(VPSC)

Self-consistent scheme

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* We start with guessing $\underline{\bar{M}^{el,(1st)}}$

1st guess.

i) → calculate Eshelby tensor $S^{el\,(1st)}_{ijkl}$

ii) → calculate $\tilde{M}^{el\,(1st)}_{ijkl}$

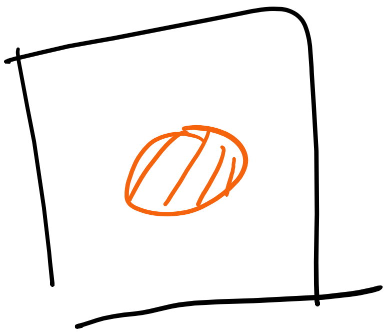
iii) → calculate B_{ijkl}

iv) → One can back-calculate $\bar{M}^{el}$ from

$$\bar{M}^{el,(2nd)} = \langle M^{el} \cdot B \rangle$$ new

→ we iteratively estimate $\boxed{\bar{M}^{el}}$

Now, what about viscoplasticity?



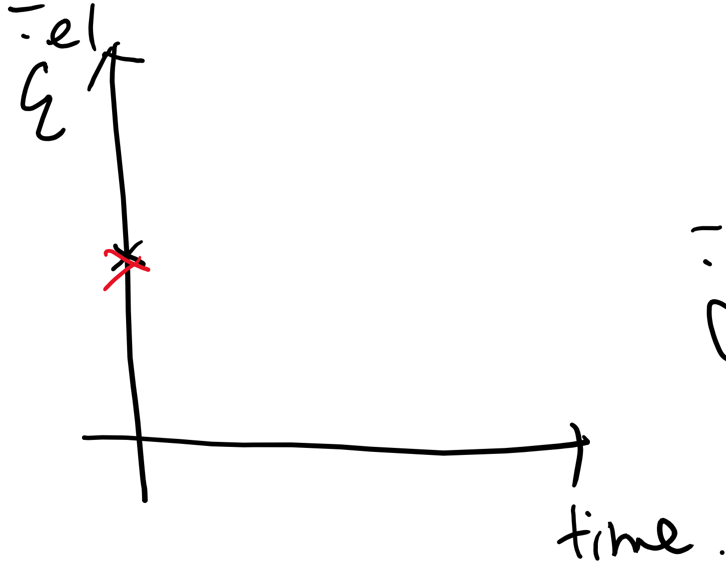
el HEM → vp HEM

$$\dot{\bar{\varepsilon}}^{el} = \bar{M}^{el} \dot{\bar{\sigma}}$$

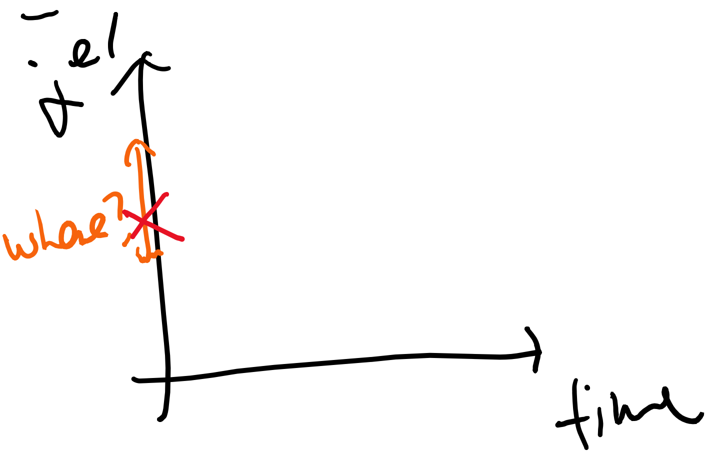
stress rate.

$$\dot{\bar{\varepsilon}}^{vp} = \bar{M}^{vp} \cdot \bar{\sigma} + (\dot{\bar{\varepsilon}}^{o})$$

not stress rate, but stress

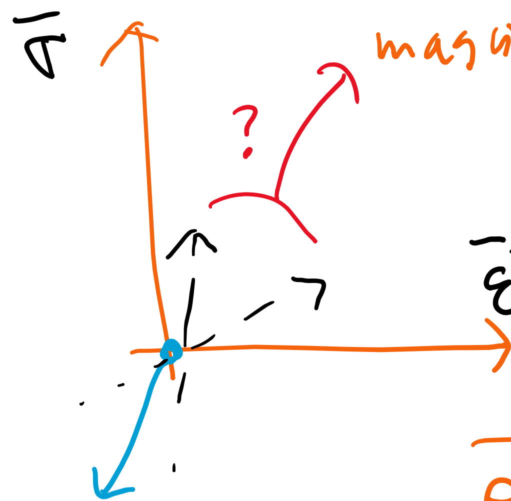


$$\dot{\bar{\sigma}}^{el} = \bar{C}^{el} \; \dot{\bar{e}}^{el}$$



direction $\left(\frac{d\bar{\varepsilon}^{el}}{dt}, \frac{d\bar{\sigma}}{dt}\right)$

