$. In this case, we choose γ so that $\dot{y}(t) = 0$. This defines the plastic flow as

$$\mathcal{L}_\mathbf{v}\mathbf{B}^E = \begin{cases} \mathbf{0}, & \text{if } y(\boldsymbol{\tau}(\mathbf{B}^E)) < 0 \text{ or if } y(\boldsymbol{\tau}(\mathbf{B}^E)) = 0 \text{ and } \beta \leq 0 \\ -\gamma\mathbf{L}, & \text{if } y(\boldsymbol{\tau}(\mathbf{B}^E)) = 0 \text{ and } \beta > 0 \end{cases} \tag{38}$$

where γ is chosen as

$$\gamma = \frac{\beta}{\frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \mathbf{L}} \tag{39}$$

3.2 Choosing the direction of the plastic flow

In order to insure that stress never leaves the feasible region, the plastic flow direction $\mathbf{L}$ only needs to have non-zero component $\frac{\partial y}{\partial \boldsymbol{\tau}}(\boldsymbol{\tau}(\mathbf{B}^E(t))) : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E}(\mathbf{B}^E(t)) : \mathbf{L}$. Thus, for a given value of $\mathbf{B}^E$, there are infinitely

many choices of $\mathbf{L}$ that will suffice in preventing stresses outside the feasible region. However, care must be taken to insure that the plastic flow does not decrease the entropy of the system. Or more specifically, that it does not instantaneously increase the rate of change of the total energy and thus violate the second law of thermodynamics [2]. Notably, the rate of change of total energy would be zero in the absence of plasticity so violating this would cause an increase in the total energy. Physically we would expect the plasticity to decrease the total energy over time. We next discuss the choice of $\mathbf{L}$ in light of the entropy concerns.

The total energy $E(t) = KE(t) + PE(t)$ satisfies (see Section 5)

$$E(t+\Delta t) - E(t) = W^{\mathbf{t}}(t, \Delta t) - \int_t^{t+\Delta t} \int_{\Omega^0} \dot{w}^P(\mathbf{X}, s) d\mathbf{X} ds \tag{40}$$

where $W^{\mathbf{t}}(t, \Delta t)$ is the work done by external traction $\mathbf{t}$ boundary conditions and $\dot{w}^P = \boldsymbol{\tau} : \mathbf{l}^P$ where $\mathbf{l}^P = -\frac{1}{2}\mathcal{L}_{\mathbf{v}}\mathbf{B}^E\mathbf{B}^{E^{-1}}$. In the absence of plasticity, the work done by the mechanical stresses is equal to the negative change in the potential, and this leads to exact conservation of energy (minus the effect of the boundary conditions and external forcing). In the case of plasticity, the total energy may go up or down from the work done by the mechanical stress, and this term quantifies that. Specifically, the plastic flow must be designed in a way that ensures non-negative $\dot{w}^P$, otherwise total energy may increase due to plasticity, which would violate the second law of thermodynamics.

The principle of maximum plastic dissipation [1] seeks to design the plastic flow in a way that maximizes $\dot{w}^P$ to respect this concern. This leads to an associative plastic flow where $\mathbf{l}^P = \gamma \frac{\partial y}{\partial \boldsymbol{\tau}}$ or $\mathcal{L}_{\mathbf{v}}\mathbf{B}^E = -2\gamma \frac{\partial y}{\partial \boldsymbol{\tau}}\mathbf{B}^E$. Unfortunately, the choice of matrix $\mathbf{L}$ in $\mathcal{L}_{\mathbf{v}}\mathbf{B}^E = -\gamma\mathbf{L}$ will effect the volume change in the plastic flow. Specifically, it can be shown that if $\mathrm{tr}(\mathbf{L}) = 0$, then the plastic flow will be volume preserving with $J^P = \det(\mathbf{F}^P) = 1$. Since the elastic potential seeks to preserve $\det(\mathbf{F}^E) = 1$ by design, a volume preserving plastic flow will produce an overall flow that tends to preserve volume. However, without $\mathrm{tr}(\mathbf{L}) = 0$ there is a potential for excessive volume loss or gain in the model and indeed simply using $\mathcal{L}_{\mathbf{v}}\mathbf{B}^E = -2\gamma \frac{\partial y}{\partial \boldsymbol{\tau}}\mathbf{B}^E$ will tend to cause excessive volume gain during sheering [3]. However, using the non-associative rule $\mathcal{L}_{\mathbf{v}}\mathbf{B}^E = -\gamma\mathbf{G}\mathbf{B}^E$, with $\mathbf{G} = \frac{\partial y}{\partial \boldsymbol{\tau}} - \frac{1}{d}\mathrm{tr}(\frac{\partial y}{\partial \boldsymbol{\tau}})\mathbf{I}$, the deviatoric part of $\frac{\partial y}{\partial \boldsymbol{\tau}}$, remedies the artifact. Furthermore, we show in Section 7 that the modification still guarantees that $\dot{w}^P$ is non-negative and thus satisfies the second law of thermodynamics. In summary, the plasticity is expressed through $\mathcal{L}_{\mathbf{v}}\mathbf{B}^E$ as

$$\mathcal{L}_{\mathbf{v}}\mathbf{B}^E = \begin{cases} \mathbf{0}, & \text{if } y(\boldsymbol{\tau}(\mathbf{B}^E)) < 0 \text{ or if } y(\boldsymbol{\tau}(\mathbf{B}^E)) = 0 \text{ and } \beta \leq 0 \\ -\gamma\mathbf{G}\mathbf{B}^E, \text{ with } \mathbf{G} = \frac{\partial y}{\partial \boldsymbol{\tau}} - \frac{1}{d}\mathrm{tr}(\frac{\partial y}{\partial \boldsymbol{\tau}})\mathbf{I}, & \text{if } y(\boldsymbol{\tau}(\mathbf{B}^E)) = 0 \text{ and } \beta > 0 \end{cases} \tag{41}$$

where, given $\mathbf{L} = \mathbf{G}\mathbf{B}^E$, γ is defined as in Equation (39).

