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# Implementation of material constitutive equations in finite element codes

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## Introduction

Why is it important to know how to implement material constitutive equations in FE codes ?

- Few constitutive equations are available in commercial codes
- Implement new constitutive equations in FE codes (ABAQUS, ANSYS, MARC, ..., ASTER, CAST3M, ..., Zébulon, WARP3D)
- Understand convergence problems

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## Outline

- Definition of a constitutive equation (FE code point of view)
- Numerical integration methods (explicites/implicites)
- Consistent tangent matrix
- Particular case : von Mises material
- Convergence

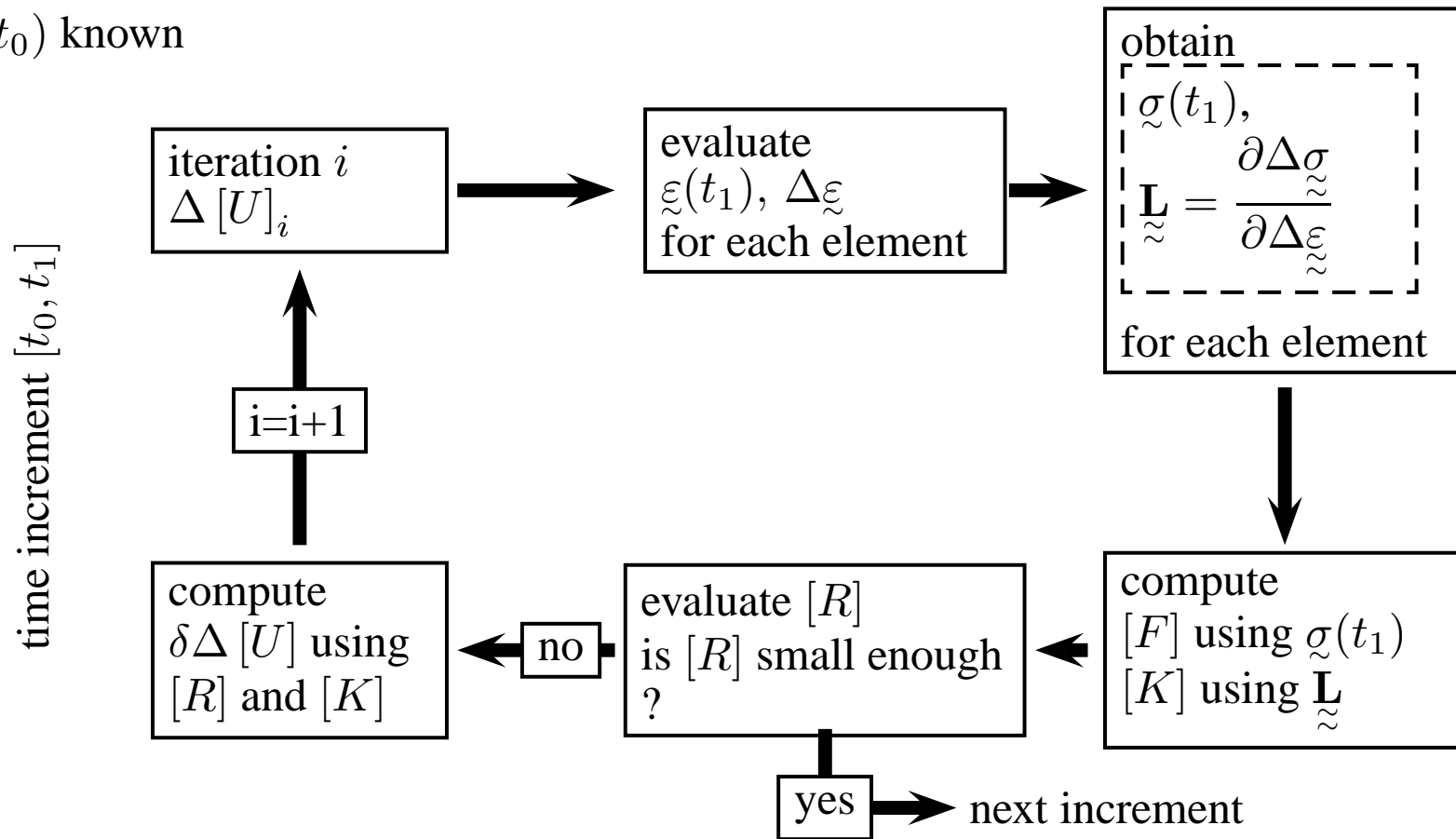
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## Definition of a constitutive equation

- For a displacement based FE formulation, nodal displacements are assumed to be known and therefore the deformations
- The constitutive equation must then supply: (i) stresses  $\underline{\sigma}$  and (ii) the consistent tangent matrix  $\underline{\underline{L}} = \partial \Delta \underline{\sigma} / \partial \Delta \underline{\varepsilon}$  for a given strain increment  $\Delta \underline{\varepsilon}$ .
- Complex constitutive equations are characterized by internal state variables  $[A]$ : the constitutive equation must provide an update of these variables consistent with the strain and time increment.

## Role of the constitutive equation in the FEM

$[U](t_0)$  known



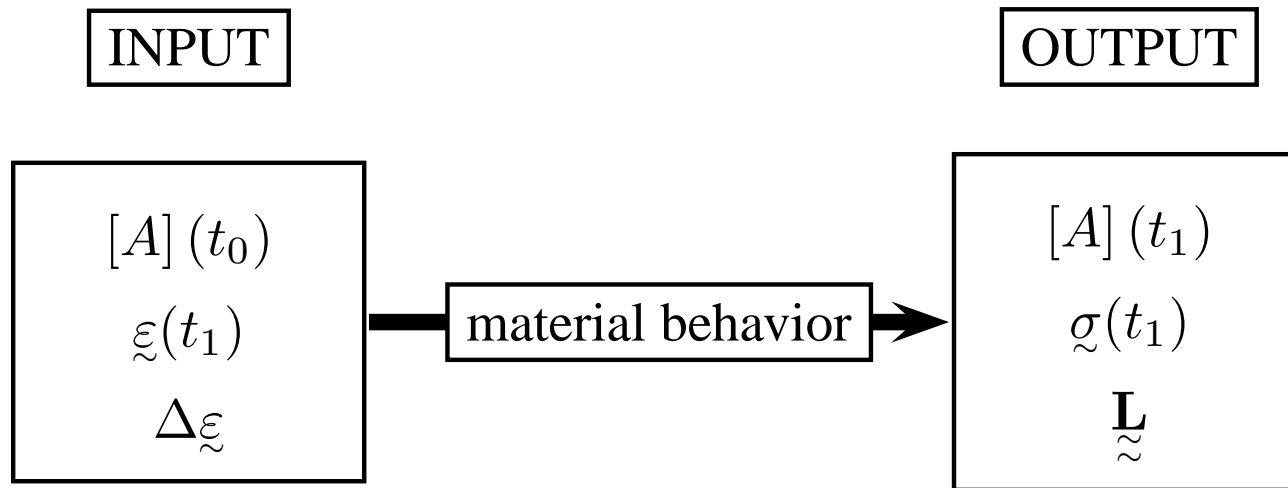
: global computation

: local time integration of the constitutive equations

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## Generic interface behavior/FEM

