Elasto-Viscoplastic Constitutive Scheme Including Isotropic and Kinematic Hardening

Aaditya Lakshmanan

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Nomenclature

$\boldsymbol{\sigma}$	Cauchy stress tensor
$\Delta\gamma^{\alpha}$	Locally converged signed slip increment corresponding to slip system α
$\boldsymbol{E^e}$	Locally converged elastic Green-Lagrange strain tensor
$\boldsymbol{F}$	Locally converged[a] deformation gradient
$\boldsymbol{F^e}$	Locally converged elastic part of deformation gradient
$\boldsymbol{F^e}(t)$	Globally converged[b] elastic part of deformation gradient
$\boldsymbol{F^p}$	Locally converged plastic part of deformation gradient
$\boldsymbol{F^p}(t)$	Globally converged plastic part of deformation gradient
$\dot{\gamma}^{\alpha}$	Slip rate on slip system α
$\boldsymbol{P}$	First Piola-Kirchoff stress tensor
$\boldsymbol{S_0^{\alpha}}$	Schmid tensor in undeformed configuration corresponding to slip system α
s^{α}	Locally converged slip resistance corresponding to slip system α
$s^{\alpha}(t)$	Globally converged slip resistance corresponding to slip system α
$\boldsymbol{T}$	Stress conjugate to Green-Lagrange elastic strain
w^{α}	Locally converged backstress on slip system α
$w^{\alpha}(t)$	Globally converged backstress on slip system α
$h_{\alpha\beta}$	Hardening coefficient determined by the interactions of the slip system pair (α, β)
$q_{\alpha\beta}$	Strength of interaction corresponding to slip system pair (α, β)

[a]Here locally converged refers to the value obtained after convergence of the local constitutive model alone
[b]Here globally converged refers to the value obtained after convergence of the global FE incremental problem

Single Crystal Constitutive Model

Here the constitutive scheme is outlined for a single crystal with isotropic and kinematic hardening. We begin with the following postulates as sufficient ingredients for a description of single crystal elasto-viscoplasticity within the framework of continuum mechanics :

1. Multiplicative decomposition of deformation gradient

$$\boldsymbol{F} = \boldsymbol{F^e}\boldsymbol{F^p} \tag{1}$$

2. Generalized Hooke's Law

$$\boldsymbol{T} = \mathcal{L} \cdot \boldsymbol{E^e} = \frac{1}{2}\mathcal{L} \cdot (\boldsymbol{F^{e}}^T\boldsymbol{F^e} - \boldsymbol{I}) \tag{2}$$

3. Plastic Kinematic Relation

$$\boldsymbol{L^p} = \dot{\boldsymbol{F^p}}\boldsymbol{F^{p-1}} = \sum_{\alpha=1}^{n_s} \dot{\gamma}^\alpha \boldsymbol{S_0^\alpha} \tag{3}$$

4. Phenomenological Viscoplastic Power Law

$$\tau^\alpha := \boldsymbol{T} : \boldsymbol{S_0^\alpha} \ ; \ \dot{\gamma}^\alpha = \dot{\gamma}^0 \left(\frac{\left|\tau^\alpha - w^\alpha\right|}{s^\alpha} \right)^m \operatorname{sign}(\tau^\alpha) \tag{4}$$

5. Isotropic Hardening Law

$$\dot{s^\alpha} = \sum_{\alpha=1}^{n_s} q_{\alpha\beta} h_0 \left(1 - \frac{s^\beta}{s^s}\right)^a \left|\dot{\gamma}^\beta\right| \tag{5}$$

6. Ohno-Wang Backstress Evolution Law

$$\dot{w_i^\alpha} = h_i \dot{\gamma}^\alpha - r_i \left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha \left|\dot{\gamma}^\alpha\right| \ , \quad (i = 1, 2) \ ; \ w^\alpha = \sum_{i=1}^{2} w_i^\alpha \tag{6}$$

Incremental Constitutive Model

We start with Eqn. (3) whose implicit time discretization yields

$$\dot{\boldsymbol{F^p}} = \left(\sum_{\alpha=1}^{n_s} \dot{\gamma}^\alpha \boldsymbol{S_0^\alpha}\right) \boldsymbol{F^p} \implies \boldsymbol{F^p} \approx \exp\left(\sum_{\alpha=1}^{n_s} \Delta\gamma^\alpha \boldsymbol{S_0^\alpha}\right) \boldsymbol{F^p}(t) \tag{7}$$

where $\approx$ is used to denote a reasonable approximation, $\Delta\gamma^\alpha = \dot{\gamma}^\alpha \Delta t$ and $\exp(\cdot)$ denotes the matrix exponential defined using a power series(Appendix A). The elastic constitutive law reads