4 Derivation of return mapping algorithm from plastic flow

The return mapping algorithm is the discrete equivalent to solving for a strain that satisfies the plastic flow rule in Equation (41) and that lies in the Drucker-Prager yield surface. In this section first we outline the method of Simo and Meschke [4] to derive the discrete equations from their continuous versions, and then we show how they can be solved leading to a procedure that computes $\mathbf{Z}(\mathbf{F}^E, \alpha)$. This procedure starts by assuming there is no plastic flow and a return mapping algorithm is derived from the flow equations that shows how to project back to the yield surface if the assumption of no plastic flow is invalid.

Consider the evolution of $\mathbf{B}^E$ from time t^n to time $t^{n+1} = t^n + \Delta t$. We consider this evolution per particle, and thus it is useful to take a Lagrangian view. We outline the notation used in the Lagrangian view in Section 5. Specifically useful here is the flow map $\boldsymbol{\phi} : \Omega^0 \times [0, T] \to \mathbb{R}^d$, and its relation to the deformation gradient $\mathbf{F} = \frac{\partial \boldsymbol{\phi}}{\partial \mathbf{X}}$. Define the time t^n configuration of the material as $\Omega^{t^n} = \left\{\tilde{\mathbf{x}} | \tilde{\mathbf{x}} = \boldsymbol{\phi}(\mathbf{X}, t^n) \text{ for some } \mathbf{X} \in \Omega^0\right\}$ and define $\tilde{\boldsymbol{\phi}} : \Omega^{t^n} \times [t^n, T] \to \mathbb{R}^d$ as $\tilde{\boldsymbol{\phi}}(\tilde{\mathbf{x}}, t) = \boldsymbol{\phi}(\boldsymbol{\phi}^{-1}(\tilde{\mathbf{x}}, t^n), t)$. Intuitively, $\tilde{\boldsymbol{\phi}}$ defines the deformation as if the time t^n configuration Ω^{t^n} of the material is the reference configuration, rather than Ω^0 as in the standard Lagrangian view. This is some times called an updated

Lagrangian view. While the deformation gradient $\mathbf{F}$ defines the deformation from the initial configuration (Ω^0) to the time t configuration (Ω^t), the Jacobian $\tilde{\mathbf{F}} = \frac{\partial \tilde{\boldsymbol{\phi}}}{\partial \tilde{\mathbf{x}}}$ defines the deformation from the time t^n configuration (Ω^{t^n}) to the time t configuration (Ω^t), where $t \geq t^n$. Also these are related as $\mathbf{F} = \tilde{\mathbf{F}}\mathbf{F}^n$, or more precisely $\mathbf{F}(\mathbf{X}, t) = \tilde{\mathbf{F}}(\boldsymbol{\phi}(\mathbf{X}, t^n), t)\mathbf{F}(\mathbf{X}, t^n)$ for all $\mathbf{X} \in \Omega^0$.

Define $\mathbf{B}^{E*} = \tilde{\mathbf{F}}^{-1}\mathbf{B}^E\tilde{\mathbf{F}}^{-T}$. Let us consider the difference between the evolution of $\mathbf{B}^{E*}$ and $\mathbf{B}^E$ in absence of plasticity at time $t^n < t < t^{n+1}$. By the definition of $\mathbf{B}^{E*}$, $\frac{D\mathbf{B}^{E*}}{Dt} = -2\gamma\tilde{\mathbf{F}}^{-1}\mathbf{G}\tilde{\mathbf{F}}\mathbf{B}^{E*}$, therefore in absence of plasticity $\mathbf{B}^{E*}$ is constant since $\frac{D\mathbf{B}^{E*}}{Dt} = \mathbf{0}$. In contrast, $\mathbf{B}^E\big|_t = \tilde{\mathbf{F}}\Big|_t \mathbf{B}^E\big|_{t^n} \tilde{\mathbf{F}}^T\Big|_t$ in the same case. In other words, $\mathbf{B}^{E*}$ is constant along characteristics except for the effect of plasticity, but at the same time $\mathbf{B}^E$ would also be stretched by the flow. This isolation of the plastic part allows for a more intuitive discretization. Specifically, combined with the initial value $\mathbf{B}^{E*}\big|_{t^n} = \mathbf{B}^E\big|_{t^n}$, we can use the exponential approximation $\mathbf{B}^{E*}\big|_{t^{n+1}} \approx \exp(-2\delta\gamma\,\tilde{\mathbf{F}}^{-1}\mathbf{G}\tilde{\mathbf{F}})\Big|_{t^{n+1}} \mathbf{B}^E\big|_{t^n}$ where $\delta\gamma \geq 0$ will be used to enforce the constraint $y(\boldsymbol{\tau}(\mathbf{B}^E\big|_{t^{n+1}})) \leq 0$. Multiplying the approximation by $\tilde{\mathbf{F}}\Big|_{t^{n+1}}$ on the left and $\tilde{\mathbf{F}}^T\Big|_{t^{n+1}}$ on the right, and recalling the definition of $\mathbf{B}^{E*}$, we obtain

$$\begin{aligned}
\mathbf{B}^E\big|_{t^{n+1}} &= \tilde{\mathbf{F}}\Big|_{t^{n+1}} \mathbf{B}^{E*}\big|_{t^{n+1}} \tilde{\mathbf{F}}^T\Big|_{t^{n+1}} \\
&\approx \tilde{\mathbf{F}}\Big|_{t^{n+1}} \exp(-2\delta\gamma\,\tilde{\mathbf{F}}^{-1}\mathbf{G}\tilde{\mathbf{F}})\Big|_{t^{n+1}} \mathbf{B}^E\big|_{t^n} \tilde{\mathbf{F}}^T\Big|_{t^{n+1}} \\
&= \tilde{\mathbf{F}}\Big|_{t^{n+1}} \tilde{\mathbf{F}}^{-1}\Big|_{t^{n+1}} \exp(-2\delta\gamma\,\mathbf{G})|_{t^{n+1}} \tilde{\mathbf{F}}\Big|_{t^{n+1}} \mathbf{B}^E\big|_{t^n} \tilde{\mathbf{F}}^T\Big|_{t^{n+1}} \\
&= \exp(-2\delta\gamma\,\mathbf{G})|_{t^{n+1}} \tilde{\mathbf{F}}\Big|_{t^{n+1}} \mathbf{B}^E\big|_{t^n} \tilde{\mathbf{F}}^T\Big|_{t^{n+1}}.
\end{aligned}$$

