

IMPLEMENTATION OF CONSTITUTIVE EQUATIONS

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Why is it important to know how to implement constitutive equations in finite element codes ?

- Few constitutive equations are available in commercial FE codes
- Implement new constitutive models in commercial codes (ABAQUS, ANSYS, MARC, . . . , Code_Aster, CAST3M, . . . , Zset, WARP3D)
- Implement specific treatment of implemented models

- “ Numerical” definition of constitutive equations
- Methods (explicit/implicit) for numerical integration
- Consistent tangent matrix
- Example : von Mises plasticity model
- Convergence

“ Numerical” definition of constitutive equations

“ Numerical” definition of constitutive equations

- In the case of a displacement based FE formulation, nodal displacements are known and deformations can be computed
- The constitutive equations are used to evaluate:
 - 1 the stress tensor $\underline{\sigma}$
 - 2 the “consistent” tangent matrix

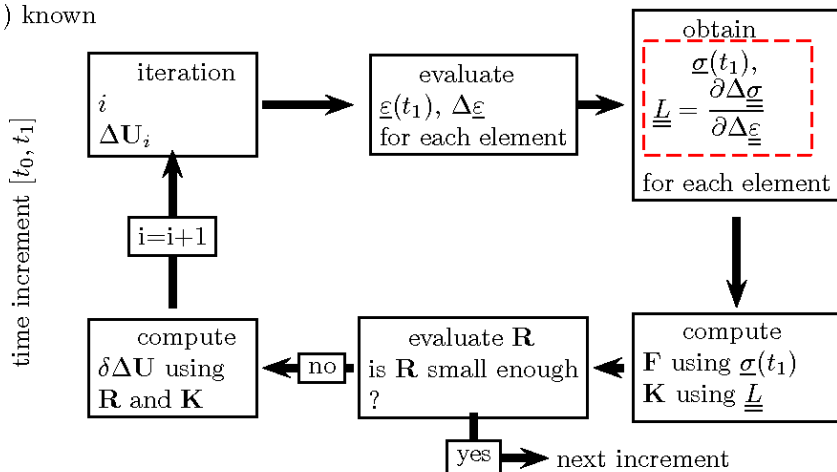
$$\underline{L} = \frac{\partial \underline{\Delta \sigma}}{\partial \underline{\Delta \varepsilon}}$$

for a given deformation increment $\underline{\Delta \varepsilon}$.

- Material behaviours are also characterized by internal variables **A**.
- The constitutive equations are used to update these variables.

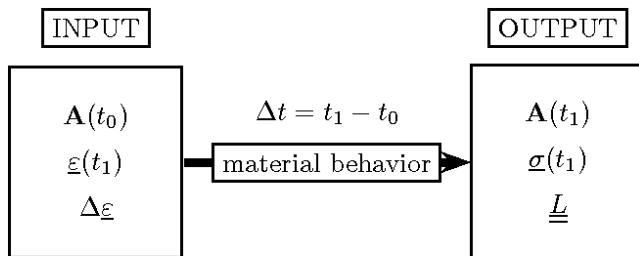
Constitutive equations within the finite element method

$\mathbf{U}(t_0)$ known



 : global computation

 : local time integration of the constitutive equations



$$\frac{d\mathbf{A}}{dt} = \dot{\mathbf{A}} = \mathbf{G}(\mathbf{A}, t)$$

$$\frac{dA_i}{dt} = \dot{A}_i = G_i(A_1, \dots, A_n, t)$$

- Time is used here to represent an imposed deformation as well as imposed **external parameters** depending on both time and position such as an temperature ($T(\vec{x}, t)$).
- Evaluation of the constitutive equations = integrate the previous system from t_0 to t_1 .
- Usually: $\mathbf{A} = (\underline{\varepsilon}_e, \dots)$ so that

$$\underline{\sigma}(t_1) = \underline{E}(t_1) : \underline{\varepsilon}_e(t_1)$$

- \underline{L} must still be computed...