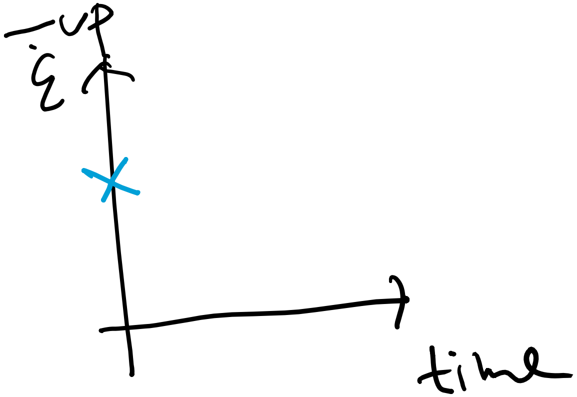
magnitude : Δt

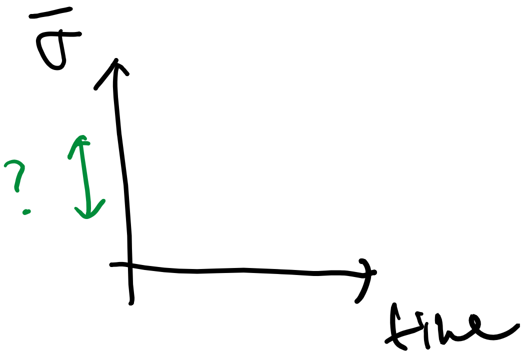


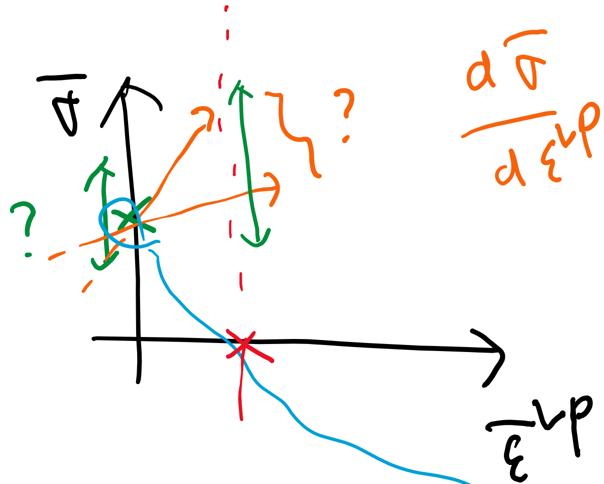
initial condition (unloaded)

$$\bar{e}^{el} = \int_0^T \dot{\bar{e}} \, dt$$

$$\bar{\sigma} = \int_0^T \dot{\bar{\sigma}} \, dt$$







$\dfrac{d\bar{\sigma}}{d\bar{\varepsilon}^{vp}}$?

δt, $\dot{\bar{\varepsilon}}^{vp}$ given

we know

$$\bar{\varepsilon} = \int_0^{0+\delta T} \dot{\bar{\varepsilon}}^{vp} dt$$

$$\bar{\varepsilon}^{vp} = \int_0^T \dot{\bar{\varepsilon}}^{vp} dt$$

at $T=0$, $\bar{\varepsilon}^{vp} = 0$

but $\dfrac{d\bar{\varepsilon}^{vp}}{dt} \neq 0$

$$\dot{\bar{\varepsilon}}^{vp} = \bar{M}^{vp} \cdot \bar{\sigma} \quad \rightarrow \quad \dot{\bar{\varepsilon}}_{ij}^{vp} = \bar{M}_{ijkl}^{vp} \bar{\sigma}_{kl}$$

correspondingly, viscoplastic behavior of grain:
constitutive

$$\longrightarrow \quad \dot{\varepsilon}_{ij}^{vp} = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}}{\underbrace{\tau}_{\text{CRSS}}} \right)^n$$