$$\begin{aligned} \boldsymbol{T} &= \frac{1}{2}\mathcal{L} \cdot \left(\boldsymbol{F^{e}}^T\boldsymbol{F^e} - \boldsymbol{I}\right) = \frac{1}{2}\mathcal{L} \cdot \left(\boldsymbol{F^{p-T}}\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{F^{p-1}} - \boldsymbol{I}\right) \\ &= \frac{1}{2}\mathcal{L} \cdot \left(\exp\left(\sum_{\alpha=1}^{n_s} -\Delta\gamma^\alpha \boldsymbol{S_0^{\alpha T}}\right) \boldsymbol{A} \exp\left(\sum_{\alpha=1}^{n_s} -\Delta\gamma^\alpha \boldsymbol{S_0^\alpha}\right) - \boldsymbol{I}\right) \end{aligned} \tag{8}$$

where $\boldsymbol{A} := \boldsymbol{F^{p-T}}(t)\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{F^{p-1}}(t)$.The implicit time-discretized version of the isotropic hardening law reads

$$s^\alpha = s^\alpha(t) + \sum_{i=1}^{n_s} q_{\alpha\beta} h_0 \left(1 - \frac{s^\beta}{s^s}\right)^a \left|\Delta\gamma^\beta\right| \tag{9}$$

The implicit time-discretized version of the Ohno-Wang backstress model reads

$$w_i^\alpha = w_i^\alpha(t) + h_i \Delta\gamma^\alpha - r_i \left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha |\Delta\gamma^\alpha| \ , \quad (i = 1, 2) \ ; \ w^\alpha = \sum_{i=1}^{2} w_i^\alpha \tag{10}$$

Knowing that the slip increments on all the slip systems are expressed in terms of $\boldsymbol{T}$ and w^α via Eqn. (31), we end up with following nonlinear system of equations

$$\boldsymbol{R_T} = \boldsymbol{T} - \frac{1}{2}\mathcal{L} \cdot \left(\exp\left(\sum_{\alpha=1}^{n_s} -\Delta\gamma^\alpha(\boldsymbol{T}, \boldsymbol{w}, \boldsymbol{s}) \boldsymbol{S_0^{\alpha T}}\right) \boldsymbol{A} \exp\left(\sum_{\alpha=1}^{n_s} -\Delta\gamma^\alpha(\boldsymbol{T}, \boldsymbol{w}, \boldsymbol{s}) \boldsymbol{S_0^{\alpha}}\right) - \boldsymbol{I} \right) = 0 \tag{11}$$

$$\boldsymbol{R}_w^{\alpha,i} = w_i^\alpha - w_i^\alpha(t) - h_i \Delta\gamma^\alpha(\boldsymbol{T}, \boldsymbol{w}, \boldsymbol{s}) + r_i \left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha |\Delta\gamma^\alpha(\boldsymbol{T}, \boldsymbol{w}, \boldsymbol{s})| = 0 \ , \ \ (i = 1, 2) \tag{12}$$

$$\boldsymbol{R}_s^\alpha = s^\alpha - s^\alpha(t) - \sum_{i=1}^{n_s} q_{\alpha\beta} h_0 \left(1 - \frac{s^\beta}{s^s}\right)^a \left|\Delta\gamma^\beta(\boldsymbol{T}, \boldsymbol{w}, \boldsymbol{s})\right| = 0 \tag{13}$$

where $\boldsymbol{w}$ denotes a vector comprising the $2n_s$ backstress components and $\boldsymbol{s}$ denotes a vector comprising the n_s slip resistances . Eqns. (11)-(13) form a total of $3n_s + 6$ equations in $3n_s + 6$ variables, whose solution we wish to obtain numerically. The numerical scheme is outlined next.

Solution to Nonlinear System

We first separate the system of $3n_s + 6$ equations into two sets - (i) involving $\boldsymbol{T}$ and $\boldsymbol{w}$ which forms $2n_s + 6$ equations, and (ii) involving $\boldsymbol{s}$ which forms n_s equations. First, values of slip resistance on all n_s slip systems are specified, which are updated iteratively as well(discussed later). Let the vector of slip resistances corresponding to the j^{th} iteration be denoted by $\boldsymbol{s}^j$. Then keeping $\boldsymbol{s}^j$ fixed, Eqns. (11)-(12) are solved using the Newton's method augmented with a cubic line search algorithm[Pre+88]. Let $[\boldsymbol{T}^n, \boldsymbol{w}^n]$ denote the estimate of the stress and backstresses at the n^{th} Newton iteration. The residual for the $(n+1)^{th}$ Newton iteration is then computed by evaluating Eqns. (11) - (12) at $[\boldsymbol{T}^n, \boldsymbol{w}^n]$. The Jacobian matrix comprises the partial derivative of the residual relative to $[\boldsymbol{T}, \boldsymbol{w}]$ evaluated at $[\boldsymbol{T}^n, \boldsymbol{w}^n]$, resulting in a $(2n_s + 6) \times$