Integration methods for constitutive equations

$$\mathbf{A}(t_1) = \mathbf{A}(t_0) + \dot{\mathbf{A}}(\mathbf{A}(t_0), t_0) \Delta t = \mathbf{A}(t_0) + \mathbf{G}(\mathbf{A}(t_0), t_0) \Delta t$$
$$\Delta \mathbf{A} = \mathbf{G}(\mathbf{A}(t_0), t_0) \Delta t$$

- The method is not stable ; it must not be employed
- Explicit ? : because $\dot{\mathbf{A}}$ is evaluated at t_0 using $(\mathbf{A}(t_0), t_0)$

- Numerical estimation of derivatives of $\dot{\mathbf{A}}$: $d\mathbf{G}/d\mathbf{A}$, $d^2\mathbf{G}/d\mathbf{A}^2$, $d^3\mathbf{G}/d\mathbf{A}^3 \dots$
- Error estimator to control the solution

The Runge–Kutta integration method is easy to set up as it only uses the differential equation:

$$\dot{\mathbf{A}} = \mathbf{G}(\mathbf{A}, t)$$

It however has some drawbacks:

- Integration may require long CPU time
- In the case of plastic material, the plastic multiplier must be computed. This can be tricky in cases where material coefficients depend on external parameters (e.g. temperature).
- The stability of the integration scheme is not certain for softening materials.

- Estimation of $\dot{\mathbf{A}}$ at time t_θ between t_0 and t_1
- $t_\theta = t_0 + \theta \Delta t$ avec $0 \leq \theta \leq 1$
- Two solutions :

$$\begin{aligned}\Delta \mathbf{A} &= \mathbf{G}(\mathbf{A}(t_0) + \theta \Delta \mathbf{A}, t_0 + \theta \Delta t) \Delta t \\ &= \mathbf{G}(\mathbf{A}_\theta, t_\theta) \Delta t \\ \Delta \mathbf{A} &= [(1 - \theta) \mathbf{G}(\mathbf{A}(t_0), t_0) + \theta \mathbf{G}(\mathbf{A}(t_1), t_1)] \Delta t \\ &= [(1 - \theta) \mathbf{G}(\mathbf{A}_0, t_0) + \theta \mathbf{G}(\mathbf{A}_0 + \Delta \mathbf{A}, t_0 + \Delta t)] \Delta t\end{aligned}$$

- Implicit i? : $\Delta \mathbf{A}$ appears on both sides of the previous equations
- Integrate the constitutive equations = solve the previous equations
- $\theta = 0 \rightarrow$ Euler
- ... in the following we will focus on the first method

- Resolution using the Newton-Raphson method
- Residual expressed as:

$$\mathbf{R}(\Delta \mathbf{A}) = \Delta \mathbf{A} - \mathbf{G}(\mathbf{A}(t_0) + \theta \Delta \mathbf{A}, t_0 + \theta \Delta t) \Delta t$$

$$R_i(\Delta A_1, \dots, \Delta A_n) = \Delta A_i - G_i(A_1(t_0) + \theta \Delta A_1, \dots, A_n(t_0) + \theta \Delta A_n) \Delta t$$

- First order Taylor expansion at s^{th} estimate $\Delta \mathbf{A}_s$

$$\mathbf{R} = \mathbf{R}(\Delta \mathbf{A}_s) + \frac{\partial \mathbf{R}}{\partial \Delta \mathbf{A}} \cdot (\Delta \mathbf{A} - \Delta \mathbf{A}_s) = \mathbf{0}$$

- Calculation of the next estimate ($s + 1$):

$$\Delta \mathbf{A}_{s+1} = \Delta \mathbf{A}_s - \left(\frac{\partial \mathbf{R}}{\partial \Delta \mathbf{A}} \right)_{\Delta \mathbf{A} = \Delta \mathbf{A}_s}^{-1} \cdot \mathbf{R}(\Delta \mathbf{A}_s)$$

- $\mathbf{J} = \partial \mathbf{R} / \partial \Delta \mathbf{A}$ ($J_{ij} = \partial R_j / \partial A_i$): Jacobian matrix, $\mathbf{J}^* = \mathbf{J}^{-1}$

- The **A** vector often holds second order tensors
- The Voigt notation is then used
- Notation

Standard notation	Preferred notation
$\underline{\underline{\varepsilon}} = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \end{pmatrix}, \quad \underline{\underline{\sigma}} = \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{pmatrix}$	$\underline{x} = \begin{pmatrix} x_{11} \\ x_{22} \\ x_{33} \\ \sqrt{2}x_{12} \\ \sqrt{2}x_{23} \\ \sqrt{2}x_{31} \end{pmatrix}$

Examples

- Additive decomposition of deformations:

$$\underline{\varepsilon} = \underline{\varepsilon}_e + \underline{\varepsilon}_p$$