- $\Delta t = t_1 - t_0$

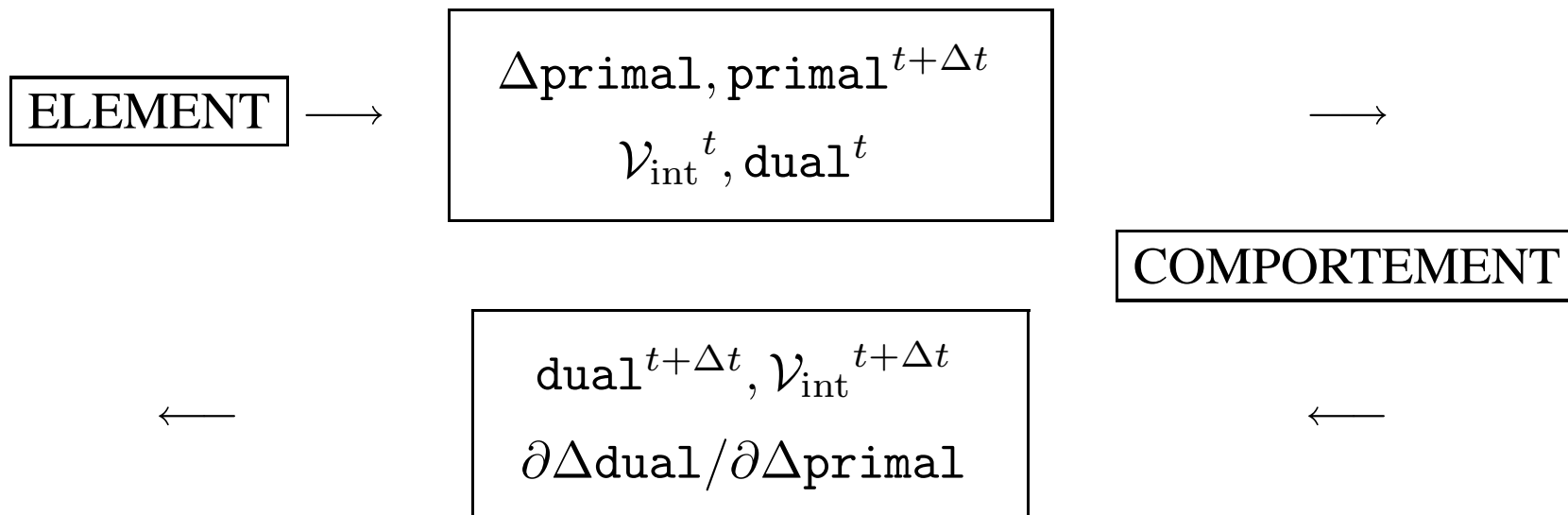


## Quantities characterising the material behavior

- Integrated variables/State variables ( $\mathcal{V}_{\text{int}}$ )
- Auxiliary variables ( $\mathcal{V}_{\text{aux}}$ )
- External parameters (EP)
- Coefficients (CO)

$$\text{CO} = \text{CO}(\text{EP}, \mathcal{V}_{\text{int}}, \mathcal{V}_{\text{aux}})$$

- Interface: input variable (primal), associated dual variable (dual), tangent matrix  $\partial\Delta\text{dual}/\partial\Delta\text{primal}$ .



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Examples of primal—dual couples

<b>problème</b>	primal	dual
mechanics (small deformation)	$\underline{\underline{\varepsilon}}$	$\underline{\underline{\sigma}}$
mechanics (finite strain)	$\underline{\underline{\mathbf{F}}}$	$\underline{\underline{\sigma}}$ ou $\underline{\underline{\mathbf{S}}}$
thermal problem	$(T, \underline{\underline{\text{grad}T})}$	$(H, \underline{\underline{\mathbf{q}}})$



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## Constitutive equations as a differential equation

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

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

- Time ( $t$ ) represents the imposed deformation but also an external parameter such as the temperature ( $T(\vec{x}, t)$ ).
- The FE evaluation of the Constitutive equation for  $(\Delta_{\underline{\varepsilon}}, \Delta)$  corresponds to the integration of the previous equation from  $t_0$  to  $t_1$ .
- In most cases:  $[A] = (\underline{\varepsilon}_e, \dots)$  so that  $\underline{\sigma}(t_1) = \underline{\mathbf{E}}(t_1) : \underline{\varepsilon}_e(t_1)$ ,
- $\underline{\mathbf{L}}$  must be computed ...

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## Integration methods of Constitutive equations

### Euler explicit method

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

- The method is not stable and should be avoided
- Explicit : because  $[\dot{A}]$  is computed at  $t_0$  for the known couple  $([A](t_0), t_0)$

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## Runge–Kutta explicit method

- Numerical estimation of the derivatives of  $[\dot{A}]$  (i.e.  $d^2 [F]_A / dt^2, d^3 [F]_A / dt^3, \dots$ )
- Error estimation to control the solution

The Runge–Kutta Integration method is easy to implement because it only uses the differential equation  $[\dot{A}] = [G] ([A], t)$ . It however has some drawbacks:

- Integration may require a large CPU time
- In the case of plastic materials, it is mandatory to compute the plastic multiplier which can be a difficult task (see below) in the case of temperature dependant material coefficients.