$(2n_s+6)$ matrix, whose submatrices take the following form

$$\left.\frac{\partial \boldsymbol{R_T}}{\partial \boldsymbol{T}}\right|_{\boldsymbol{T}^n,\boldsymbol{w}^n} = \mathcal{I}_s + \sum_{\alpha=1}^{n_s}(\mathcal{L}\cdot \boldsymbol{C}^{\alpha,n,j})\otimes(\kappa_n^\alpha \boldsymbol{M}^\alpha) \;\; ; \;\; \left.\frac{\partial \boldsymbol{R_T}}{\partial w_i^\alpha}\right|_{\boldsymbol{T}^n,\boldsymbol{w}^n} = -\kappa_n^\alpha \mathcal{L}\cdot \boldsymbol{C}^{\alpha,n,j} \tag{14}$$

$$\boldsymbol{M}^\alpha := \boldsymbol{S_0^\alpha} + \boldsymbol{S_0^{\alpha T}} - \mathrm{diag}(\boldsymbol{S_0^\alpha}) \;\; ; \;\; \kappa_n^\alpha := \frac{\Delta\gamma^0 m}{s^{\alpha,j}}\left(\frac{\left|\boldsymbol{T}^n : \boldsymbol{S_0^\alpha} - w^{\alpha,n}\right|}{s^{\alpha,j}}\right)^{m-1}$$

$$\boldsymbol{C}^{\alpha,n,j} := \left(\left.\frac{\partial(\exp\boldsymbol{M})}{\partial \boldsymbol{M}}\right|_{-\boldsymbol{L^p}^T_{n,j}\Delta t} : \boldsymbol{S_0^{\alpha T}}\right)\boldsymbol{A}\,\exp\left(\sum_{\alpha=1}^{n_s} -\Delta\gamma^\alpha(\boldsymbol{T},\boldsymbol{w},\boldsymbol{s})\boldsymbol{S_0^\alpha}\right)$$

$$\boldsymbol{L^p}_{n,j} = \sum_{\alpha=1}^{n_s}\dot{\gamma}^\alpha(\boldsymbol{T}^n,\boldsymbol{w}^n,\boldsymbol{s}^j)\boldsymbol{S_0^\alpha}$$

$$\left.\frac{\partial \boldsymbol{R}_w^{\alpha,i}}{\partial \boldsymbol{T}}\right|_{\boldsymbol{T}^n,\boldsymbol{w}^n} = -\left(h_i\kappa_n^\alpha - \left(\frac{|w_i^{\alpha,n}|}{b_i}\right)^{m_i} r_i w_i^{\alpha,n}\kappa_n^\alpha \mathrm{sign}(\boldsymbol{T}^n : \boldsymbol{S_0^\alpha} - w^{\alpha,n})\right)\boldsymbol{M}^\alpha \tag{15}$$

$$\begin{aligned}\left.\frac{\partial \boldsymbol{R}_w^{\alpha,i}}{\partial w_j^\beta}\right|_{\boldsymbol{T}^n,\boldsymbol{w}^n} &= \delta_{\alpha\beta}\delta_{ij} + h_i\delta_{\alpha\beta}\kappa_n^\alpha + \delta_{\alpha\beta}\delta_{ij}(m_i+1)r_i\left(\frac{|w_i^{\alpha,n}|}{b_i}\right)^{m_i}|\Delta\gamma^\alpha(\boldsymbol{T}^n,\boldsymbol{w}^n)| \;\; \text{(no sum)}\\ &- \delta_{\alpha\beta}r_i\left(\frac{|w_i^{\alpha,n}|}{b_i}\right)^{m_i} w_i^{\alpha,n}\kappa_n^\alpha\mathrm{sign}(\boldsymbol{T}^n : \boldsymbol{S_0^\alpha} - w^{\alpha,n}) \qquad \text{(no sum)}\end{aligned} \tag{16}$$

where $\mathcal{I}_s$ represents the fourth-order identity tensor with the symmetry constraint because $\boldsymbol{T}$ is symmetric. $\mathrm{diag}(\boldsymbol{M})$ denotes a diagonal matrix with the main diagonal coinciding with that of $\boldsymbol{M}$ and remaining entries zero. $\boldsymbol{C}^{\alpha,n,j}$ involves evaluating the directional derivative of the matrix exponential whose theoretical and numerical implementation is outlined in Appendix (A). Once convergence of $[\boldsymbol{T},\boldsymbol{w}]$ is ensured to set tolerances, we can compute the converged values of $\Delta\gamma^{\alpha,j}$ which is then used to update the slip resistance using Eqn. (9) yielding

$$s^{\alpha,j+1} = s^\alpha(t) + \sum_{i=1}^{n_s} q_{\alpha\beta}h_0\left(1-\frac{s^{\beta,j}}{s^s}\right)^a\left|\Delta\gamma^{\beta,j}\right| \tag{17}$$