- Yield surface

$$\phi = \sigma_{eq} - R(p)$$

- Normality

$$\dot{\underline{\varepsilon}}_p = \dot{p} \frac{\partial \phi}{\partial \underline{\sigma}} = \frac{3}{2} \dot{p} \frac{\underline{s}}{\sigma_{eq}} = \dot{p} \underline{n}$$

- Internal variables : $(\underline{\varepsilon}_e, p)$

- Calculation of \dot{p} using the consistency condition: $\dot{\phi} = 0$

$$\dot{\phi} = \frac{\partial \phi}{\partial \underline{\underline{\sigma}}} : \dot{\underline{\underline{\sigma}}} + \frac{\partial \phi}{\partial p} \dot{p} = \underline{n} : \dot{\underline{\underline{\sigma}}} - H \dot{p}$$

- avec $\underline{\underline{\sigma}} = \underline{\underline{E}} : \underline{\underline{\varepsilon}}_e = \underline{\underline{E}} : (\underline{\underline{\varepsilon}} - \underline{\underline{\varepsilon}}_p) \rightarrow \dot{\underline{\underline{\sigma}}} = \underline{\underline{E}} : \dot{\underline{\underline{\varepsilon}}}_e = \underline{\underline{E}} : (\dot{\underline{\underline{\varepsilon}}} - \dot{\underline{\underline{\varepsilon}}}_p)$
- Finally one gets

$$\dot{p} = \frac{\underline{n} : \underline{\underline{E}} : \dot{\underline{\underline{\varepsilon}}}}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

- System of differential equations to be solved

$$\text{sur } \underline{\underline{\varepsilon}}_e \quad \dot{\underline{\underline{\varepsilon}}}_e = \dot{\underline{\underline{\varepsilon}}} - \dot{p} \underline{n}$$

$$\text{sur } p \quad \dot{p} = \frac{\underline{n} : \underline{\underline{E}} : \dot{\underline{\underline{\varepsilon}}}}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

- Attention must be paid on dependences on external parameters (temperature...)
- Ready for explicit Runge–Kutta integration !

$$\begin{aligned}\underline{\dot{\varepsilon}}_e &= \underline{\dot{\varepsilon}} - \dot{p}\underline{n} & \rightarrow & \Delta\underline{\varepsilon}_e = \Delta\underline{\varepsilon} - \Delta p \underline{n} \\ \dot{p} &= \frac{\underline{n} : \underline{E} : \underline{\dot{\varepsilon}}}{\underline{n} : \underline{E} : \underline{n} + H} & \rightarrow & \Delta p = \frac{\underline{n} : \underline{E} : \Delta\underline{\varepsilon}}{\underline{n} : \underline{E} : \underline{n} + H}\end{aligned}$$



- Evaluation of \underline{n} , \underline{E} , H ? ... at time $t_\theta = t_0 + \theta\Delta t$.
- Application :

$$\underline{n} = \frac{3}{2} \frac{\underline{s}^\theta}{\sigma_{eq}^\theta} \quad \text{avec} \quad \underline{\sigma}^\theta = \underline{E}^\theta : \underline{\varepsilon}_e^\theta \quad \underline{\varepsilon}_e^\theta = \underline{\varepsilon}_e^0 + \theta \Delta \underline{\varepsilon}_e$$

$$\underline{E}^\theta = \underline{E}(T^\theta) = \underline{E}(T^0 + \theta \Delta T)$$

$$H^\theta = H(p^\theta) = H(p^0 + \theta \Delta p)$$

- The equation

$$\Delta p = \frac{\underline{n} : \underline{\underline{E}} : \Delta \underline{\varepsilon}}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

is correct but may be replaced by:

$$\phi = \sigma_{\text{eq}} - R(p) = 0$$



This equation is wrong if R depends on an external parameter as in that case:

$$\dot{p} = \frac{\underline{n} : \underline{\underline{E}} : \dot{\underline{\varepsilon}} - R_{,T} \dot{T}}{\underline{n} : \underline{\underline{E}} : \underline{n} + H} \rightarrow \Delta p = \frac{\underline{n} : \underline{\underline{E}} : \Delta \underline{\varepsilon} - R_{,T} \delta T}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

The incremental equation is then

$$\Delta p = \frac{\underline{n}^\theta : \underline{\underline{E}}^\theta : \Delta \underline{\varepsilon} - R_{,T}^\theta \Delta T}{\underline{n}^\theta : \underline{\underline{E}}^\theta : \underline{n}^\theta + H^\theta}$$