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## Runge–Kutta Method

Using a Taylor expansion, one gets for a time increment  $[t, t + \Delta t]$  (which can differ from the FE time step  $[t_0, t_1]$ ):

$$\{v\}(t + \Delta t) = \{v\}(t) + \{\dot{v}\}(t)\Delta t + O(\Delta t^2)$$

The accuracy of the Euler integration is therefore of magnitude  $O(\Delta t^2)$ . Based on this first estimation of the increment, another one can be performed using the mid-point (i.e.  $t + \Delta t/2$ ). Let:

$$\{\delta v_1\} = \Delta t \{\dot{v}\}(t)$$

and

$$\begin{aligned} \{\delta v_2\} &= \Delta t \{\dot{v}\}\left(t + \frac{\Delta t}{2}, \{v\}(t) + \frac{1}{2}\{\delta v_1\}\right) \\ &= \Delta t \left( \{\dot{v}\}(t) + \frac{\Delta t}{2} \{\ddot{v}\}(t) \right) \\ &= \{\delta v_1\} + \frac{\Delta t^2}{2} \{\ddot{v}\}(t) \end{aligned}$$

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This provides one way to estimate  $\{\ddot{v}\}(t)$ . The second order Taylor expansion is:

$$\{v\}(t + \Delta t) = \{v\}(t) + \{\dot{v}\}(t)\Delta t + \{\ddot{v}\}(t)\frac{\Delta t^2}{2} + O(\Delta t^3)$$

which can be simplified using the previous estimate of  $\{\ddot{v}\}(t)$ :

$$\{v\}(t + \Delta t) = \{v\}(t) + \{\delta v_2\} + O(\Delta t^3)$$

The precision has been improved ( $O(\Delta t^3)$  instead of  $O(\Delta t^2)$ ). This is a second order method.

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The procedure can be generalized. This leads to a 4th order Runge–Kutta method which is written as:

$$\{\delta v_1\} = \Delta t \{\dot{v}\} (t, \{v\})$$

$$\{\delta v_2\} = \Delta t \{\dot{v}\} \left( t + \frac{\Delta t}{2}, \{v\} + \frac{1}{2} \{\delta v_1\} \right)$$

$$\{\delta v_3\} = \Delta t \{\dot{v}\} \left( t + \frac{\Delta t}{2}, \{v\} + \frac{1}{2} \{\delta v_2\} \right)$$

$$\{\delta v_4\} = \Delta t \{\dot{v}\} (t + \Delta t, \{v\} + \{\delta v_3\})$$

$$\{v\} (t + \Delta t) = \{v\} (t) + \frac{1}{6} \{\delta v_1\} + \frac{1}{3} \{\delta v_2\} + \frac{1}{3} \{\delta v_3\} + \frac{1}{6} \{\delta v_4\} + O(\Delta t^5)$$

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## Runge–Kutta Method : error control

Aim: Obtain a given precision while minimize the computational effort

Make large time steps when the  $\{\dot{v}\}$  function varies little and smaller time steps if its evolution is rapid.

Let  $\Delta t$  be the time increment over which the itegration has to be performed. It can be divided into  $n$  sub-steps so that:

$$\Delta t = \sum_k \delta t_k$$

The error is estimated be applying the RK4 method

one time step       $\delta t$        $\rightarrow \{v_1\}$

two time steps     $\delta t/2$      $\rightarrow \{v_2\}$

This corresponds to 11 evaluations of  $\{\dot{v}\}$ .

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Let  $\{v\}(t + \delta t)$  be the exact solution; one gets

$$\begin{aligned}\{v\}(t + \delta t) &= \{v_1\} + (\delta t)^5 \{\phi\} + O(\delta t^6) \\ \{v\}(t + \delta t) &= \{v_2\} + 2(\delta t/2)^5 \{\phi\} + O(\delta t^6)\end{aligned}$$

$$\{\phi\} \approx \text{constant} \approx \frac{1}{5!} \{v^{(5)}\}$$

The difference between both estimations is an indicator the error:

$$\{E\} = \{v_2\} - \{v_1\}$$

This difference has to be kept smaller than a prescribed precision by adjusting  $\delta t$ . This equation can be solved neglecting  $O(\delta t^6)$  terms:

$$\{v\}(t + \delta t) = \{v_2\} + \frac{1}{15} \{E\} + O(\delta t^6)$$

This is a better estimation (5th order).



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$\{E\}$  can then be used to modify the time step. Let  $\{E^0\}$  be the requested precision (note that the precision is a vector).

$$\text{if } E_i < E_i^0, \forall i$$

The time step can be increased

$$\text{if } \exists i, E_i > E_i^0$$

The time step must be decreased

The time step is corrected by the following factor:

$$\alpha = \min_i \left| \frac{E_i^0}{E_i} \right|^{0.2}$$

as the error varies as  $\delta t^5$  for the 4th order Runge–Kutta method.

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$\{E^0\}$  must now be chosen.

The required precision must be obtained over the whole time increment  $\Delta t$  and not only on local sub steps  $\delta t_k$ . In that case the error is best defined as:

$$E_i^0 = \epsilon \delta t \left| \frac{dv_i}{dt} \right| = \epsilon |\delta v_i|$$

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## Implicite methods (or $\theta$ -methods)

- Evaluate  $[\dot{A}]$  at  $t_\theta$  between  $t_0$  et  $t_1$
- $t_\theta = t_0 + \theta\Delta t$  with  $0 \leq \theta \leq 1$
- Two solutions :

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

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

- Implicit :  $\Delta [A]$  appears on both left and right handsides of the previous equations
- Integrate the constitutive equation = solve the implicit equations
- $\theta = 0 \rightarrow$  Euler
- ...in the following the first method will only be considered

- Solution obtained by the Newton-Raphson method

- Write a residual vector

$$[R] (\Delta [A]) = \Delta [A] - [G] ([A] (t_0) + \theta \Delta [A] , t_0 + \theta \Delta t) \Delta t$$

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

- 1st order Taylor expansion around an estimation  $\Delta [A]_s$ :

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

- Construction of the next estimation:

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

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

## Note

- The internal variable vector  $[A]$  often contains 2nd order tensors
- The Voigt notation is used.

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

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## Integration — Simple Example : von Mises plasticity

- Additive Decomposition of deformations :

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

- Flow surface

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

- Normality

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

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

- $\dot{p}$  is computed using the consistency condition:  $\dot{\phi} = 0$

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

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



- so that:


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

- Differential equations to be integrated:

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

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



-  Pay attention to the dependance on external parameters (temperature...)
- Ready for the Runge–Kutta integration



## von Mises plasticity : implicit integration

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



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

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

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

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

- The equation

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

is exact but can be replaced by:

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



It is wrong if  $R$  depends on an external parameter (temperature,...) as:

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

The correct incremental equation is then:

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

This method should be avoided !