Using the notation $\hat{\mathbf{B}}^E = \tilde{\mathbf{F}}\Big|_{t^{n+1}} \mathbf{B}^E\big|_{t^n} \tilde{\mathbf{F}}^T\Big|_{t^{n+1}}$, we are looking for a solution pair $\delta\gamma$ and $\mathbf{B}^E\big|_{t^{n+1}}$ such that

$$\mathbf{B}^E\big|_{t^{n+1}} = \exp\left(-2\delta\gamma\,\mathbf{G}(\boldsymbol{\tau}(\mathbf{B}^E\big|_{t^{n+1}}))\right)\hat{\mathbf{B}}^E, \tag{42}$$

and constraint $y(\boldsymbol{\tau}(\mathbf{B}^E\big|_{t^{n+1}})) \leq 0$ is satisfied. Note that $\hat{\mathbf{B}}^E$ is the elastic strain we would get without the effect of plasticity. For example if $y(\boldsymbol{\tau}(\hat{\mathbf{B}}^E)) \leq 0$, then $\delta\gamma = 0$ and $\mathbf{B}^E\big|_{t^{n+1}} = \hat{\mathbf{B}}^E$ is the trivial solution pair and there is no plastic flow. In this sense, we can see that $\hat{\mathbf{B}}^E$ can be considered as the trial elastic state obtained without any plastic flow. If this does not satisfy the constraint, $\delta\gamma$ and $\mathbf{B}^E\big|_{t^{n+1}}$ must be defined to "project" $\hat{\mathbf{B}}^E$ to $\mathbf{B}^E\big|_{t^{n+1}}$.

We use this process to define the projection $\mathbf{Z}(\mathbf{F}^E, \alpha)$. $\mathbf{F}^E$ is considered the trial elastic state, one obtained in the absence of plastic flow. Thus, $\hat{\mathbf{B}}^E = \mathbf{F}^E\mathbf{F}^{E^T}$ and we seek the solution of Equation 42 to define the projection to $\mathbf{B}^E\big|_{t^{n+1}}$, from which we can determine $\mathbf{Z}(\mathbf{F}^E, \alpha)$. This can be done most easily by considering the singular value decomposition of $\mathbf{F}^E$.

If the singular value decomposition of $\mathbf{F}^E$ is given by $\mathbf{F}^E = \mathbf{U}^E\boldsymbol{\Sigma}^E\mathbf{V}^{E^T}$, then $\hat{\mathbf{B}}^E = \mathbf{F}^E\mathbf{F}^{E^T} = \mathbf{U}^E\boldsymbol{\Sigma}^{E^2}\mathbf{U}^{E^T}$. It can be shown that $\mathbf{U}$ diagonalizes $\mathbf{G}(\boldsymbol{\tau}(\mathbf{B}^E\big|_{t^{n+1}}))$ and $\mathbf{B}^E\big|_{t^{n+1}}$ (i.e. $\mathbf{G}(\boldsymbol{\tau}(\mathbf{B}^E\big|_{t^{n+1}})) = \mathbf{U}^E\hat{\mathbf{G}}(\boldsymbol{\Sigma}^{E,n+1})\mathbf{U}^{E^T}$, and $\mathbf{B}^E\big|_{t^{n+1}} = \mathbf{U}^E\left(\boldsymbol{\Sigma}^{E,n+1}\right)^2\mathbf{U}^{E^T}$), then we may write (42) as

$$\mathbf{U}^E\left(\boldsymbol{\Sigma}^{E,n+1}\right)^2\mathbf{U}^{E^T} = \exp\left(-2\delta\gamma\mathbf{U}^E\hat{\mathbf{G}}(\boldsymbol{\Sigma}^{E,n+1})\mathbf{U}^{E^T}\right)\mathbf{U}^E\boldsymbol{\Sigma}^{E^2}\mathbf{U}^{E^T} = \mathbf{U}^E\exp\left(-2\delta\gamma\hat{\mathbf{G}}(\boldsymbol{\Sigma}^{E,n+1})\right)\boldsymbol{\Sigma}^{E^2}\mathbf{U}^{E^T}. \tag{43}$$

Multiplying both sides of Equation (43) by $\mathbf{U}^{E^T}$ on the left and by $\mathbf{U}^E$ on the right, and taking log results in

$$2\ln\left(\boldsymbol{\Sigma}^{E,n+1}\right) = -2\delta\gamma\hat{\mathbf{G}}(\boldsymbol{\Sigma}^E) + 2\ln\left(\boldsymbol{\Sigma}^E\right). \tag{44}$$

The model that we choose uses the Hencky-strain as a measure of deformation. By defining

$$\boldsymbol{\epsilon}^E := \ln\boldsymbol{\Sigma}^E \quad \text{and} \quad \mathbf{H}^E := \ln\boldsymbol{\Sigma}^{E,n+1}, \tag{45}$$

we may simplify and rearrange Equation (44)

$$\boldsymbol{\epsilon}^E - \mathbf{H}^E = \delta\gamma\hat{\mathbf{G}}. \tag{46}$$