Let $\mathcal{J}$ and $\boldsymbol{R}$ denote the Jacobian matrix and the residual vector respectively assembled as

$$\mathcal{J} = \begin{bmatrix}\frac{\partial \boldsymbol{R_T}}{\partial \boldsymbol{T}} & \frac{\partial \boldsymbol{R_T}}{\partial \boldsymbol{w}}\\ \frac{\partial \boldsymbol{R_w}}{\partial \boldsymbol{T}} & \frac{\partial \boldsymbol{R_w}}{\partial \boldsymbol{w}}\end{bmatrix}_{\boldsymbol{T}^n,\boldsymbol{w}^n} \;,\;\; \boldsymbol{R} = \begin{bmatrix}\boldsymbol{R_T}\\ \boldsymbol{R_w}\end{bmatrix}_{\boldsymbol{T}^n,\boldsymbol{w}^n} \tag{18}$$

For the purpose of the line search algorithm the following quantities are necessary inputs and are computed from the quantities defined previously.

$$\begin{aligned} f = 0.5\boldsymbol{R}\cdot\boldsymbol{R}\;,\;\; \boldsymbol{s}^n &= \begin{bmatrix}\boldsymbol{T}^n\\ \boldsymbol{w}^n\end{bmatrix}\\ \boldsymbol{d}^n = -\mathcal{J}^{-1}\boldsymbol{R}\;,\;\; \boldsymbol{g}^n &= 0.5(\mathcal{J}+\mathcal{J}^T)\boldsymbol{R}\end{aligned} \tag{19}$$

where f denotes the value of the objective function, $\boldsymbol{s}^n$ the current state, $\boldsymbol{d}^n$ the search direction and $\boldsymbol{g}^n$ the gradient of f.

The iterative update of $\boldsymbol{s}$ coupled with the Newton's method for updating $[\boldsymbol{T},\boldsymbol{w}]$ is continued until the slip resistances, intermediate stresses and backstresses converge within set tolerances. The converged intermediate stress and slip resistance from the previous increment are chosen as starting guesses for the numerical scheme.

Algorithmic Tangent Modulus

We would like to compute an estimate of the tangent modulus denoted as $\mathcal{T}$ and defined by the differential relation $\delta\boldsymbol{P} = \mathcal{T} \cdot \delta\boldsymbol{F}$. We start with the relation between $\boldsymbol{\sigma}$, $\boldsymbol{T}$ and $\boldsymbol{P}$ which are

$$\boldsymbol{P} = \det(\boldsymbol{F})\boldsymbol{\sigma}\boldsymbol{F}^{-T} \tag{20}$$

$$\boldsymbol{T} = \det(\boldsymbol{F^e})\boldsymbol{F^{e-1}}\boldsymbol{\sigma}\boldsymbol{F^{e-T}} \tag{21}$$

The additional restriction that plastic deformation is isochoric implies $\det(\boldsymbol{F^p}) = 1 \implies \det(\boldsymbol{F}) = \det(\boldsymbol{F^e})$. Then

$$\boldsymbol{P} = \boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} \tag{22}$$

Computing the variation of the LHS and RHS results in

$$\begin{aligned}\delta\boldsymbol{P} &= \delta(\boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T}) \\ &= \delta\boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} + \boldsymbol{F^e}\delta\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} + \boldsymbol{F^e}\boldsymbol{T}\delta\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} + \boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\delta(\boldsymbol{F}^{-T})\end{aligned} \tag{23}$$

From the elastic constitutive relation we have

$$\begin{aligned}\boldsymbol{T} &= \mathcal{L}\cdot\boldsymbol{E}^e = \frac{1}{2}\mathcal{L}\cdot\left(\boldsymbol{F^{e}}^T\boldsymbol{F^e} - \boldsymbol{I}\right) \\ \implies \delta\boldsymbol{T} &= \frac{1}{2}\mathcal{L}\cdot\left(\delta\boldsymbol{F^{e}}^T\boldsymbol{F^e} + \boldsymbol{F^{e}}^T\delta\boldsymbol{F^e}\right) = \mathcal{L}\cdot\left(\boldsymbol{F^{e}}^T\delta\boldsymbol{F^e}\right)\end{aligned} \tag{24}$$

where the last equality follows due to the minor symmetries of $\mathcal{L}$. Additionally, $\delta(\boldsymbol{F}^{-T})$ can be obtained as follows

$$\begin{aligned}&\boldsymbol{F}\boldsymbol{F}^{-1} = \boldsymbol{I} \implies \delta\boldsymbol{F}\boldsymbol{F}^{-1} + \boldsymbol{F}\delta(\boldsymbol{F}^{-1}) = \boldsymbol{0} \\ &\implies \delta\boldsymbol{F}^{-1} = -\boldsymbol{F}^{-1}\delta\boldsymbol{F}\boldsymbol{F}^{-1} \implies \delta\boldsymbol{F}^{-T} = -\boldsymbol{F}^{-T}\delta\boldsymbol{F}^T\boldsymbol{F}^{-T}\end{aligned} \tag{25}$$