The method must be avoided and it is better to use the yield condition $\phi = \sigma_{\text{eq}} - R(p) = 0$

- N.B.: in the following the superscript $^\theta$ will be omitted for the sake of simplicity

$$\underline{R}_e = \Delta \underline{\varepsilon}_e + \Delta p \underline{\eta} - \Delta \varepsilon$$

$$R_p = \phi = \sigma_{\text{eq}} - R(p)$$

$$\mathbf{R} = (R_e, R_p)$$

- Writing using sub-blocks

$$\mathbf{J} = \left(\begin{array}{c|c} \frac{\partial \underline{R}_e}{\partial \Delta \underline{\varepsilon}_e} & \frac{\partial \underline{R}_e}{\partial \Delta \underline{p}} \\ \hline \frac{\partial \underline{R}_p}{\partial \Delta \underline{\varepsilon}_e} & \frac{\partial \underline{R}_p}{\partial \Delta \underline{p}} \end{array} \right) = \left(\begin{array}{c|c} \underline{T4} & \underline{T2} \\ \hline \underline{T2} & \underline{Sc} \end{array} \right)$$

Calculation of the derivatives of $\underline{R}_e = \Delta \underline{\varepsilon}_e + \Delta p \underline{n}^\theta - \Delta \varepsilon$

$$\frac{\partial \underline{R}_e}{\partial \Delta \underline{\varepsilon}_e} = \underline{1} + \Delta p \frac{\partial \underline{n}}{\partial \underline{\sigma}} : \frac{\partial \underline{\sigma}}{\partial \underline{\varepsilon}_e} : \frac{\partial \underline{\varepsilon}_e}{\partial \Delta \underline{\varepsilon}_e}$$

$$\frac{\partial \underline{n}}{\partial \underline{\sigma}} = \underline{N} = \frac{1}{\sigma_{eq}} \left(\frac{3}{2} \underline{J} - \underline{n} \otimes \underline{n} \right)$$

where \underline{J} is such that $\underline{J} : \underline{a} = \text{deviator}(\underline{a})$

$$\frac{\partial \underline{\sigma}}{\partial \underline{\varepsilon}_e} = \underline{E}$$

$$\frac{\partial \underline{\varepsilon}_e}{\partial \Delta \underline{\varepsilon}_e} = \theta \underline{1}$$

so that:

$$\frac{\partial \underline{R}_e}{\partial \Delta \underline{\varepsilon}_e} = \underline{1} + \theta \underline{N} : \underline{E}$$

$$\frac{\partial \underline{R}_e}{\partial \Delta p} = \underline{n}$$

Calculation of the derivatives of $R_p = \sigma_{\text{eq}} - R(p)$

$$\boxed{\frac{\partial R_p}{\partial \underline{\Delta \underline{\varepsilon}_e}}} = \frac{\partial \sigma_{\text{eq}}}{\partial \underline{\sigma}} : \frac{\partial \underline{\sigma}}{\partial \underline{\varepsilon}_e} : \frac{\partial \underline{\varepsilon}_e}{\partial \underline{\Delta \underline{\varepsilon}_e}} = \boxed{\theta \underline{n} : \underline{\underline{E}}}$$

$$\boxed{\frac{\partial R_p}{\partial \Delta p}} = -\frac{\partial R}{\partial p} \frac{\partial p}{\partial \Delta p} = \boxed{-\theta H}$$

- **Tangent matrix**

$$\underline{\dot{\sigma}} = \underline{\underline{L}}_p : \underline{\dot{\epsilon}}$$

- Calculation :

$$\underline{\dot{\sigma}} = \underline{\underline{E}} : (\underline{\dot{\epsilon}} - \dot{p}\underline{n}) \quad \diamond$$

and

$$\dot{p} = \frac{\underline{n} : \underline{\underline{E}} : \underline{\dot{\epsilon}}}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

imply that

$$\underline{\underline{L}}_p = \underline{\underline{E}} - \frac{(\underline{\underline{E}} : \underline{n}) \otimes (\underline{n} : \underline{\underline{E}})}{\underline{n} : \underline{\underline{E}} : \underline{n} + H}$$