This is our discrete flow rule. In the return mapping algorithm, we want to solve for $\mathbf{H}^E$ satisfies Equation (46) subject to the constraint

$$y(\boldsymbol{\tau}(\mathbf{H}^E)) \leq 0. \tag{47}$$

Solving Equation (46) and (47) can be seen as a ray-cone intersection problem, see Figure 9 in the paper. Before proceeding, we introduce the deviatoric operator to act on matrices:

$$\text{dev}(\mathbf{A}) := \mathbf{A} - \frac{1}{d}\text{tr}(\mathbf{A})\mathbf{I}, \tag{48}$$

i.e. $\text{dev}(\mathbf{A})$ gives the deviatoric part of any arbitrary square matrix $\mathbf{A}$ of size $d \times d$. Equation (46) has no solution if $\text{tr}(\boldsymbol{\epsilon}^E) \geq 0$. In this case the sand is in extension and we project to the tip $\mathbf{H}^E = \mathbf{0}$. We have $\mathbf{G} = \text{dev}(\frac{\partial y}{\partial \boldsymbol{\tau}})$, and $\frac{\partial y}{\partial \boldsymbol{\tau}} = \alpha\mathbf{I} + \frac{\text{dev}(\boldsymbol{\tau})}{\|\text{dev}(\boldsymbol{\tau})\|_F}$, thus $\mathbf{G}$ is simply $\frac{\text{dev}(\boldsymbol{\tau})}{\|\text{dev}(\boldsymbol{\tau})\|_F}$. In principal space this becomes $\hat{\mathbf{G}} = \frac{\text{dev}(\hat{\boldsymbol{\tau}})}{\|\text{dev}(\hat{\boldsymbol{\tau}})\|_F}$, where $\hat{\boldsymbol{\tau}}$ and $\hat{\mathbf{G}}$ are diagonal. From (§6.1) we have $\hat{\boldsymbol{\tau}} = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}^E} = 2\mu\mathbf{H}^E + \lambda\text{tr}(\mathbf{H}^E)\mathbf{I}$ because we use the energy density $\psi(\boldsymbol{\epsilon}^E) = \mu\text{tr}((\boldsymbol{\epsilon}^E)^2) + \frac{1}{2}\lambda\text{tr}(\boldsymbol{\epsilon}^E)^2$. Thus $\hat{\mathbf{G}} = \frac{\text{dev}(\mathbf{H}^E)}{\|\text{dev}(\mathbf{H}^E)\|_F}$. Using Equation (46), we can see that $\text{tr}(\boldsymbol{\epsilon}) = \text{tr}(\mathbf{H}^E)$, since $\text{tr}(\hat{\mathbf{G}}) = 0$. Thus $\text{dev}(\boldsymbol{\epsilon}^E) - \text{dev}(\mathbf{H}^E) = \delta\gamma\frac{\text{dev}(\mathbf{H}^E)}{\|\text{dev}(\mathbf{H}^E)\|_F}$, and collecting like terms we have $\text{dev}(\boldsymbol{\epsilon}^E) = \left(1 + \frac{\delta\gamma}{\|\text{dev}(\mathbf{H}^E)\|_F}\right)\text{dev}(\mathbf{H}^E)$. Thus $\hat{\mathbf{G}} = \frac{\text{dev}(\boldsymbol{\epsilon}^E)}{\|\text{dev}(\boldsymbol{\epsilon}^E)\|_F}$. Then plugging the equation for the ray $\mathbf{H}^E = \boldsymbol{\epsilon}^E - \delta\gamma\frac{\text{dev}(\boldsymbol{\epsilon}^E)}{\|\text{dev}(\boldsymbol{\epsilon}^E)\|_F}$, into the equation for the cone $y(\boldsymbol{\tau}(\mathbf{H}^E)) = \mathbf{0}$, and solving for $\delta\gamma$, we obtain

$$\delta\gamma = \|\text{dev}(\boldsymbol{\epsilon}^E)\|_F + \left(\frac{d\lambda + 2\mu}{2\mu}\right)\text{tr}(\boldsymbol{\epsilon}^E)\alpha. \tag{49}$$

If $\delta\gamma \leq 0$ we intersect the cone from the inside and thus don't need to project and have $\mathbf{H}^E = \boldsymbol{\epsilon}^E$. Otherwise we project to the cone and $\mathbf{H}^E = \boldsymbol{\epsilon}^E - \delta\gamma\hat{\boldsymbol{\epsilon}}^E$. Finally, we return $\mathbf{Z}(\mathbf{F}^E, \alpha) = \mathbf{U}e^{\mathbf{H}^E}\mathbf{V}^T$.

5 Energy and plasticity

Here we discuss the notion of total, kinetic and potential energy in the context of elastoplasticity. It is important to carefully consider the effect the plastic flow will have on the rate of change of total energy. The plastic flow should not increase the rate of change of total energy. Using a hyperelastic constitutive model for the elastic stress implies that the rate of change of total energy in the absence of plasticity will be zero. We take a Lagrangian view of the continuum for these derivations. We define a number of quantities here for completeness but refer the reader to the texts of Gonzalez and Stuart [2] and Bonet and Wood [1] for more detail on Lagrangian and Eulerian descriptions of the continuum.

We use $\boldsymbol{\phi} : \Omega^0 \times [0, T] \to \mathbb{R}^d$ to denote the flow map of the material (where $d = 2$ or 3 is the number of space dimensions). The Lagrangian view identifies particles of the continuum with their initial positions. Ω^0 is the set of all initial positions of particles in the material. We use $\mathbf{X}$ to represent points in Ω^0. We use $\Omega^t = \left\{\mathbf{x} |\ \mathbf{x} = \boldsymbol{\phi}(\mathbf{X}, t) \text{ for some } \mathbf{X} \in \Omega^0\right\}$ to represent the time t configuration of the material. In other words, $\boldsymbol{\phi}(\cdot, t) : \Omega^0 \to \Omega^t$ and $\boldsymbol{\phi}(\mathbf{X}, t)$ is the location of particle $\mathbf{X}$ at time t. Thus $\boldsymbol{\phi}(\mathbf{X}, t)$ is the trajectory of the material point $\mathbf{X}$ over time, and $\mathbf{V}(\mathbf{X}, t) = \frac{\partial \boldsymbol{\phi}}{\partial t}(\mathbf{X}, t)$ is its velocity and $\mathbf{A}(\mathbf{X}, t) = \frac{\partial^2 \boldsymbol{\phi}}{\partial t^2}(\mathbf{X}, t)$ is its acceleration. Note also that the deformation gradient is related to the flow map as $\mathbf{F} = \frac{\partial \boldsymbol{\phi}}{\partial \mathbf{X}}$. The flow map is invertible (a fundamental assumption of continuum mechanics) and its inverse $\boldsymbol{\phi}^{-1}$ can be used to define any function over Ω^0 as a function over Ω^t. For example, the Eulerian velocity is related to the flow map as $\mathbf{v}(\mathbf{x}, t) = \mathbf{V}(\boldsymbol{\phi}^{-1}(\mathbf{x}, t), t)$. We can also define a Lagrangian version of the mass density $R : \Omega^0 \times [0, T] \to \mathbb{R}$ with $R(\mathbf{X}, t) = \rho(\phi(\mathbf{X}, t), t)$ and $\rho(\mathbf{x}, t) = R(\boldsymbol{\phi}^{-1}(\mathbf{x}, t), t)$.