This vp formulation is not "linear" relationship between $\dot{\varepsilon}^{vp}$ and σ

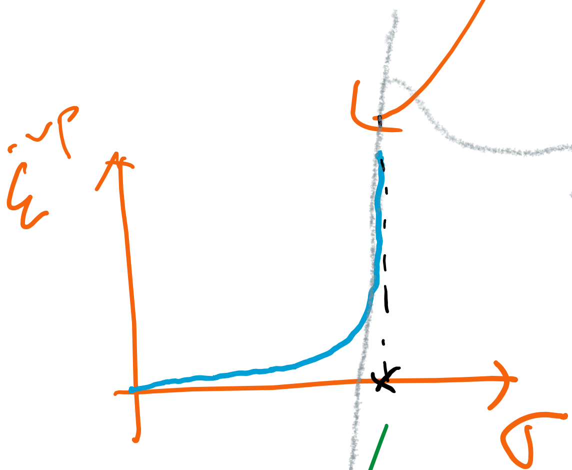
* Nevertheless, we need "linear" relationship to use Eshelby's approach

$$\dot{\varepsilon}^{vp}_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m^s_{kl}\sigma_{kl}}{\tau} \right)^n$$

$$\rightarrow \quad \dot{\varepsilon}^{vp}_{ij} = M^{vp}_{ijkl}\,\sigma_{kl}$$

similar to $\dot{\bar{\varepsilon}}^{vp}_{ij} = \bar{M}^{vp}_{ijkl}\,\bar{\sigma}_{kl}$

how?



$m_{kl}\sigma_{kl} \simeq \tau$

$$\dot{\varepsilon}^{vp} = M^{vp}_0\,\sigma + \dot{\varepsilon}^0$$

this is easily estimated

this is not so!

$$M^{vp} = \frac{\partial \dot{\varepsilon}^{vp}}{\partial \sigma} \;\Big|\; \rightarrow \; M^{vp}_{ijkl} = \frac{\partial \dot{\varepsilon}^{vp}_{ij}}{\partial \sigma_{kl}}$$

$$\frac{\partial \dot{\varepsilon}_{ij}^{vp}}{\partial \sigma_{kl}} = \frac{\partial \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m:\sigma}{\tau} \right)^n}{\partial \sigma_{kl}}$$

$$= \dot{\gamma}_0 \sum_s m_{ij}^s \frac{\partial \left(\frac{m:\sigma}{\tau} \right)^n}{\partial \sigma_{kl}}$$

$$= \dot{\gamma}_0 \sum_s m_{ij}^s \cdot n \cdot \left(\frac{m^s:\sigma}{\tau} \right)^{n-1} \cdot \frac{\partial \left\{ \frac{m^s:\sigma}{\tau} \right\}}{\partial \sigma_{kl}}$$

$$= \dot{\gamma}_0 \sum_s m_{ij}^s \cdot n \left(\frac{m^s:\sigma}{\tau} \right)^{n-1} : \frac{1}{\tau} \frac{\partial (m^s:\sigma)}{\partial \sigma_{kl}}$$

$$m^s : \sigma = \sum_i \sum_j m^s_{ij} \sigma_{ij} = m^s_{11}\sigma_{11} + m^s_{12}\sigma_{12} + m^s_{13}\sigma_{13} + \cdots + m^s_{33}\sigma_{33}$$

→ we're looking for $\left(\frac{\partial\, m^s : \sigma}{\partial \sigma_{kl}}\right)$ during pause of

$M^{vp}_{ijkl} \quad \frac{\partial \dot{\varepsilon}^{vp}_{ij}}{\partial \sigma_{kl}}$

say, $\frac{\partial \dot{\varepsilon}^{vp}_{11}}{\partial \sigma_{32}}$?