Substituting Eqns. (24)-(25) in Eqn. (23) results in

$$\begin{aligned}\delta\boldsymbol{P} &= \delta\boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} + \boldsymbol{F^e}\mathcal{L}\cdot\left(\boldsymbol{F^{e}}^T\delta\boldsymbol{F^e}\right)\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} \\ &\quad + \boldsymbol{F^e}\boldsymbol{T}\delta\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T} - \boldsymbol{F^e}\boldsymbol{T}\boldsymbol{F^{e}}^T\boldsymbol{F}^{-T}\delta\boldsymbol{F}^T\boldsymbol{F}^{-T}\end{aligned} \tag{26}$$

Then the computation of $\mathcal{T}$ depends completely on the computation of $\mathcal{F}$ defined by the differential relation $\delta\boldsymbol{F^e} = \mathcal{F}\cdot\delta\boldsymbol{F}$. To accomplish this we invoke the following relationships

$$\boldsymbol{F} = \boldsymbol{F^e}\boldsymbol{F^p} \implies \delta\boldsymbol{F} = \delta\boldsymbol{F^e}\boldsymbol{F^p} + \boldsymbol{F^e}\delta\boldsymbol{F^p} \tag{27}$$

Additionally

$$\begin{aligned}\dot{\boldsymbol{F}}^{\boldsymbol{p}} = \boldsymbol{L^p}\boldsymbol{F^p} &\implies \boldsymbol{F^p} \approx \exp\left(\boldsymbol{L^p}\Delta t\right)\boldsymbol{F^p}(t) \\ &= \exp\left(\sum_{\alpha=1}^{n_s}\dot{\gamma}^\alpha\Delta t\boldsymbol{S_0^\alpha}\right)\boldsymbol{F^p}(t) = \exp\left(\sum_{\alpha=1}^{n_s}\Delta\gamma^\alpha\boldsymbol{S_0^\alpha}\right)\boldsymbol{F^p}(t)\end{aligned} \tag{28}$$

where $\Delta\gamma^\alpha := \dot{\gamma}^\alpha\Delta t$ Define the quantity $\mathcal{P}$ by $\delta\boldsymbol{F^p} = \mathcal{P}\cdot\delta\boldsymbol{F^e}$. Then Eqn. (27) takes the form

$$\delta\boldsymbol{F} = \delta\boldsymbol{F^e}\boldsymbol{F^p} + \boldsymbol{F^e}\left(\mathcal{P}\delta\boldsymbol{F^e}\right) \tag{29}$$

Taking a variation of the LHS and RHS of Eqn. (28) results in

$$\begin{aligned}
\delta \boldsymbol{F^p} &= \delta\left(\exp\left(\sum_{n=1}^{n_s} \Delta\gamma^\alpha \boldsymbol{S_0^\alpha}\right)\right)\boldsymbol{F^p}(t) = \frac{\partial(\exp \boldsymbol{M})}{\partial \boldsymbol{M}}\Big|_{\boldsymbol{L^p}\Delta t} : \left(\sum_{\alpha=1}^{n_s} \delta\Delta\gamma^\alpha \boldsymbol{S_0^\alpha}\right)\boldsymbol{F^p}(t) \\
&= \left(\sum_{\alpha=1}^{n_s} \frac{\partial(\exp \boldsymbol{M})}{\partial \boldsymbol{M}}\Big|_{\boldsymbol{L^p}\Delta t} : \boldsymbol{S_0^\alpha}\delta\Delta\gamma^\alpha\right)\boldsymbol{F^p}(t) \\
&= \sum_{\alpha=1}^{n_s}\left(\frac{\partial(\exp \boldsymbol{M})}{\partial \boldsymbol{M}}\Big|_{\boldsymbol{L^p}\Delta t} : \boldsymbol{S_0^\alpha}\right)\boldsymbol{F^p}(t).\left(\frac{\partial\Delta\gamma^\alpha}{\partial \boldsymbol{F^e}} : \delta \boldsymbol{F^e}\right) \qquad (30)
\end{aligned}$$

In the viscoplastic constitutive model, slip increments are expressed phenomenologically as follows

$$\Delta\gamma^\alpha = \Delta\gamma^0\left(\frac{\left|\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right|}{s^\alpha}\right)^m \operatorname{sign}\left(\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right) \qquad (31)$$