The Lagrangian view presents more options when defining stresses, for example while the Cauchy stress ($\boldsymbol{\sigma}$) relates area weighted normals in the current configuration (Ω^t) to surface tractions, the first Piola-Kirchhoff Stress ($\mathbf{P}$) relates area weighted normals in the initial configuration (Ω^0) to surface tractions. We will use the first Piola-Kirchhoff stress tensor in our discussion of energy.

We can also express the governing equations in the Lagrangian view. Conservation of mass, in the Lagrangian view is

$$R(\mathbf{X},t)J(\mathbf{X},t) = R(\mathbf{X},0), \quad \mathbf{X} \in \Omega^0,\ t \in [0,T] \tag{50}$$

where recall that $J(\mathbf{X},t) = \det(\mathbf{F}(\mathbf{X},t))$. Conservation of linear momentum results in force density balance

$$R(\mathbf{X},0)\mathbf{A}(\mathbf{X},t) = \nabla^{\mathbf{X}} \cdot \mathbf{P}(\mathbf{X},t), \quad \mathbf{X} \in \Omega^0,\ t \in [0,T]. \tag{51}$$

Note that this equation has units of force density but is otherwise just Newton's second law generalized to the continuum.

5.1 Work done by elastic deformation

The work done by the elastic forces (W^e) is defined to be (see [1])

$$W^e(T) = \int_0^T \int_{\Omega^0} P_{ij,j} V_i d\mathbf{X} dt. \tag{52}$$

Here we use the convention that $P_{ij,k}$ represents $\frac{\partial P_{ij}}{\partial X_k}$ and unless otherwise stated, we use the Einstein summation conventions where repeated indices are summed over their ranges. With this in mind, the work can be rewritten by using integration by parts, this satisfies

$$\int_0^T \int_{\Omega^0} P_{ij,j} V_i d\mathbf{X} dt = \int_0^T \int_{\Omega^0} (P_{ij}V_i)_{,j} - P_{ij}V_{i,j} d\mathbf{X} dt = \int_0^T \int_{\partial\Omega^0} t_i V_i dS(\mathbf{X}) - \int_{\Omega^0} P_{ij}V_{i,j} d\mathbf{X} dt \tag{53}$$

where $t_i = P_{ij}N_j$ is the applied traction boundary condition. Now since

$$\frac{d}{dt}\int_{\Omega^0} \psi(\mathbf{F}(\mathbf{X},t)) d\mathbf{X} = \int_{\Omega^0} \frac{d\psi}{dF_{ij}}(\mathbf{F}(\mathbf{X},t)) V_{i,j}(\mathbf{X},t) d\mathbf{X} = \int_{\Omega^0} P_{ij}V_{i,j} d\mathbf{X} \tag{54}$$

we can say

$$\begin{aligned} W^e(T) &= W^{\mathbf{t}}(T) - \int_0^T \frac{d}{dt}\int_{\Omega^0} \psi(\mathbf{F}(\mathbf{X},t)) d\mathbf{X} dt \\ &= W^{\mathbf{t}}(T) - \int_{\Omega^0} \psi(\mathbf{F}(\mathbf{X},T)) d\mathbf{X} + \int_{\Omega^0} \psi(\mathbf{F}(\mathbf{X},0)) d\mathbf{X} \\ &= W^{\mathbf{t}}(T) - PE(T) + PE(0) \end{aligned}$$

where $W^t(T) = \int_0^T \int_{\partial\Omega^0} t_i V_i dS(\mathbf{X}) dt$ is defined to be the work done by the boundary forces and $PE(t)$ is the elastic potential at time t. The kinetic energy $KE(t)$ is

$$KE(t) = \int_{\Omega_0} \frac{1}{2}\mathbf{V}(\mathbf{X},t)^T \big(R(\mathbf{X},0)\mathbf{V}(\mathbf{X},t)\big) d\mathbf{X} \tag{55}$$

The rate of change of kinetic energy density is:

$$\frac{d}{dt}\left[\frac{1}{2}\mathbf{V}(\mathbf{X},t)^T \big(R(\mathbf{X},0)\mathbf{V}(\mathbf{X},t)\big)\right] = R(\mathbf{X},0)\mathbf{A}(\mathbf{X},t) \cdot \mathbf{V}(\mathbf{X},t) \tag{56}$$

and assuming

$$R(\mathbf{X},0)\mathbf{A}(\mathbf{X},t) = \nabla^{\mathbf{X}} \cdot \mathbf{P} \tag{57}$$

we get

$$\int_0^T \int_{\Omega_0} \frac{d}{dt}\left[\frac{1}{2}\mathbf{V}(\mathbf{X},t)^T \big(R(\mathbf{X},0)\mathbf{V}(\mathbf{X},t)\big)\right] d\mathbf{X} dt = KE(T) - KE(0) = W^e \tag{58}$$

and also

$$KE(T) - KE(0) + PE(T) - PE(0) = W^{\mathbf{t}}(T) \tag{59}$$

5.2 Plastic flow rate and potential

With plasticity we have $\mathbf{F} = \mathbf{F}^E\mathbf{F}^P$ and $\dot{\mathbf{F}} = \dot{\mathbf{F}}^E\mathbf{F}^P + \mathbf{F}^E\dot{\mathbf{F}}^P$. Also,