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## Residual vector

$$R_e = \Delta \xi_e + \Delta p \mathbf{n}^\theta - \Delta \varepsilon$$

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

$$R = (R_e, R_p)$$

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## Jacobian matrix ... a tough job

- The Jacobian matrix can be written by blocks:

$$[J] = \begin{pmatrix} \frac{\partial R_e}{\partial \Delta \tilde{\varepsilon}_e} & \frac{\partial R_e}{\partial \Delta p} \\ \frac{\partial R_p}{\partial \Delta \tilde{\varepsilon}_e} & \frac{\partial R_p}{\partial \Delta p} \end{pmatrix}$$

## Computation of the blocks related to $R_e = \Delta \xi_e + \Delta p \mathbf{n}^\theta - \Delta \varepsilon$

$$\frac{\partial R_e}{\partial \Delta \xi_e} = \underset{\sim}{\mathbf{1}} + \Delta p \frac{\partial \underset{\sim}{\mathbf{n}}}{\partial \underset{\sim}{\sigma}} : \frac{\partial \underset{\sim}{\sigma}}{\partial \xi_e} : \frac{\partial \xi_e}{\partial \Delta \xi_e}$$

$$\underset{\sim}{\mathbf{N}} \qquad \underset{\sim}{\mathbf{E}}^\theta \qquad \theta \underset{\sim}{\mathbf{1}}$$

$$\underset{\sim}{\mathbf{N}} = \frac{1}{\sigma_{\text{eq}}} \left( \frac{3}{2} \underset{\sim}{\mathbf{J}} - \underset{\sim}{\mathbf{n}} \otimes \underset{\sim}{\mathbf{n}} \right)$$

$$\Rightarrow \frac{\partial R_e}{\partial \Delta \xi_e} = \underset{\sim}{\mathbf{1}} + \Delta p \underset{\sim}{\mathbf{N}}^\theta : \underset{\sim}{\mathbf{E}}^\theta$$

$$\frac{\partial R_e}{\partial \Delta p} = \underset{\sim}{\mathbf{n}}^\theta$$

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**Computation of the blocks related to  $R_p = \sigma_{\text{eq}}^\theta - R(p^\theta)$**

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

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

## Tangent matrix vs. consistent tangent matrix

- Tangent matrix

$$\dot{\underline{\underline{\sigma}}} = \underline{\underline{\mathbf{L}}}_p : \dot{\underline{\underline{\varepsilon}}}$$

- Calculated as:

$$\dot{\underline{\underline{\sigma}}} = \underline{\underline{\mathbf{E}}} : (\dot{\underline{\underline{\varepsilon}}} - \dot{p} \underline{\underline{\mathbf{n}}}) \quad \img alt="Warning triangle icon" data-bbox="561 386 621 451"/>$$

and

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

imply

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

- Consistent tangent matrix

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

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

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

...

it can be shown that

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



## Automatic and generic computation of the consistent tangent matrix

- Internal variables and residuals can be expressed in a very general way as:

$$\begin{aligned}[A] &= (\underline{\xi}_e, [a]) \\ [R] &= ([R]_e, [R]_a) \\ [R]_e &= \Delta \underline{\xi}_e + \Delta \underline{\xi}_{\text{irr}} - \Delta \underline{\xi}\end{aligned}$$

- Influence of a small variation of  $\Delta \underline{\xi}$  on the internal variables  $(\underline{\xi}_e, [a])$  ? (around the solution)
- $[R]$  must stay null

$$\begin{aligned}\delta [R] = [0] &= \delta \begin{pmatrix} \Delta \underline{\xi}_e + \Delta \underline{\xi}_{\text{irr}} \\ [R]_a \end{pmatrix} - \delta \begin{pmatrix} \Delta \underline{\xi} \\ [0] \end{pmatrix} \\ \delta [R] &= \frac{\partial [R]}{\partial [A]} - \begin{pmatrix} \delta \Delta \underline{\xi} \\ [0] \end{pmatrix} = [J] \cdot \delta \Delta A - \begin{pmatrix} \delta \Delta \underline{\xi} \\ [0] \end{pmatrix}\end{aligned}$$

- Consequently

$$\delta\Delta A = [J]^{-1} \cdot \begin{pmatrix} \delta\Delta_{\tilde{\xi}} \\ [0] \end{pmatrix}$$

- $[J]^{-1}$  can be divided in sub-blocks:

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

- One therefore gets :

$$\delta\Delta_{\tilde{\xi}_e} = [J]_{ee}^* \cdot \delta\Delta_{\tilde{\xi}}$$

- Using the Hooke law (elasticity):

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

so that:

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

- The consistent tangent matrix is therefore given by:

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

- In case where  $\underline{\underline{\mathbf{E}}}$  depends on an internal variable (e.g.  $d$ =damage) then

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

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

## Explicit/Implicit

Explicit	Implicit
easy to implement	difficult to implement
slow	fast
$\mathbf{L}_{\approx}$ ?	direct computation of $\mathbf{L}_{\approx}$

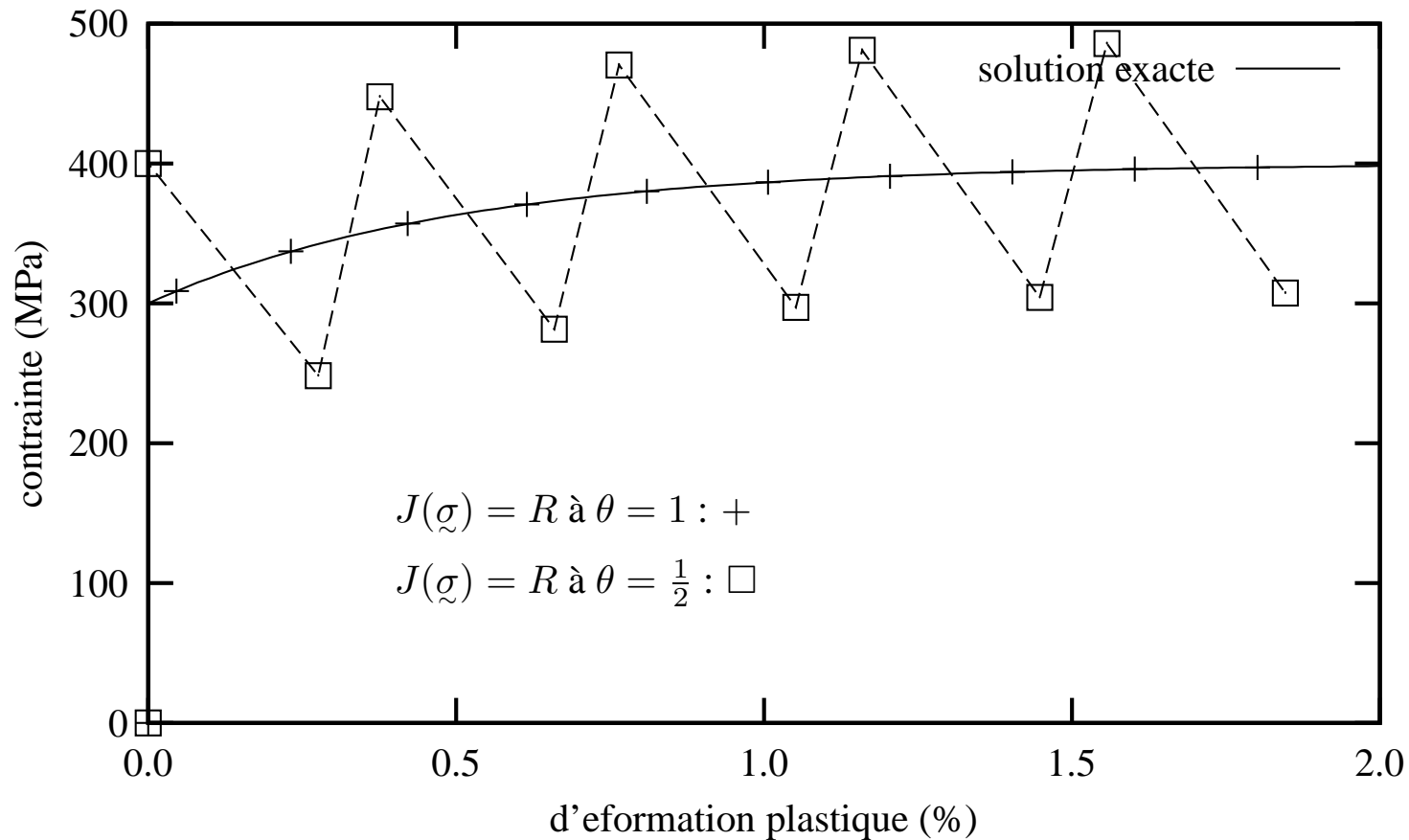
- $\mathbf{L}_{\approx}$  can be evaluated by perturbation