Assuming $\operatorname{sign}\left(\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right)$ remains unchanged upon computing the variation, we have

$$\begin{aligned}
\delta(\Delta\gamma^\alpha) &= \Delta\gamma^0\delta\left[\left(\frac{\left|\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right|}{s^\alpha}\right)^m\right]\operatorname{sign}(\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha) \\
&= \Delta\gamma^0 m\left(\frac{\left|\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right|}{s^\alpha}\right)^{m-1}\cdot\delta\left(\frac{\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha}{s^\alpha}\right) \\
&= \Delta\gamma^0 m\left(\frac{\left|\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha\right|}{s^\alpha}\right)^{m-1}\left(\frac{\delta\boldsymbol{T} : \boldsymbol{S_0^\alpha} - \delta w^\alpha}{s^\alpha} - \left(\frac{\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha}{s^\alpha.s^\alpha}\right)\delta s^\alpha\right) \\
&= \kappa^\alpha\left(\delta\boldsymbol{T} : \boldsymbol{S_0^\alpha} - \delta w^\alpha - \left(\frac{\boldsymbol{T} : \boldsymbol{S_0^\alpha} - w^\alpha}{s^\alpha}\right)\delta s^\alpha\right) \\
\implies \delta(\Delta\gamma^\alpha) &+ \kappa^\alpha\delta w^\alpha + \frac{m\Delta\gamma^\alpha}{s^\alpha}\delta s^\alpha = \kappa^\alpha\delta\boldsymbol{T} : \boldsymbol{S_0^\alpha} \qquad (32)
\end{aligned}$$

Now we invoke specific evolutionary equations prescribed for s^α and w^α to compute δs^α and δw^α respectively.

$$\begin{aligned}
\dot{s^\alpha} &= \sum_{\beta=1}^{n_s} h_{\alpha\beta}\left|\dot{\gamma}^\beta\right| = \sum_{\beta=1}^{n_s} q_{\alpha\beta}h_\beta\left|\dot{\gamma}^\beta\right| = \sum_{\beta=1}^{n_s} q_{\alpha\beta}h_0\left(1 - \frac{s^\beta}{s^s}\right)^a\left|\dot{\gamma}^\beta\right| \\
\implies s^\alpha &= s^\alpha(t) + \sum_{\beta=1}^{n_s} q_{\alpha\beta}h_0\left(1 - \frac{s^\beta}{s^s}\right)^a\left|\Delta\gamma^\beta\right| \\
\implies \delta s^\alpha &= \sum_{\beta=1}^{n_s} q_{\alpha\beta}h_0\left(1 - \frac{s^\beta}{s^s}\right)^a\delta(\Delta\gamma^\beta).\operatorname{sign}(\Delta\gamma^\beta) - \sum_{\beta=1}^{n_s}\frac{q_{\alpha\beta}h_0 a}{s_s}\left(1 - \frac{s^\beta}{s^s}\right)^{a-1}\left|\Delta\gamma^\beta\right|\delta s^\beta \\
\implies \sum_{\beta=1}^{n_s}&\left(\delta_{\alpha\beta} + \frac{q_{\alpha\beta}h_0 a}{s_s}\left(1 - \frac{s^\beta}{s^s}\right)^{a-1}\left|\Delta\gamma^\beta\right|\right)\delta s^\beta = \sum_{\beta=1}^{n_s} q_{\alpha\beta}h_0\left(1 - \frac{s^\beta}{s^s}\right)^a\delta(\Delta\gamma^\beta).\operatorname{sign}(\Delta\gamma^\beta) \\
\implies [\delta s] &= \boldsymbol{P}^{-1}.\boldsymbol{Q}[\delta(\Delta\gamma)] \qquad (33)
\end{aligned}$$

$$
\begin{aligned}
\dot{w_i^\alpha} &= h_i\dot{\gamma}^\alpha - r_i\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha\,|\dot{\gamma}^\alpha| \qquad (i=1,2) \\
\implies w_i^\alpha &= w_i^\alpha(t) + h_i\Delta\gamma^\alpha - r_i\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha|\Delta\gamma^\alpha| \\
\implies \delta w_i^\alpha &= h_i\delta(\Delta\gamma^\alpha) - r_i\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha \mathrm{sign}(\Delta\gamma^\alpha)\delta(\Delta\gamma^\alpha) - r_i(m_i+1)\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i}|\Delta\gamma^\alpha|\delta w_i^\alpha \\
\implies \delta w_i^\alpha &= \frac{h_i - r_i\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha \mathrm{sign}(\Delta\gamma^\alpha)}{1 + r_i(m_i+1)\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i}|\Delta\gamma^\alpha|}\delta(\Delta\gamma^\alpha) \\
\implies \delta w^\alpha &= \sum_{i=1}^{2}\frac{h_i - r_i\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i} w_i^\alpha \mathrm{sign}(\Delta\gamma^\alpha)}{1 + r_i(m_i+1)\left(\frac{|w_i^\alpha|}{b_i}\right)^{m_i}|\Delta\gamma^\alpha|}\delta(\Delta\gamma^\alpha) \qquad (34)
\end{aligned}
$$