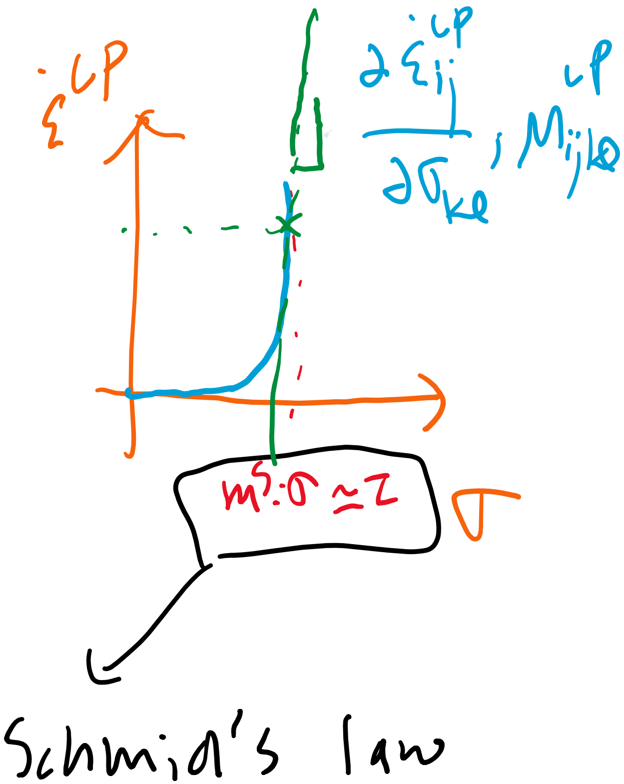
$$\frac{\partial \left(m^s_{11}\sigma_{11} + m^s_{12}\sigma_{12} + \cdots + m^s_{33}\sigma_{33} \right)}{\partial \sigma_{32}} = m^s_{32}$$

$$\therefore \frac{\partial\, m^s : \sigma}{\partial \sigma_{kl}} = m^s_{kl}$$

$$\frac{\partial \dot{\varepsilon}_{ij}^{cp}}{\partial \sigma_{kl}} = \dot{\gamma}_0 \sum_s m_{ij}^s \cdot n \cdot \frac{1}{\tau^s}\left(\frac{m^s:\sigma}{\tau^s}\right)^{n-1} \cdot m_{kl}^s$$

$$= n\,\dot{\gamma}_0 \sum_s \frac{m_{ij}^s\, m_{kl}^s}{\tau^s}\left(\frac{m^s:\sigma}{\tau^s}\right)^{n-1}$$

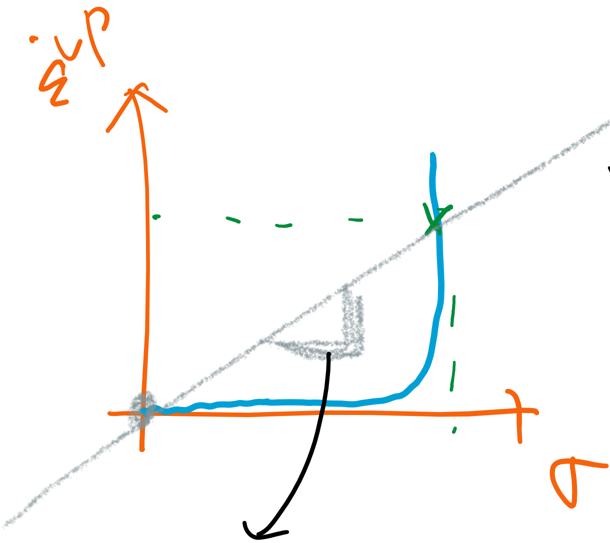
$\rightarrow$ tangential to curve



$\dot{\varepsilon}^{0}$ is seeming difficult to determine.

instead of using tangential, what about secant?

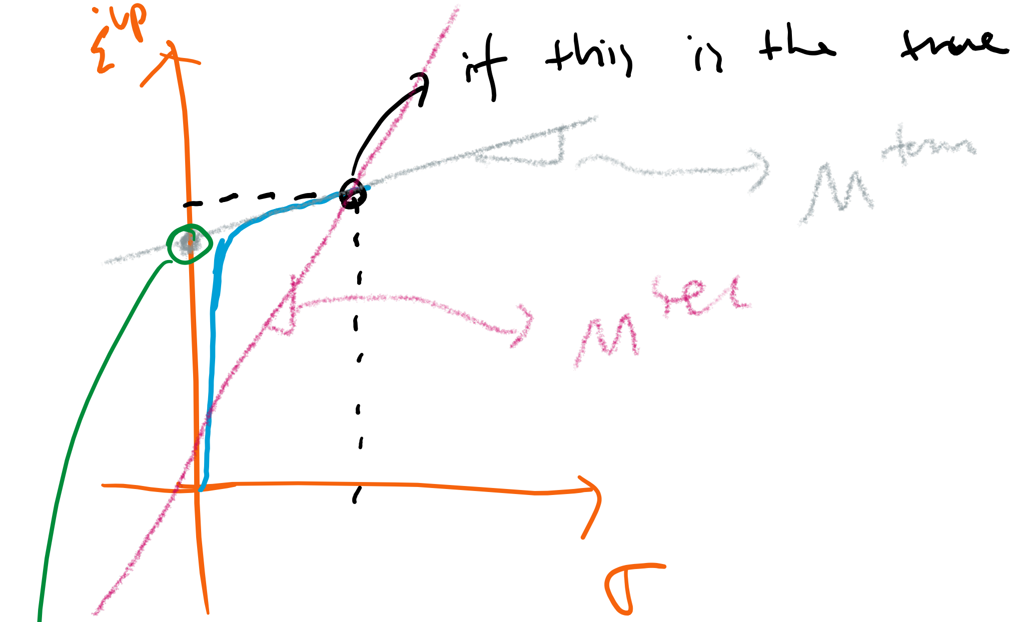
That means ...