- The tangent matrix cannot be defined for viscoplastic materials

- “Consistent” tangent matrix

$$\underline{\underline{L}}_c = \frac{\partial \Delta \underline{\underline{\sigma}}}{\partial \Delta \underline{\underline{\varepsilon}}}$$

$$\Delta \underline{\underline{\sigma}} = \underline{\underline{E}} : (\Delta : \underline{\underline{\varepsilon}} - \Delta p \underline{\underline{n}})$$

- calculation

$$\begin{aligned} \delta \Delta \underline{\underline{\sigma}} &= \underline{\underline{E}} : (\delta \Delta \underline{\underline{\varepsilon}} - \delta \Delta p \underline{\underline{n}} - \Delta p \delta \underline{\underline{n}}) \\ \underline{\underline{E}} : (\delta \Delta \underline{\underline{\varepsilon}} - \delta \Delta p \underline{\underline{n}}) &= \underline{\underline{L}}_p : \delta \Delta \underline{\underline{\varepsilon}} \\ \Delta p \delta \underline{\underline{n}} &= \Delta p \frac{\partial \underline{\underline{n}}}{\partial \underline{\underline{\sigma}}} : \frac{\partial \underline{\underline{\sigma}}}{\partial \Delta \underline{\underline{\varepsilon}}} : \delta \Delta \underline{\underline{\varepsilon}} = \Delta p \underline{\underline{N}} : \underline{\underline{E}} : \delta \Delta \underline{\underline{\varepsilon}} + \dots \end{aligned}$$

so that

$$\underline{\underline{L}}_c \approx \underline{\underline{L}}_p - \Delta p \underline{\underline{E}} : \underline{\underline{N}} : \underline{\underline{E}} + O(\Delta p^2)$$

- The consistent tangent matrix can be defined for viscoplastic materials

- It is generally possible to write:

$$\begin{aligned}\mathbf{A} &= (\underline{\varepsilon}_e, \mathbf{a}) \\ \mathbf{R} &= (\mathbf{R}_e, \mathbf{R}_a) \\ \mathbf{R}_e &= \Delta \underline{\varepsilon}_e + \Delta \underline{\varepsilon}_{irr} - \Delta \underline{\varepsilon}\end{aligned}$$

- Influence of a variation of $\Delta \underline{\varepsilon}$ on the variations of integrated variables $(\underline{\varepsilon}_e, \mathbf{a})$?
- At the solution point \mathbf{R} must remain equal to $\mathbf{0}$

$$\delta \mathbf{R} = \mathbf{0} = \delta \begin{pmatrix} \Delta \underline{\varepsilon}_e + \Delta \underline{\varepsilon}_{irr} \\ \mathbf{R}_a \end{pmatrix} - \delta \begin{pmatrix} \Delta \underline{\varepsilon} \\ \mathbf{0} \end{pmatrix}$$

$$\delta \mathbf{R} = \frac{\partial \mathbf{R}}{\partial \mathbf{A}} \cdot \begin{pmatrix} \delta \Delta \underline{\varepsilon} \\ \mathbf{0} \end{pmatrix} = \mathbf{J} \cdot \delta \Delta \mathbf{A} - \begin{pmatrix} \delta \Delta \underline{\varepsilon} \\ \mathbf{0} \end{pmatrix}$$

- Therefore

$$\delta \Delta \mathbf{A} = \mathbf{J}^{-1} \cdot \begin{pmatrix} \delta \Delta \underline{\varepsilon} \\ \mathbf{0} \end{pmatrix}$$

- \mathbf{J}^{-1} can be expressed using sub-blocks

$$\mathbf{J}^{-1} = \mathbf{J}^* = \begin{pmatrix} \mathbf{J}_{ee}^* & \mathbf{J}_{ea}^* \\ \mathbf{J}_{ae}^* & \mathbf{J}_{aa}^* \end{pmatrix},$$

- so that

$$\delta \Delta \underline{\underline{\varepsilon}}_e = \mathbf{J}_{ee}^* \cdot \delta \Delta \underline{\underline{\varepsilon}}$$

- Using Hooke's law:

$$\underline{\underline{\sigma}}(t_1) = \underline{\underline{\sigma}}(t_0) + \Delta \underline{\underline{\sigma}} = \underline{\underline{E}}(t_1) : \underline{\underline{\varepsilon}}_e(t_1) = \underline{\underline{E}}(t_1) : (\underline{\underline{\varepsilon}}_e(t_0) + \Delta \underline{\underline{\varepsilon}}_e)$$

therefore

$$\delta \Delta \underline{\underline{\sigma}} = \underline{\underline{E}}(t_1) : \delta \Delta \underline{\underline{\varepsilon}}_e = \underline{\underline{E}}(t_1) : \underline{\underline{J}}_{ee}^* : \delta \Delta \underline{\underline{\varepsilon}}$$