$$\dot{\mathbf{F}}^E = \dot{\mathbf{F}}\mathbf{F}^{P^{-1}} - \mathbf{F}^E\dot{\mathbf{F}}^P\mathbf{F}^{P^{-1}} \tag{60}$$

etc. The elastic potential energy is defined as

$$PE(t) = \int_{\Omega_0} \psi(\mathbf{F}^E(\mathbf{X},t))d\mathbf{X} \tag{61}$$

and its rate of change is

$$\begin{aligned}\frac{d}{dt}PE(t) &= \int_{\Omega_0} \frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E(\mathbf{X},t))\dot{F}^E_{ij}(\mathbf{X},t)d\mathbf{X} \\ &= \int_{\Omega_0} \frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E)F^{P^{-T}}_{jk}\dot{F}_{ik} - F^{E^T}_{ki}\frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E)F^{P^{-T}}_{jl}\dot{F}^P_{kl}d\mathbf{X}.\end{aligned}$$

The integral above motivates the definition of the first Piola-Kirchhoff Stress in the presence of plasticity as $P_{ik} = \frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E)F^{P^{-T}}_{jk}$ or

$$\mathbf{P}(\mathbf{X},t) = \frac{\partial\psi}{\partial\mathbf{F}}(\mathbf{F}^E(\mathbf{X},t))\mathbf{F}^{P^{-T}}(\mathbf{X},t). \tag{62}$$

With this definition, the work done by the mechanical forces is

$$\begin{aligned}W^e(T) &= \int_0^T\int_{\Omega_0} P_{ij,j}(\mathbf{X},t)V_i(\mathbf{X},t)d\mathbf{X}dt \\ &= W^{\mathbf{t}}(T) - \int_0^T\int_{\Omega_0}\frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E)\dot{F}_{ik}F^{P^{-T}}_{jk}d\mathbf{X}dt\end{aligned}$$

5.3 Stress power density

Define the stress power density as

$$\dot{w}(\mathbf{X},t) = \tau_{ij}(\mathbf{X},t)l_{ij}(\mathbf{X},t) = P_{ij}(\mathbf{X},t)\dot{F}_{ij}(\mathbf{X},t) \tag{63}$$

with $\mathbf{l} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ and $\boldsymbol{\tau} = J\boldsymbol{\sigma} = \mathbf{P}\mathbf{F}^T$. Also define

$$\dot{w}^e(\mathbf{X},t) = \tau_{ij}(\mathbf{X},t)l^e_{ij}(\mathbf{X},t) = \frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E(\mathbf{X},t))\dot{F}^E_{ij}(\mathbf{X},t) \tag{64}$$

with $\mathbf{l}^E = \dot{\mathbf{F}}^E\mathbf{F}^{E^{-1}}$. $\dot{w}^e(\mathbf{X},t)$ is then the rate of change in elastic potential density since

$$\frac{d}{dt}PE(t) = \int_{\Omega_0}\frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E(\mathbf{X},t))\dot{F}^E_{ij}(\mathbf{X},t)d\mathbf{X} = \int_{\Omega_0}\dot{w}^e(\mathbf{X},t)d\mathbf{X} \tag{65}$$

Next, defining

$$\dot{w}^p(\mathbf{X},t) = F^{E^T}_{ki}\frac{\partial\psi}{\partial F_{ij}}(\mathbf{F}^E)F^{P^{-T}}_{jl}\dot{F}^P_{kl} = P_{il}F^E_{ik}\dot{F}^P_{kl} \tag{66}$$

gives

$$\dot{w}(\mathbf{X},t) = \dot{w}^e(\mathbf{X},t) + \dot{w}^p(\mathbf{X},t). \tag{67}$$

The term $\mathbf{F}^E\dot{\mathbf{F}^P}$ is referred to as the plastic rate of deformation [1]. The work can then expressed as

$$W^e(T) = \int_0^T\int_{\partial\Omega^0} t_iV_idS(\mathbf{X}) - \int_{\Omega^0}P_{ij}V_{i,j}d\mathbf{X}dt = W^{\mathbf{t}}(T) - \int_0^T\int_{\Omega_0}\dot{w}^e(\mathbf{X},t) + \dot{w}^p(\mathbf{X},t)d\mathbf{X}dt \tag{68}$$

and then also

$$KE(T) - KE(0) = W^{\mathbf{t}}(T) - \int_0^T \int_{\Omega_0} \dot{w}^e(\mathbf{X},t) + \dot{w}^p(\mathbf{X},t) d\mathbf{X} dt$$
$$= W^{\mathbf{t}}(T) - PE(T) + PE(0) - \int_0^T \int_{\Omega_0} \dot{w}^p(\mathbf{X},t) d\mathbf{X} dt$$

and thus

$$KE(T) - KE(0) + PE(T) - PE(0) = W^{\mathbf{t}}(T) - \int_0^T \int_{\Omega_0} \dot{w}^p(\mathbf{X},t) d\mathbf{X} dt. \tag{69}$$

This motivates why $\dot{w}^p(\mathbf{X},t)$ is often referred to as "plastic dissipation rate".

6 Hencky Strain Derivative Lemma

Consider symmetric positive definite matrix $\mathbf{B} \in \mathbb{R}^{d\times d}$ with $d = 2$ or 3. Use $\mathbf{B} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ to denote the eigenvalue decomposition of $\mathbf{B}$ where $\mathbf{\Lambda}$ is diagonal and positive definite. Define $\boldsymbol{\epsilon}(\mathbf{B}) = \frac{1}{2}\ln(\mathbf{B}) = \mathbf{U}\ln(\mathbf{\Lambda}^{\frac{1}{2}})\mathbf{U}^T$. For example if $\mathbf{B} = \mathbf{F}\mathbf{F}^T$, then $\boldsymbol{\epsilon}$ is the Hencky strain. We can also write $\mathbf{B}(\boldsymbol{\epsilon}) = e^{2\boldsymbol{\epsilon}}$.