what if we use this approximation?

That corresponds to

$$M_{ijkl}^{secant,vp} = \dot{\gamma}_0 \sum_s \frac{m_{ij}^s m_{kl}^s}{\tau} \left(\frac{m:\sigma}{\tau} \right)^{n-1}$$

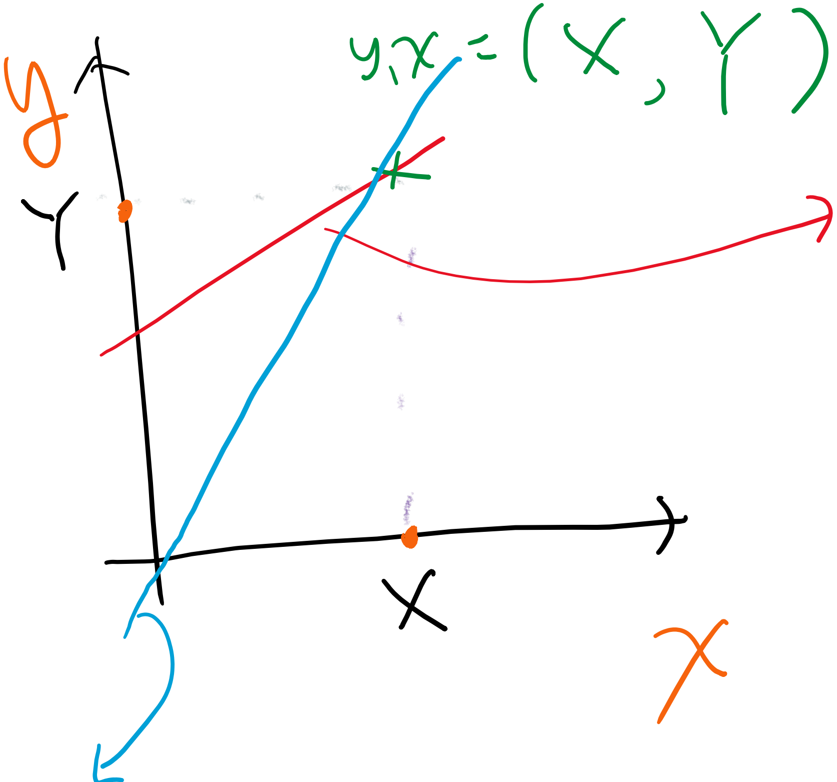


unknown.

I don't know

$$y = ax + b$$

$$M^{sec} \times \sigma$$



The true line func.

→ $y = ax + b$

and that satisfies.

$$Y = aX + b$$

$y = Ax$

→ $Y = A \cdot X$

what we want is express b by knowns. X, Y, A and a

→ $aX + b = AX$

→ $b = \underbrace{A}_{\text{secant}}X - \underbrace{a}_{\text{tangent}}X$.

$M_{ijkl}^{tan,vp}$ $\quad M_{ijkl}^{sec,vp}$, $\dot{\varepsilon}^{vp}$, σ

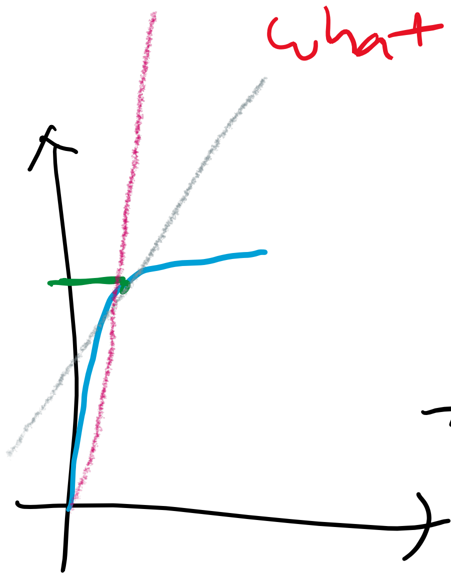
$\dot{\varepsilon}^{vp,0}$?