$$L_{ijkl} = \frac{\sigma_{ij}(\Delta \tilde{\varepsilon} + \delta \varepsilon \mu_{\approx}^{kl}) - \sigma_{ij}(\Delta \tilde{\varepsilon})}{\delta \varepsilon}$$

## Choosing de $\theta$ in the case of plasticity

The hardening law is

$$R(p) = 300 + 100(1 - \exp(-200p)) \quad \text{MPa}$$



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## Solution(s)

- Use  $\theta = 1$
- Write the residual  $R_p$  for  $\theta = 1$

$$R_e = \Delta \tilde{\xi}_e + \Delta p \tilde{\mathbf{n}}^\theta - \Delta \varepsilon$$

$$R_p = \sigma_{\text{eq}}^1 - R(p^1)$$

- Internal variables must be evaluated at both  $t_\theta$  ( $R_e$ ) and  $t_1 = t + \Delta t$  ( $R_p$ ) !

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## Plasticity : variable temperature

It is assumed that the flow stress  $R$  depends on temperature  $T$  The consistency condition is expressed as:

$$\dot{f} = \underline{\underline{\mathbf{n}}} : \underline{\underline{\dot{\boldsymbol{\sigma}}}} - R_{,p}\dot{p} - R_{,T}\dot{T} = 0$$

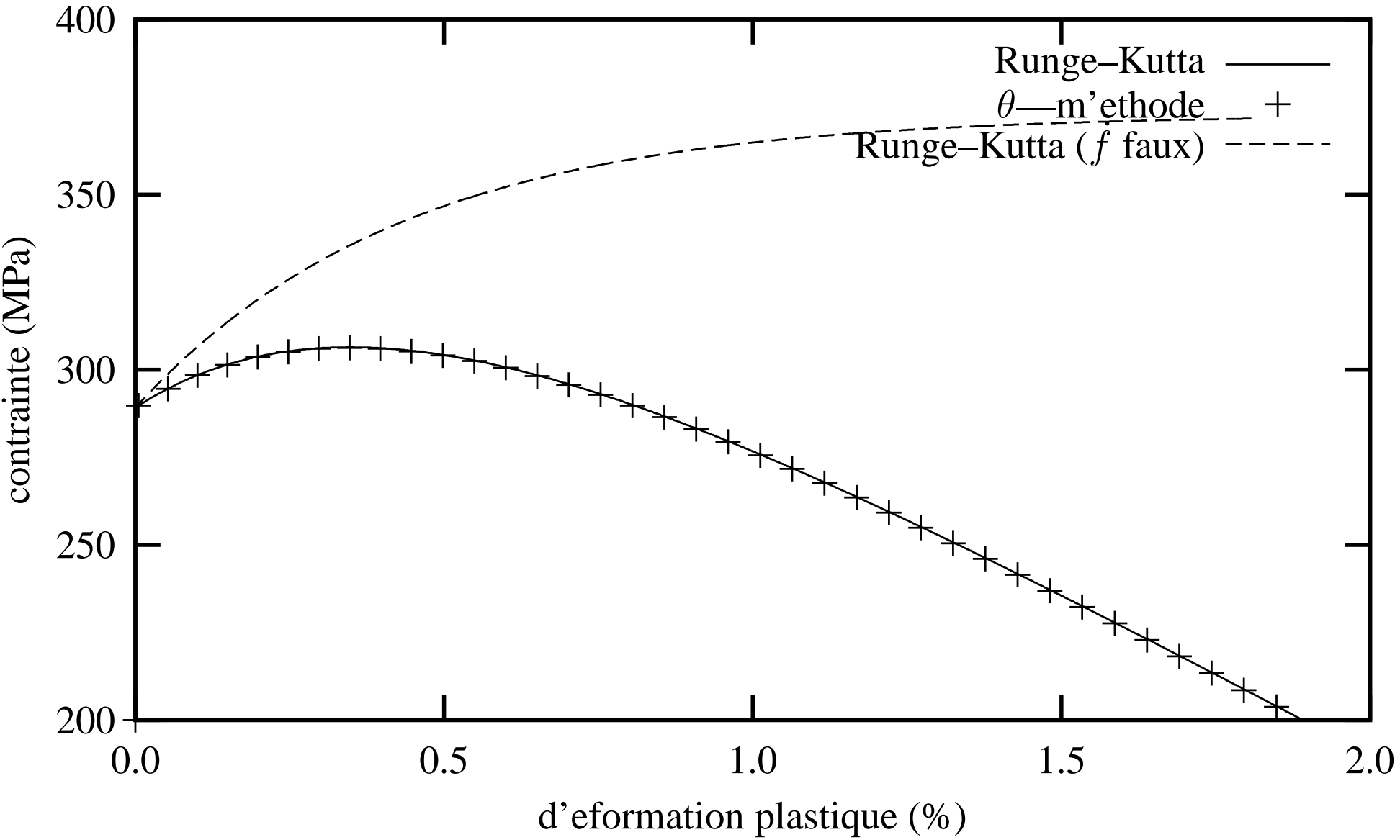
and one gets

$$\dot{p} = \frac{\underline{\underline{\mathbf{n}}} : \underline{\underline{\mathbf{C}}} : \underline{\underline{\dot{\boldsymbol{\epsilon}}}}_t - R_{,T}\dot{T}}{R_{,p} + \underline{\underline{\mathbf{n}}} : \underline{\underline{\mathbf{C}}} : \underline{\underline{\mathbf{n}}}}$$

using the previous exemple with:

$$R(p, T) = [300 + 100(1 - \exp(-200p))][1 - T/200]$$

it is shown the omitting the  $R_{,T}\dot{T}$  term in the consistency condition leads to wrong results:





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In the case where the elasticity coefficients also depend on temperature, this dependence must also be accounted for while writing the consistency condition. The plastic multiplier is then expressed as:

$$\dot{p} = \frac{\underline{\mathbf{n}} : \underline{\mathbf{C}} : \dot{\underline{\epsilon}}_t - \dot{T} \underline{\mathbf{n}} : \underline{\mathbf{C}}_{,T} : \epsilon_e - R_{,T} \dot{T}}{R_{,p} + \underline{\mathbf{n}} : \underline{\mathbf{C}} : \underline{\mathbf{n}}}$$

It may become difficult to take into account the various possible dependancies when several external parameters are prescribed.

This problems are avoided in the case of the  $\theta$ -method as in all case the yield condition is deirctly used  $f_{t+\Delta t} = 0$  and not  $\dot{f} = 0$ .

## Prandtl–Reuss law: creep

In the case of a viscous material,  $\dot{p}$  is directly obtained from the creep law:

$$\dot{p} = \phi(\underline{\sigma}, A_i)$$

$\theta$ -method:

$$r_p = \Delta p - \Delta t \phi(J - R, \dots)_\theta = 0$$

The partial derivatives related to the computation of the Jacobian matrix are:

$$\frac{\partial r_p}{\partial \Delta \underline{\xi}_e} = -\theta \Delta t \phi_{,\omega} \underline{\mathbf{C}} : \underline{\mathbf{n}}$$

$$\frac{\partial r_p}{\partial \Delta p} = 1 + \theta \Delta t R_{,p} \phi_{,\omega}$$

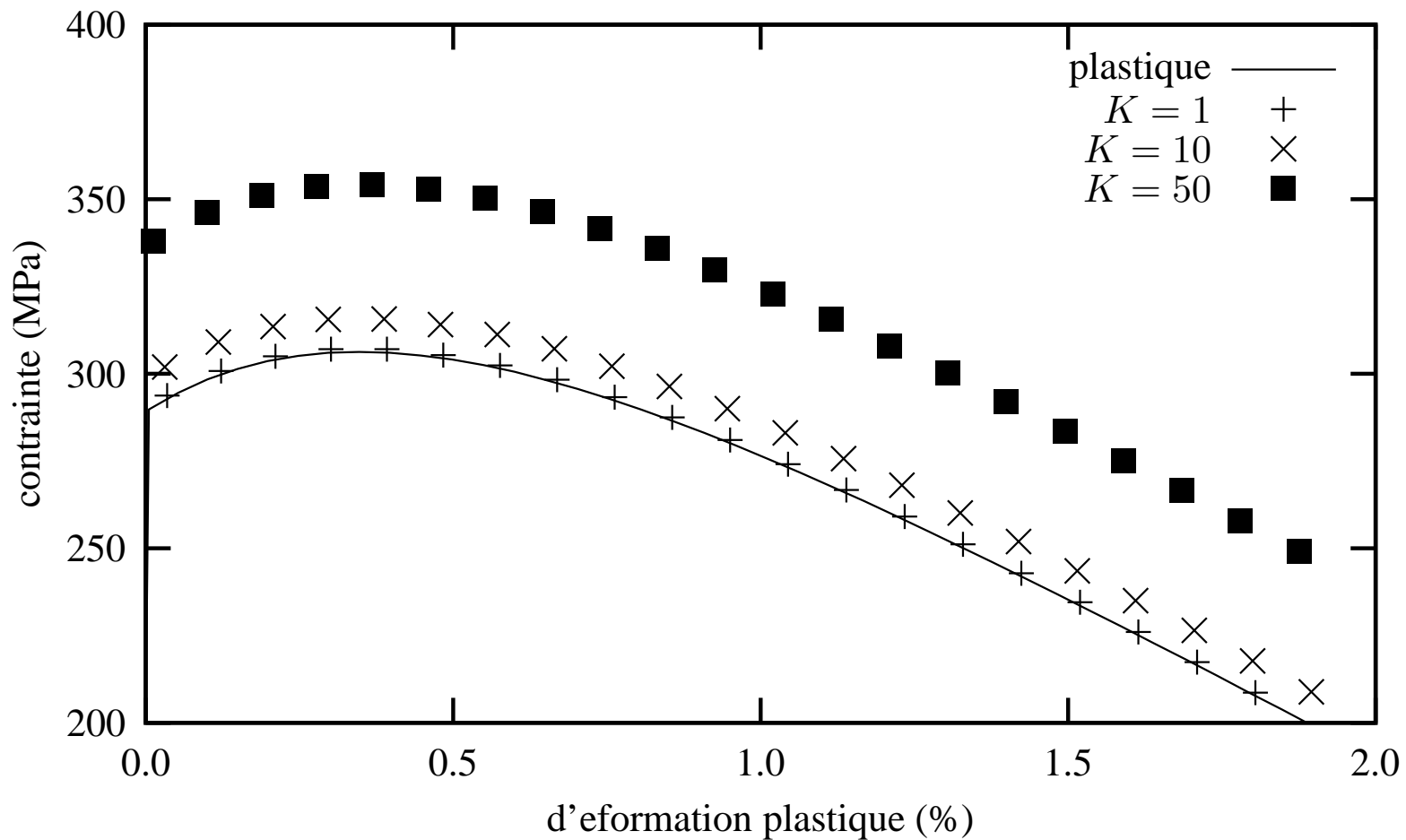
There are not longer problems related to the calculation of the consistency condition. A “creep law” can be used to mimic plasticity. For instance using a Norton law

$$\phi(\omega) = \left\langle \frac{\omega}{K} \right\rangle^n$$

if  $n$  is high enough, one gets

$$J - R \simeq K$$

- example with  $n = 10$  and  $K = 1, 10, 50$ . When  $K$  is small enough, the viscoplastic solution tends towards the plastic solution



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## Multi-kinematic law : constitutive equations

- The law is expressed using the following state internal variables

$\underline{\underline{\epsilon}}_e$  elastic strain tensor

$\underline{\underline{\alpha}}_i$  kinematic hardening variable tensors

$r$  isotropic hardening variable

- The following variable is an auxiliary variable:

$p$  cumulated plastic strain

Forces associated to the state variables are:

$$\begin{aligned}\underline{\underline{\sigma}} &= \underline{\underline{\mathbf{C}}} : \underline{\underline{\epsilon}}_e \\ \underline{\underline{\mathbf{X}}}_i &= \underline{\underline{\mathbf{C}}}_i : \underline{\underline{\alpha}}_i \\ R &= cr\end{aligned}$$

- The back-stress  $\underline{\underline{\mathbf{X}}}$  is given by:

$$\underline{\underline{\mathbf{X}}} = \sum_i \underline{\underline{\mathbf{X}}}_i$$

The evolution laws are given by:

$$\begin{aligned}\dot{\underline{\underline{\xi}}}_e + \dot{\underline{\underline{\xi}}}_p &= \dot{\underline{\underline{\xi}}}_t \\ \dot{\underline{\underline{\alpha}}}_i &= \dot{\underline{\underline{\xi}}}_p - \dot{p} \underline{\underline{\mathbf{D}}}_i : \underline{\underline{\alpha}}_i \\ \dot{r} &= \dot{p} - \dot{p} b r\end{aligned}$$

- The plasticity criterion is given by:

$$f = \|\underline{\underline{\sigma}} - \underline{\underline{\mathbf{X}}}\|_M - \sigma_y - R \geq 0$$

$\sigma_y$  is the size of the initial elastic domain. The norm  $\|\cdot\|_M$  is used to model plastic anisotropy:

$$\|\underline{\underline{\mathbf{a}}}\|_M = \left( \underline{\underline{\mathbf{a}}} : \underline{\underline{\mathbf{M}}} : \underline{\underline{\mathbf{a}}} \right)^{\frac{1}{2}}$$

where  $\underline{\underline{\mathbf{M}}}$  is a fourth order tensor such that  $\underline{\underline{\mathbf{M}}} : \underline{\underline{\mathbf{1}}} = \underline{\underline{\mathbf{0}}}$ .

- In the viscous case (studied in the following)

$$\dot{p} = \phi(f, \dots)$$

- The flow direction (normality) is expressed as:

$$\underline{\mathbf{n}} = \frac{\partial f}{\partial \underline{\boldsymbol{\sigma}}} = \frac{1}{\|\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}}\|_M} \underline{\mathbf{M}} : (\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}})$$

- To compute the Jacobian matrix, the following tensor is also needed:

$$\underline{\mathbf{N}} = \frac{\partial \underline{\mathbf{n}}}{\partial \underline{\boldsymbol{\sigma}}} = \frac{\partial^2 f}{\partial \underline{\boldsymbol{\sigma}}^2} = \frac{1}{\|\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}}\|_M} \left( \underline{\mathbf{M}} - \frac{1}{\|\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}}\|_M^2} \underline{\mathbf{M}} : (\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}}) \otimes \underline{\mathbf{M}} : (\underline{\boldsymbol{\sigma}} - \underline{\mathbf{X}}) \right)$$

- $\underline{\mathbf{C}}_i$ ,  $\underline{\mathbf{D}}_i$  and  $\underline{\mathbf{M}}$  are used to model anisotropy. The isotropic case corresponds to:

$$\underline{\mathbf{C}}_i = C_i \underline{\mathbf{1}}, \underline{\mathbf{D}}_i = D_i \underline{\mathbf{1}} \text{ and } \underline{\mathbf{M}} = \underline{\mathbf{J}}.$$

- Runge–Kutta is straightforward !

## Multi-kinematic law : $\theta$ -method

- The time discretization of the previous equations leads to:

$$\begin{aligned} \mathbf{r}_e &= \Delta \underline{\xi}_e + \Delta p \mathbf{n} - \Delta \underline{\xi}_t = \mathbf{0} \\ \mathbf{r}_{\alpha_i} &= \Delta \underline{\alpha}_i - \Delta p \mathbf{n} + \Delta p \mathbf{D}_i : \underline{\alpha}_i + \theta D_i \Delta \underline{\alpha}_i \Delta p = \mathbf{0} \\ r_r &= \Delta r - \Delta p (1 - br) = 0 \\ r_p &= \Delta p - \phi(f, \dots) \Delta t = 0 \end{aligned}$$

- Variables  $\underline{\xi}_e$ ,  $\underline{\alpha}_i$ ,  $r$  are considered e time  $t + \theta \Delta t$  and are equal to:  $\underline{\xi}_e(t) + \theta \Delta \underline{\xi}_e$ ,  $\underline{\alpha}_i(t) + \theta \Delta \underline{\alpha}_i$ ,  $r + \theta \Delta r$ .
- Plasticity can be treated writting:

$$r_p = \left\| \underline{\sigma} - \underline{\mathbf{X}} \right\|_M - R - \sigma_y = 0 \Big|_1$$

- The Jacobian matrix is expressed in the following slides ...

$$\underline{\mathbf{r}}_e = \Delta \underline{\boldsymbol{\epsilon}}_e + \Delta p \underline{\mathbf{n}} - \Delta \underline{\boldsymbol{\epsilon}}_t = \underline{\mathbf{0}}$$

$$\frac{\partial \underline{\mathbf{r}}_e}{\partial \Delta \underline{\boldsymbol{\epsilon}}_e} = \underline{\mathbf{1}} + \theta \Delta p \underline{\mathbf{N}} \underline{\mathbf{C}}$$

$$\frac{\partial \underline{\mathbf{r}}_e}{\partial \Delta \alpha_i} = \Delta p \frac{\partial \underline{\mathbf{n}}}{\partial \underline{\mathbf{X}}_i} \frac{\partial \underline{\mathbf{X}}_i}{\partial \alpha_i} \frac{\partial \alpha_i}{\partial \Delta \alpha_i} = -\theta \Delta p \underline{\mathbf{N}} \underline{\mathbf{C}}_i$$

$$\frac{\partial \underline{\mathbf{r}}_e}{\partial \Delta r} = 0$$

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



$$\mathbf{r}_{\alpha_i} = \Delta \alpha_i - \Delta p \mathbf{n} + \Delta p \mathbf{D}_i : \alpha_i + \theta D_i \Delta \alpha_i \Delta p = \mathbf{0}$$

$$\frac{\partial \mathbf{r}_{\alpha_i}}{\partial \Delta \xi_e} = -\Delta p \frac{\partial \mathbf{n}}{\partial \sigma} \frac{\partial \sigma}{\partial \xi_e} \frac{\partial \xi_e}{\partial \Delta \xi_e} = -\theta \Delta p \mathbf{N} \mathbf{C}$$

$$\frac{\partial \mathbf{r}_{\alpha_i}}{\partial \Delta \alpha_i} = \mathbf{1} + \theta \Delta p \mathbf{D}_i$$

$$\frac{\partial \mathbf{r}_{\alpha_i}}{\partial \Delta r} = 0$$

$$\frac{\partial \mathbf{r}_{\alpha_i}}{\partial \Delta p} = -\mathbf{n} + \mathbf{D}_i : \alpha_i$$