Lemma: Suppose that $f(\mathbf{B})$ is a scalar function of $\mathbf{B}$ which is invariant under coordinate changes, and $\hat{f}(\boldsymbol{\epsilon}) = f(\mathbf{B}(\boldsymbol{\epsilon}))$, then $\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}} = 2\frac{\partial f}{\partial \mathbf{B}}\mathbf{B}$.

Proof: First note that $\hat{f}$ will also be invariant under coordinate change and therefore can be written as a function of the invariants of $\boldsymbol{\epsilon}$. That is $\hat{f}(\boldsymbol{\epsilon}) = \tilde{f}(I_1, I_2, I_3)$. This means we have $\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}} = \frac{\partial \tilde{f}}{\partial I_1}\frac{\partial I_1}{\partial \boldsymbol{\epsilon}} + \frac{\partial \tilde{f}}{\partial I_2}\frac{\partial I_2}{\partial \boldsymbol{\epsilon}} + \frac{\partial \tilde{f}}{\partial J}\frac{\partial J}{\partial \boldsymbol{\epsilon}}$ where $\frac{\partial I_1}{\partial \boldsymbol{\epsilon}} = \mathbf{I}$, $\frac{\partial I_2}{\partial \boldsymbol{\epsilon}} = I_1\mathbf{I} - \boldsymbol{\epsilon}^T$, $\frac{\partial J}{\partial \boldsymbol{\epsilon}} = J\boldsymbol{\epsilon}^{-T}$. Therefore, if $\boldsymbol{\epsilon}$ is diagonal then $\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}$ will be as well. Note that from frame invariance we have $\hat{f}(\boldsymbol{\epsilon}) = \hat{f}(\mathbf{R}^T\boldsymbol{\epsilon}\mathbf{R})$ for any rotation $\mathbf{R}$. Which means

$$\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}} : \delta\boldsymbol{\epsilon} = \left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\mathbf{R}^T\boldsymbol{\epsilon}\mathbf{R}} : \mathbf{R}^T\delta\boldsymbol{\epsilon}\mathbf{R}$$
$$\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}} : \delta\boldsymbol{\epsilon} = \mathbf{R}\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\mathbf{R}^T\boldsymbol{\epsilon}\mathbf{R}} \mathbf{R}^T : \delta\boldsymbol{\epsilon}$$
$$\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}} = \mathbf{R}\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\mathbf{R}^T\boldsymbol{\epsilon}\mathbf{R}} \mathbf{R}^T$$
$$\mathbf{R}\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}} \mathbf{R}^T = \left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\mathbf{R}^T\boldsymbol{\epsilon}\mathbf{R}}$$

Plugging in $\mathbf{R} = \mathbf{U}$ we have $\mathbf{U}\left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\boldsymbol{\epsilon}}\mathbf{U}^T = \left.\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\right|_{\mathbf{U}^T\boldsymbol{\epsilon}\mathbf{U}}$ and is therefore diagonal.

Deriving

$$\frac{\partial f}{\partial \mathbf{B}} : \delta\mathbf{B} = \frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}} : \delta\boldsymbol{\epsilon}$$
$$= \mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U} : \mathbf{U}^T\delta\boldsymbol{\epsilon}\mathbf{U}$$
$$= \mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U} : \mathrm{diag}(\mathbf{U}^T\delta\boldsymbol{\epsilon}\mathbf{U})$$

From $\boldsymbol{\epsilon} = \frac{1}{2}\mathbf{U}\log(\boldsymbol{\Lambda})\mathbf{U}^T$ we have

$$\begin{aligned}\delta\boldsymbol{\epsilon} &= \frac{1}{2}(\delta\mathbf{U}\log(\boldsymbol{\Lambda})\mathbf{U}^T + \mathbf{U}\delta\boldsymbol{\Lambda}\boldsymbol{\Lambda}^{-1}\mathbf{U}^T + \mathbf{U}\log(\boldsymbol{\Lambda})\delta\mathbf{U}^T)\\ \mathbf{U}^T\delta\boldsymbol{\epsilon}\mathbf{U} &= \frac{1}{2}(\mathbf{U}^T\delta\mathbf{U}\log(\boldsymbol{\Lambda}) + \delta\boldsymbol{\Lambda}\boldsymbol{\Lambda}^{-1} + \log(\boldsymbol{\Lambda})\delta\mathbf{U}^T\mathbf{U})\end{aligned}$$

Since $\mathbf{U}$ is orthonormal $\mathbf{U}^T\delta\mathbf{U}$ is skew and therefore $\mathrm{diag}(\mathbf{U}^T\delta\boldsymbol{\epsilon}\mathbf{U}) = \mathrm{diag}(\delta\boldsymbol{\Lambda})\boldsymbol{\Lambda}^{-1}$. Similarly from $\mathbf{B} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$ we have $\mathrm{diag}(\mathbf{U}^T\delta\mathbf{B}\mathbf{U}) = \frac{1}{2}\mathrm{diag}(\delta\boldsymbol{\Lambda})$. Continuing the derivation we have

$$\begin{aligned}\frac{\partial f}{\partial \mathbf{B}} : \delta\mathbf{B} &= \frac{1}{2}\mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U} : \mathrm{diag}(\delta\boldsymbol{\Lambda})\boldsymbol{\Lambda}^{-1}\\ &= \frac{1}{2}\mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U} : \mathrm{diag}(\mathbf{U}^T\delta\mathbf{B}\mathbf{U})\boldsymbol{\Lambda}^{-1}\\ &= \frac{1}{2}\mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U}\boldsymbol{\Lambda}^{-1} : \mathrm{diag}(\mathbf{U}^T\delta\mathbf{B}\mathbf{U})\\ &= \frac{1}{2}\mathbf{U}^T\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U}\boldsymbol{\Lambda}^{-1} : \mathbf{U}^T\delta\mathbf{B}\mathbf{U}\\ &= \frac{1}{2}\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{U}\boldsymbol{\Lambda}^{-1}\mathbf{U}^T : \delta\mathbf{B}\\ &= \frac{1}{2}\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{B}^{-1} : \delta\mathbf{B}\end{aligned}$$

Thus $\frac{\partial f}{\partial \mathbf{B}} = \frac{1}{2}\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}}\mathbf{B}^{-1}$ which yields $\frac{\partial \hat{f}}{\partial \boldsymbol{\epsilon}} = 2\frac{\partial f}{\partial \mathbf{B}}\mathbf{B}$.