the intercept

or, back-extrapolated term.

$$\dot{\varepsilon}^{vp,0} = \boxed{M^{sec} \cdot \sigma} - M^{tan}\sigma$$

what is this?



$$M_{ijkl}^{sec} = \sum_s \dot{\gamma}_0 \left(\frac{m_{ij}^s m_{kl}^s}{\tau}\right)\left(\frac{m^s : \sigma}{\tau}\right)^{n-1}$$

$$\to M_{ijkl}^{sec}\sigma_{kl}$$

$$= \sum_s \dot{\gamma}_0 \frac{m_{ij}^s m_{kl}^s \sigma_{kl}}{\tau}\left(\frac{m^s : \sigma}{\tau}\right)^{n-1}$$

$$= \sum_s \dot{\gamma}_0 m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}}{\tau}\right)\left(\quad\right)^{n-1}$$

$$M^{sec} : \sigma = \dot{\varepsilon}^{vp}$$

Similar to the Elastic HEM, Elastic inclusion,

$$(\dot{\varepsilon}^{el} - \dot{\bar{\varepsilon}}^{el}) = -\tilde{M}^{el}(\dot{\sigma} - \dot{\bar{\sigma}})$$

we suggest

$$\underbrace{(\dot{\varepsilon}^{vp}} - \dot{\bar{\varepsilon}}^{vp}) = -\tilde{M}^{vp}(\sigma - \bar{\sigma})$$

$$\tilde{M}^{vp} = (I - S^{vp})^{-1} : S^{vp} : \bar{M}^{vp}$$

$$M^{vp}\sigma + \dot{\varepsilon}^{0} - (\bar{M}^{vp}\bar{\sigma} + \dot{\bar{\varepsilon}}^{0}) = -\tilde{M}^{vp}\sigma + \tilde{M}^{vp}\bar{\sigma}$$

$$\rightarrow \quad (M^{vp} + \tilde{M}^{vp})\sigma = (\bar{M}^{vp} + \tilde{M}^{vp})\bar{\sigma} + \dot{\bar{\varepsilon}}^{0} - \dot{\varepsilon}^{0}$$

$$\rightarrow \quad \sigma = (M^{vp} + \tilde{M}^{vp})^{-1}(\bar{M}^{vp} + \tilde{M}^{vp})\bar{\sigma} + (M^{vp} + \tilde{M}^{vp})^{-1}(\dot{\bar{\varepsilon}}^{0} - \dot{\varepsilon}^{0})$$

$$\sigma = \underbrace{\left(M^{vp} + \tilde{M}^{vp}\right)^{-1}\left(\bar{M}^{vp} + \tilde{M}^{vp}\right)}_{\beta} \bar{\sigma} + \underbrace{\left(M^{vp} + \tilde{M}^{vp}\right)^{-1}\left(\bar{\dot{\varepsilon}}^{vp} - \bar{\dot{\varepsilon}}^{\circ}\right)}_{b}$$

$$\sigma = \beta : \bar{\sigma} + b$$

β & b are functions of $\tilde{M}^{vp}$, M^{vp}, $\bar{M}^{vp}$ ...

$\bar{\dot{\varepsilon}}^{\circ}$

unknown priories.

$$\bar{\dot{\varepsilon}}^{vp} = \langle \dot{\varepsilon}^{vp} \rangle$$

$$\bar{\dot{\varepsilon}}^{vp} = \bar{M}^{vp} \bar{\sigma} + \bar{\dot{\varepsilon}}^{0}$$

$$\dot{\varepsilon}^{vp} = M^{vp} \sigma + \dot{\varepsilon}^{0}$$

$$\langle \dot{\varepsilon}^{vp} \rangle = \langle M^{vp} \sigma \rangle + \langle \dot{\varepsilon}^{0} \rangle = \bar{M}^{vp} \bar{\sigma} + \bar{\dot{\varepsilon}}^{0}$$

$$\sigma = B \bar{\sigma} + b$$

$$\langle M^{vp} B \bar{\sigma} + M^{vp} b \rangle + \langle \dot{\varepsilon}^{0} \rangle = \bar{M}^{vp} \bar{\sigma} + \bar{\dot{\varepsilon}}^{0}$$