Substituting Eqns. (33)-(34) in the LHS and Eqn. (24) in the RHS of Eqn. (32) results in a matrix-vector equation that relates the 12 element vector $\delta(\boldsymbol{\Delta\gamma})$ to the 9 element vector $[\delta\boldsymbol{F^e}]$, resulting in an equation of the form

$$\boldsymbol{M}.\delta(\boldsymbol{\Delta\gamma}) = \boldsymbol{N}.[\delta\boldsymbol{F^e}] \qquad (35)$$

where $\delta(\boldsymbol{\Delta\gamma})$ is a 12×1 vector, $\boldsymbol{M}$ a 12×12 matrix, $[\delta\boldsymbol{F^e}]$ a 9×1 vector and $\boldsymbol{N}$ a 12×9 matrix. If $\boldsymbol{M}$ is invertible then

$$\delta(\boldsymbol{\Delta\gamma}) = \boldsymbol{M}^{-1}\boldsymbol{N}.[\delta\boldsymbol{F^e}] \qquad (36)$$

which can be substituted in Eqn. (30) to obtain $\mathcal{P}$. Substituting $\mathcal{P}$ in Eqn. (27) results in construction of $\mathcal{F}$, which on substituting in Eqn. (26) completes the computation of $\mathcal{T}$.

Appendices

A. Matrix Exponential Tensorial Derivative

Here I demonstrate how the Gâteaux derivative of the matrix exponential can be computed. A more comprehensive review of tensorial derivatives of tensor-valued functions is presented in [Its02] while it's importance in the context of rate-independent and rate-dependent crystal plasticity constitutive models is covered in [Sou01]. Let $\mathcal{M}_n$ denote the space of all $n\times n$ matrices, closed under addition, scalar multiplication and matrix multiplication. Further let $\exp : \mathcal{M}_n \to \mathcal{M}_n$ denote the matrix exponential, which maps any $n\times n$ matrix $\boldsymbol{M}$ to another $n\times n$ matrix $\boldsymbol{M}_e$ via the following series

$$\boldsymbol{M}_e = \exp(\boldsymbol{M}) = \boldsymbol{I} + \boldsymbol{M} + \frac{1}{2!}\boldsymbol{M}^2 + \ldots + \frac{1}{k!}\boldsymbol{M}^k + \ldots \qquad (37)$$

It is already known that the matrix exponential is well-defined, i.e., the series in Eqn. (37) is convergent for any arbitrary choice of $\boldsymbol{M}$. We wish to compute the Gâteaux derivative or the directional derivative of this exponential map. In other words, the following limit is of interest to us

$$\left.\frac{\partial(\exp\boldsymbol{M})}{\partial\boldsymbol{M}}\right|_{\boldsymbol{M}} : \boldsymbol{H} = \mathcal{D}\exp(\boldsymbol{M})_{\boldsymbol{H}} := \lim_{t\to 0}\frac{\exp\left(\boldsymbol{M}+t\boldsymbol{H}\right)-\exp\left(\boldsymbol{M}\right)}{t} \tag{38}$$

where $\boldsymbol{H} \in \mathcal{M}_n$. Eqn. (38) is precisely the directional derivative of the exponential map evaluated at $\boldsymbol{M}$ along the direction $\boldsymbol{H}$. Then

$$\begin{aligned}
\mathcal{D}\exp(\boldsymbol{M})_{\boldsymbol{H}} &= \lim_{t\to 0}\frac{\exp\left(\boldsymbol{M}+t\boldsymbol{H}\right)-\exp\left(\boldsymbol{M}\right)}{t}\\
&= \lim_{t\to 0}\frac{1}{t}\left(\sum_{k=0}^{\infty}\frac{1}{k!}(\boldsymbol{M}+t\boldsymbol{H})^k - \sum_{k=0}^{\infty}\frac{1}{k!}\boldsymbol{M}^k\right)\\
&= \lim_{t\to 0}\left[\boldsymbol{H} + \frac{1}{2!}\left(\boldsymbol{H}\boldsymbol{M}+\boldsymbol{M}\boldsymbol{H}\right) + \frac{1}{3!}\left(\boldsymbol{H}\boldsymbol{M}^2+\boldsymbol{M}\boldsymbol{H}\boldsymbol{M}+\boldsymbol{M}^2\boldsymbol{H}\right)+\ldots\right] + \underbrace{\lim_{t\to 0}\mathcal{O}(t)}_{0}\\
&= \sum_{k=0}^{\infty}\frac{1}{(k+1)!}\left(\sum_{l=0}^{k}\boldsymbol{M}^{k-l}\boldsymbol{H}\boldsymbol{M}^{l}\right)
\end{aligned} \tag{39}$$

The final expression in Eqn. (37) is the directional derivative of the matrix exponential evaluated at $\boldsymbol{M}$ along $\boldsymbol{H}$. Now construct a $2n \times 2n$ matrix $\boldsymbol{P}$ as follows :

$$\boldsymbol{P} = \begin{bmatrix}\boldsymbol{M} & \boldsymbol{H}\\ \boldsymbol{0} & \boldsymbol{M}\end{bmatrix} \tag{40}$$