- Finally

$$\underline{\underline{L}}_c = \underline{\underline{E}}(t_1) : \underline{\underline{J}}_{ee}^*$$

- In cases where $\underline{\underline{E}}$ depends on an integrated variable (e.g. d = damage) the calculation is more difficult

$$\Delta \underline{\underline{\sigma}} = \frac{\partial \underline{\underline{E}}}{\partial d} \delta \Delta d : \underline{\underline{\varepsilon}}_e + \underline{\underline{E}}(t_1) : \Delta \underline{\underline{\varepsilon}}_e$$

$$\underline{\underline{L}}_c = \frac{\partial \underline{\underline{E}}}{\partial d} : (\underline{\underline{\varepsilon}}_e \otimes \mathbf{J}_{de}^*) + \underline{\underline{E}} : \underline{\underline{J}}_{ee}^*$$

Explicit versus Implicit integration

Explicit	Implicit
easy to implement	difficult to implement
time consuming	efficient
$\underline{\underline{L}}_c$?	calculation of $\underline{\underline{L}}_c$

- $\underline{\underline{L}}_c$ can be evaluated using a perturbation method

$$L_{ijkl}^c = \frac{\sigma_{ij}(\Delta \underline{\underline{\varepsilon}} + \delta \varepsilon \underline{\underline{\mu}}^{kl}) - \sigma_{ij}(\Delta \underline{\underline{\varepsilon}})}{\delta \varepsilon}$$

- The tensor $\underline{\underline{\mu}}^{kl}$ is such that:

$$\mu_{ij}^{kl} = \delta_{ik} \delta_{lj}$$

- To introduce rate dependency (viscoplastity) the above equations need to be slightly modified
- Additive decomposition of deformations:

$$\underline{\varepsilon} = \underline{\varepsilon}_e + \underline{\varepsilon}_p$$

- Yield surface

$$\phi = \sigma_{eq} - R(p)$$

- Normality

$$\dot{\underline{\varepsilon}}_p = \dot{p} \frac{\partial \phi}{\partial \underline{\sigma}}$$

- ϕ can now be positive
- \dot{p} is given by a specific material dependent law

$$\dot{p} = \mathcal{F}(\phi)$$

\mathcal{F} is such that $\mathcal{F}(x) = 0$ if $x \leq 0$

- For instance (Norton law)

$$\dot{p} = \left\langle \frac{\phi}{K} \right\rangle^n$$

- Differential equations to be integrated are therefore

$$\begin{aligned}\dot{\underline{\varepsilon}}_e &= \dot{\underline{\varepsilon}} - \dot{p} \underline{n} \\ \dot{p} &= \left\langle \frac{\phi}{K} \right\rangle^n\end{aligned}$$

- Runge-Kutta integration is straightforward
- For the implicit integration

$$\begin{aligned}\underline{R}_e &= \Delta \underline{\varepsilon}_e + \Delta p \underline{n} - \Delta \underline{\varepsilon} \\ R_p &= \Delta p - \mathcal{F}(\phi) \Delta t\end{aligned}$$

- Evaluation of the Jacobian matrix: only the derivatives of R_p have to be re-computed with $\mathcal{F}' = \partial \mathcal{F} / \partial \phi$

$$\begin{aligned}\frac{\partial R_p}{\partial \Delta \underline{\varepsilon}_e} &= -\Delta t \frac{\partial \mathcal{F}}{\partial \phi} \frac{\partial \phi}{\partial \underline{\sigma}} : \frac{\partial \underline{\sigma}}{\partial \underline{\varepsilon}_e} : \frac{\partial \underline{\varepsilon}_e}{\partial \Delta \underline{\varepsilon}_e} = -\theta \Delta t \mathcal{F}' \underline{n} : \underline{\underline{E}} \\ \frac{\partial R_p}{\partial \Delta p} &= -\Delta t \frac{\partial \mathcal{F}}{\partial \phi} \frac{\partial \phi}{\partial R} \frac{\partial R}{\partial p} \frac{\partial p}{\partial \Delta p} = -\theta \Delta t \mathcal{F}' H\end{aligned}$$