$$\langle M^{vp} B \rangle \bar{\sigma} + \langle M^{vp} b \rangle + \langle \dot{\varepsilon}^{0} \rangle = \bar{M}^{vp} \cdot \bar{\sigma} + \bar{\dot{\varepsilon}}^{0}$$

$$\therefore \quad \bar{M}^{vp} = \langle M^{vp} B \rangle$$

$$\bar{\dot{\varepsilon}}^{0} = \langle M^{vp} b \rangle + \langle \dot{\varepsilon}^{0} \rangle = \langle M^{vp} b + \dot{\varepsilon}^{0} \rangle$$

* We assume that $\bar{\dot{\varepsilon}}^{up}$ is fully imposed.

→ with that we start by using Taylor's assumption

$$\dot{\varepsilon}_{ij} = \bar{\dot{\varepsilon}}^{up}_{ij}$$

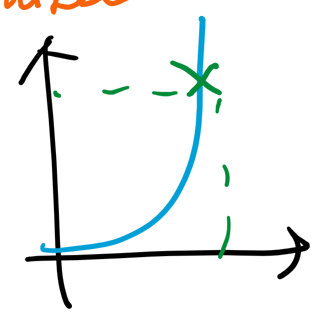
→ using the power law obtain σ? , how?

$$\dot{\varepsilon}_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m^s_{kl}\sigma_{kl}}{\tau} \right)^n$$

we'll over it separately.

inverse approach.

Lemlenten



→ Then we have $(\dot{\varepsilon}^{up}, \sigma)$

~ we need M^{up}, $\dot{\varepsilon}^{up,0}$

→ calculate B, b with "guessed" $\bar{M}^{up}$, $\bar{\dot{\xi}}^{0,up}$

$$\tilde{M}^{up} \leftarrow S^{up}$$

$$B = \left(M^{up} + \tilde{M}^{up}\right)^{-1}\left(\bar{M}^{up} + \tilde{M}^{up}\right)$$

$$b = \left(M^{up} + \tilde{M}^{up}\right)^{-1}\left(\bar{\dot{\xi}}^{up} - \bar{\dot{\xi}}^{0}\right)$$

→ Now, new guess

$$\bar{M}^{up} = \langle M^{up} B \rangle$$

$$\bar{\dot{\xi}}^{0} = \langle M^{up} b + \dot{\xi}^{0} \rangle$$

* With the new $\bar{M}^{vp}$, $\bar{\dot{\varepsilon}}^{0}$ solve the macro constitutive eq.

$$\bar{\dot{\varepsilon}}^{vp} = \bar{M}^{vp} \cdot \bar{\sigma} + \bar{\dot{\varepsilon}}^{0}$$

* Check if $\bar{\sigma} = \langle \sigma \rangle$ & $\bar{\dot{\varepsilon}}^{vp} = \langle \dot{\varepsilon}^{vp} \rangle$

* if not iterate.

The numerical recipe of VPSC.

$\boxed{\text{initial guess}}$ on $\bar{M}^{vp}$, $\dot{\bar{\varepsilon}}^{0}$ → solving Eq. gives $\bar{\sigma}$ and $\dot{\bar{\varepsilon}}^{vp}$

* Eshelby, S^{vp}
* B, b, $\tilde{M}$
* $\bar{M}^{vp}$, $\dot{\bar{\varepsilon}}^{0}$

* Solve $\dot{\bar{\varepsilon}}^{vp} = \bar{M}^{vp}\bar{\sigma} + \dot{\bar{\varepsilon}}^{0}$
* Solve to obtain σ, "NR" → This will be discussed in what follows.
* Using σ, obtain $\dot{\varepsilon}^{vp}$, M^{vp}, $\dot{\varepsilon}^{vp,0}$
* Check $\langle\sigma\rangle = \bar{\sigma}$ $\langle\dot{\varepsilon}^{vp}\rangle = \dot{\bar{\varepsilon}}^{vp}$

$$\dot{\varepsilon}_{ij} = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}}{\tau} \right)^n$$ → its explicit inverse form is not available...