6.1 The relationship between $\boldsymbol{\tau}$ and $\boldsymbol{\epsilon}$

Claim: For any isotropic constitutive model ψ, $\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}}$.

Proof: We have

$$\begin{aligned}\mathbf{P} &= \frac{\partial \psi}{\partial \mathbf{F}}\\ \mathbf{P} &= \frac{\partial \tilde{\psi}}{\partial \mathbf{B}}\mathbf{F} + \mathbf{F}^T\frac{\partial \tilde{\psi}}{\partial \mathbf{B}}\\ \mathbf{P} &= 2\frac{\partial \tilde{\psi}}{\partial \mathbf{B}}\mathbf{F}\\ \mathbf{P}\mathbf{F}^T &= 2\frac{\partial \tilde{\psi}}{\partial \mathbf{B}}\mathbf{F}\mathbf{F}^T\\ \boldsymbol{\tau} &= 2\frac{\partial \tilde{\psi}}{\partial \mathbf{B}}\mathbf{B}.\end{aligned}$$

By the Hencky strain derivative lemma applied to $\tilde{\psi}(\mathbf{B})$ we have $\boldsymbol{\tau} = \frac{\partial \psi}{\partial \boldsymbol{\epsilon}}$.

7 Plastic Dissipation is Nonnegative

Recall that we have previously defined $\mathbf{s} = \boldsymbol{\tau} - \frac{1}{d}\mathrm{tr}(\boldsymbol{\tau})$, and that $\mathbf{G} = \frac{\partial y}{\partial \boldsymbol{\tau}} - \frac{1}{d}\mathrm{tr}(\frac{\partial y}{\partial \boldsymbol{\tau}})\mathbf{I}$, i.e. it satisfies $\mathbf{G} = -\gamma \mathcal{L}_{\mathbf{v}} \mathbf{B}^E \mathbf{B}^{E^{-1}}$ (e.g. see Section (§3.2)). Therefore

$$\begin{aligned}
\dot{w}^P &= \boldsymbol{\tau} : \mathbf{l}^P \\
&= -\boldsymbol{\tau} : \frac{1}{2}\mathcal{L}_{\mathbf{v}} \mathbf{B}^E \mathbf{B}^{E^{-1}} \\
&= \gamma \boldsymbol{\tau} : \mathbf{G} \\
&= \frac{\gamma}{\|\mathbf{s}\|_F} \boldsymbol{\tau} : \mathbf{s} \\
&= \frac{\gamma}{\|\mathbf{s}\|_F} \left(\mathbf{s} + \frac{1}{d}\mathrm{tr}(\boldsymbol{\tau})\mathbf{I} \right) : \mathbf{s} \\
&= \gamma \|\mathbf{s}\|_F .
\end{aligned}$$

Thus all that remains to prove is that $\gamma \geq 0$. To do this we use the constraint that $\frac{\partial y}{\partial t} \leq 0$ when $y = 0$.

$$\begin{aligned}
\frac{\partial y}{\partial t} &= \frac{\partial y}{\partial \boldsymbol{\tau}} : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E} : \dot{\mathbf{B}}^E \\
&= \frac{\partial y}{\partial \boldsymbol{\tau}} : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E} : \left(\mathbf{l}\mathbf{B}^E + \mathbf{B}^E \mathbf{l}^T - 2\gamma \frac{\partial y}{\partial \boldsymbol{\tau}} \mathbf{B}^E \right) \\
&= \underbrace{\frac{\partial y}{\partial \boldsymbol{\tau}} : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E} : \left(\mathbf{l}\mathbf{B}^E + \mathbf{B}^E \mathbf{l}^T \right)}_{\eta} - 2\gamma \underbrace{\frac{\partial y}{\partial \boldsymbol{\tau}} : \frac{\partial \boldsymbol{\tau}}{\partial \mathbf{B}^E} : \left(\frac{\partial y}{\partial \boldsymbol{\tau}} \mathbf{B}^E \right)}_{\nu} .
\end{aligned}$$

So

$$0 = \eta - 2\gamma\nu \Longrightarrow \gamma = \frac{\eta}{2\nu}$$

Note that η is what $\frac{\partial y}{\partial t}$ would be in the absence of plastic flow. Thus if $\eta \leq 0$ the material is deforming in such a way that the yield function is going down, and therefore is undergoing elastic deformation which means $\gamma = 0$. Otherwise $\eta > 0$ and

$$\begin{aligned}
\nu &= \frac{\partial y}{\partial \mathbf{B}^E} : \left(2\frac{\mathbf{s}}{\|\mathbf{s}\|_F} \mathbf{B}^E \right) \\
&= 2\frac{\partial y}{\partial \mathbf{B}^E} \mathbf{B}^E : \frac{\mathbf{s}}{\|\mathbf{s}\|_F} .
\end{aligned}$$

Applying the Hencky strain derivative lemma to y we have

$$\begin{aligned}
\nu &= \frac{\partial y}{\partial \boldsymbol{\epsilon}^E} : \frac{\mathbf{s}}{\|\mathbf{s}\|_F} \\
&= \frac{\partial y}{\partial \boldsymbol{\tau}} : \frac{\partial \boldsymbol{\tau}}{\partial \boldsymbol{\epsilon}^E} : \frac{\mathbf{s}}{\|\mathbf{s}\|_F} \\
&= \left(\frac{\mathbf{s}}{\|\mathbf{s}\|} + \tilde{\eta}\mathbf{I} \right) : \mathbb{C} : \frac{\mathbf{s}}{\|\mathbf{s}\|_F} \\
&= 2\mu \|\mathbf{s}\|_F .
\end{aligned}$$

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