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$$r_r = \Delta r - \Delta p(1 - br) = 0$$

$$\frac{\partial r_r}{\partial \Delta \xi_e} = \underset{\sim}{0}$$

$$\frac{\partial r_r}{\partial \Delta \alpha_i} = \underset{\sim}{0}$$

$$\frac{\partial r_r}{\partial \Delta r} = 1 + \theta \Delta p d$$

$$\frac{\partial r_r}{\partial \Delta p} = br$$

$$\boxed{r_p = \Delta p - \phi(f, \dots) \Delta t}$$

$$\frac{\partial r_p}{\partial \Delta \xi_e} = - \frac{\partial F}{\partial f} \frac{\partial f}{\partial \sigma} \frac{\partial \sigma}{\partial \xi_e} \frac{\partial \xi_e}{\partial \Delta \xi_e} = -\theta \Delta t \phi_{,f} \mathbf{n} : \mathbf{C}_{\xi_e}$$

$$\frac{\partial r_p}{\partial \Delta \alpha_i} = \theta \Delta t \phi_{,f} \mathbf{n} : \mathbf{C}_i$$

$$\frac{\partial r_p}{\partial \Delta r} = - \frac{\partial \phi}{\partial R} \frac{\partial R}{\partial r} \frac{\partial r}{\partial \Delta r} \Delta t = \theta \Delta t c \phi_{,f}$$

$$\frac{\partial r_p}{\partial \Delta p} = 1$$

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## Multi-kinematic law : static recovery

Static recovery can easily be added by modifying the evolution laws for the hardening (both isotropic and kinematic) variables:

$$\begin{aligned}\dot{\underline{\alpha}}_i &= \dot{\underline{\epsilon}}_p - \dot{p} \underline{\mathbf{D}}_i : \underline{\alpha}_i - \underline{\mathbf{S}}_i : \underline{\alpha}_i \\ \dot{r} &= \dot{p} - \dot{p}br - sr\end{aligned}$$

In the calculation of the Jacobian matrix, the following terms must be added:

$$\begin{aligned}-\theta \Delta t \underline{\mathbf{S}}_i &\quad \dot{\alpha} \quad \partial \underline{\mathbf{r}}_{\alpha_i} / \partial \Delta \alpha_i \\ -\theta \Delta t s &\quad \dot{r} \quad \partial \underline{\mathbf{r}}_{\alpha_i} / \partial \Delta r\end{aligned}$$

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## Multi-kinematic law : variable temperature

- Material coefficients may depend on external parameters and state variables
- These coefficients must be evaluated at  $t$ ,  $t + \theta\Delta t$  or  $t + \Delta t$ .
- In the case of the Runge–Kutta integration, using a viscous creep law allows to bypass the computation of the plastic multiplier using the consistency condition.
- An error is often done...

The relationships

$$\underline{\tilde{\mathbf{X}}} = \frac{2}{3}C\tilde{\underline{\alpha}} \quad \dot{\tilde{\underline{\alpha}}} = \dot{\tilde{\underline{\epsilon}}}_p - \frac{3}{2}\dot{p}\frac{D}{C}\tilde{\underline{\alpha}}$$

are replaced by

$$\dot{\tilde{\underline{\mathbf{X}}}} = \frac{2}{3}C\dot{\tilde{\underline{\epsilon}}}_p - D\dot{p}\tilde{\underline{\mathbf{X}}}$$

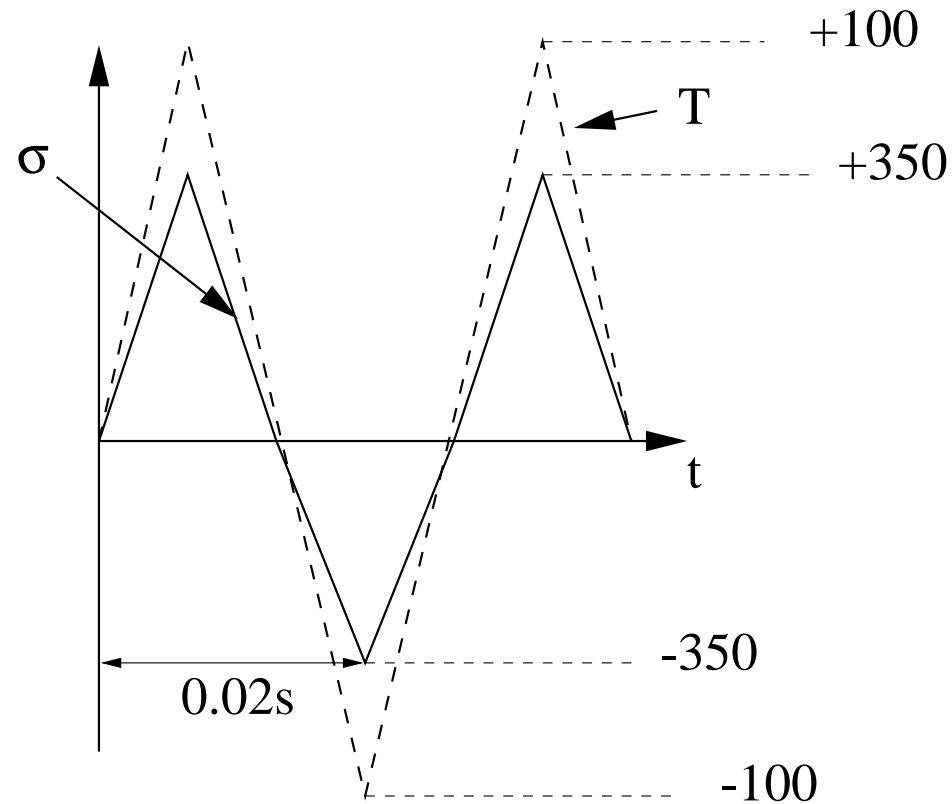
which is only valid if  $C$  is a constant. In fact:

$$\dot{\tilde{\underline{\mathbf{X}}}} = \frac{2}{3}d(C\tilde{\underline{\alpha}})/dt = \frac{2}{3}C_{,T}\dot{T}\tilde{\underline{\alpha}} + \frac{2}{3}C\dot{\tilde{\underline{\alpha}}}$$

- Comparaision of the results with

$$\begin{array}{l} C = 30000(1 - T/200) \quad D = 200 \\ K = 20 \quad n = 10 \quad R = 300 \quad E = 200000 \end{array}$$

and the following load path



In both cases, ratchetting is obtained but the results strongly differ