→ we start from the interaction eq.

$$\left(\dot{\varepsilon}^{up} - \bar{\dot{\varepsilon}}^{up} \right) = - \tilde{m}^{up} \left(\sigma - \bar{\sigma} \right)$$

→ this need S^{up} & $\bar{m}^{up}$

we assume this by (m^{up})

once $\bar{m}^{up}$ $(\bar{\dot{\varepsilon}}^{0})$ are given,

These two can be fully obtained.

$$\dot{\varepsilon}^{up} = \dot{\gamma}_0 \sum_s m_{ij}^s \left(\frac{m^s : \sigma}{\tau} \right)^n$$

→ next page.

$$\left(\dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m_{ij}\sigma}{\tau}\right)^n - \bar{\dot{\epsilon}}^{vp}\right) = -\tilde{\mu}^{vp}\left(\sigma - \bar{\sigma}\right)$$

we have guessed properties.

These two are unknown.

Now, we want to obtain "σ" that satisfy the above using Newton Raphson method.

What's Newton Raphson method?

we rearrange the interaction Eq.

$$\dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m:\sigma}{\tau}\right)^n + \tilde{M}^{up}_{ijkl}\sigma_{ijkl} - \bar{\dot{\varepsilon}}^{up}_{ij} - \tilde{M}^{up}_{ijkl}\bar{\sigma}_{kl} = 0$$

for each (i, j) pair

say, ↳ D_{ij}

$$F_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m:\sigma}{\tau}\right)^n + \tilde{M}^{up}_{ijkl}\sigma_{kl} + D_{ij}$$

we want to find σ that makes $F_{ij}(\sigma)$ zero

→ need Jacobian. $\dfrac{\partial F_{ij}}{\partial \sigma_{kl}}$

$$= M^{tan} + \tilde{M}^{up}_{ijkl}$$

if we fix $\tilde{M}^{up}$, $\bar{\dot{\varepsilon}}^{up}$, $\bar{\sigma}$

Once the Jacobian is found, we iteratively perform below calculation

$$\sigma_{ij}^{new} = \sigma_{ij}^{old} - J_{ijkl}^{-1} F_{kl}$$

Once we'd found the solution of

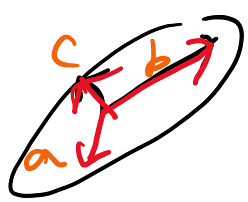
$$\bar{\dot{\varepsilon}}^{vp} = \bar{M}^{vp} \cdot \sigma + \bar{\dot{\varepsilon}}^{0}$$

remember that's pertaining to a specific state of polycrystal.

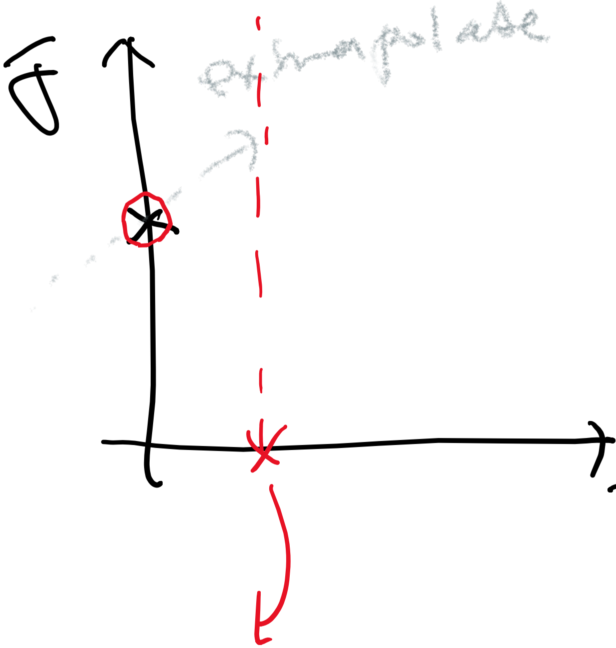
characteristics of polycrystals in VPSC

* τ_c, m^s ← crystal structure and orientation

* The shape of inclusion. and orientation



ratio a : b : c



$$\bar{\varepsilon}^{pl}(t) = \int_0^t \dot{\bar{\varepsilon}}^{pl} \, dt$$

update the state of poly crystal.

* hardening
* crystal reorientation (texture)
* inclusion shape, orientation

τ^s, S^{vp}

m^s_{ij}

If you plan to study how the Eshelby tensor is obtained, you should start looking up —

* differential Eq. { Solution using Green function.
* Linear Algebra.
* Matrix
* Vector analysis, vector field { line integration ...
* Tensor Algebra
* Fourier transformation.
* Numerical analysis
  { numerical integration }
* Continuum mechanics