Computing a few powers of $\boldsymbol{P}$ and representing it in the block matrix form

$$\boldsymbol{P}^1 = \begin{bmatrix}\boldsymbol{M} & \boldsymbol{H}\\ \boldsymbol{0} & \boldsymbol{M}\end{bmatrix},\ \boldsymbol{P}^2 = \begin{bmatrix}\boldsymbol{M}^2 & \boldsymbol{M}\boldsymbol{H}+\boldsymbol{H}\boldsymbol{M}\\ \boldsymbol{0} & \boldsymbol{M}^2\end{bmatrix},\ \boldsymbol{P}^3 = \begin{bmatrix}\boldsymbol{M}^3 & \boldsymbol{M}^2\boldsymbol{H}+\boldsymbol{M}\boldsymbol{H}\boldsymbol{M}+\boldsymbol{H}\boldsymbol{M}^2\\ \boldsymbol{0} & \boldsymbol{M}^3\end{bmatrix},\ \ldots$$

Paying attention to the $(1,2)$ block for each power of $\boldsymbol{P}$, we observe successive contributions to the sum in Eqn. (39) appearing exactly once. Then it is clear that

$$\mathcal{D}\exp(\boldsymbol{M})_{\boldsymbol{H}} = \left[\sum_{k=1}^{\infty}\frac{1}{k!}\boldsymbol{P}^k\right]_{(1,2)} = \left[\exp(\boldsymbol{P})\right]_{(1,2)} \tag{41}$$

Eqn. (41) implies that computing $\mathcal{D}\exp(\boldsymbol{M})_{\boldsymbol{H}}$ reduces to evaluating $\exp(\boldsymbol{P})$. This is has already been implemented in the function `dexpm` which forms a part of (**Manopt**), a MATLAB toolbox for optimization on manifolds ([Bou+14]). I present an alternative procedure without the need to compute the exponential of a $2n \times 2n$ matrix, and that is based on the following property.

Theorem : The directional derivative of the exponential map can be expressed as

$$\mathcal{D}\exp(\boldsymbol{M})_{\boldsymbol{H}} = \sum_{i=0}^{\infty}\frac{1}{i!}\boldsymbol{T}_i$$

where the sequence $\{\boldsymbol{T}_i\}$ possesses the following generating function

$$\boldsymbol{T}_i = \boldsymbol{M}.\boldsymbol{T}_{i-1} + \boldsymbol{T}_{i-1}.\boldsymbol{M} - \boldsymbol{M}.\boldsymbol{T}_{i-2}.\boldsymbol{M}\quad \forall i \in \{2,3,4,\ldots,\}\ ;\quad \boldsymbol{T}_1 = \boldsymbol{H},\ \boldsymbol{T}_0 = \boldsymbol{0} \tag{42}$$

Proof. From Eqn. (39) we have

$$
\begin{aligned}
&\boldsymbol{T}_{i-1} = \sum_{l=0}^{i-1} \boldsymbol{M}^{i-1-l}\boldsymbol{H}\boldsymbol{M}^{l} \ ; \ \boldsymbol{T}_{i-2} = \sum_{l=0}^{i-2} \boldsymbol{M}^{i-2-l}\boldsymbol{H}\boldsymbol{M}^{l} \\
&\implies \boldsymbol{M}.\boldsymbol{T}_{i-1} + \boldsymbol{T}_{i-1}.\boldsymbol{M} - \boldsymbol{M}.\boldsymbol{T}_{i-2}.\boldsymbol{M} \\
&\quad = \sum_{l=0}^{i-1} \boldsymbol{M}^{i-l}\boldsymbol{H}\boldsymbol{M}^{l} + \sum_{l=0}^{i-1} \boldsymbol{M}^{i-1-l}\boldsymbol{H}\boldsymbol{M}^{l+1} - \sum_{l=0}^{i-2} \boldsymbol{M}^{i-1-l}\boldsymbol{H}\boldsymbol{M}^{l+1} \\
&\quad = \sum_{l=0}^{i-1} \boldsymbol{M}^{i-l}\boldsymbol{H}\boldsymbol{M}^{l} + \boldsymbol{H}\boldsymbol{M}^{i} + \cancel{\sum_{l=0}^{i-2} \boldsymbol{M}^{i-1-l}\boldsymbol{H}\boldsymbol{M}^{l+1}} - \cancel{\sum_{l=0}^{i-2} \boldsymbol{M}^{i-1-l}\boldsymbol{H}\boldsymbol{M}^{l+1}} \\
&\quad = \sum_{l=0}^{i} \boldsymbol{M}^{i-l}\boldsymbol{H}\boldsymbol{M}^{l} = \boldsymbol{T}_{i}
\end{aligned}
$$

□

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