Plasticity in FEniCS

Piotr Minakowski

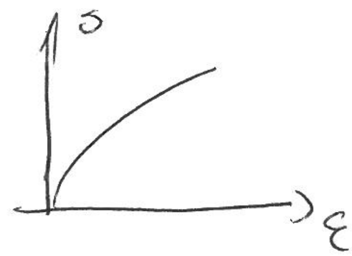
Institute of Applied Mathematics and Mechanics, University of Warsaw
E-mail: minak@mimuw.edu.pl
Mathematical Institute, Charles University
E-mail: minak@karlin.mff.cuni.cz

SEMINÁŘ O SOFTWARU PRO GEOFYZIKY aneb Jednoocí slepým

Outline

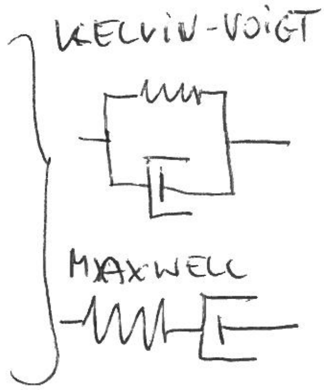
Jednoocí slepým Plasticity in FEniCS

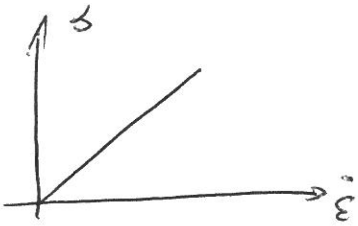
1 1D analogue



elastic

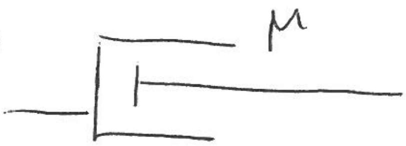
$\sigma = E\varepsilon$

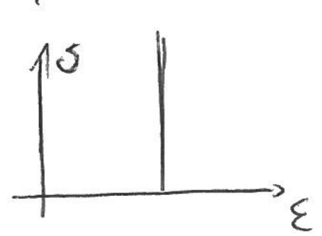




viscous

$\sigma = \mu\dot{\varepsilon}$

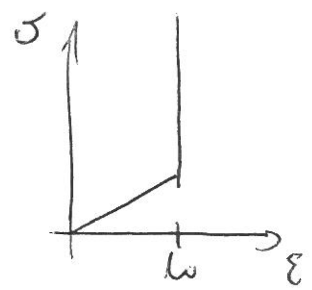


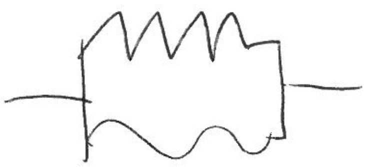


string

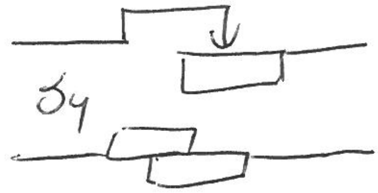
$|\varepsilon| < l_0$

example:





PLASTIC / FRICTIONAL ELEMENT



Response

$\dot{\varepsilon}_p = 0 \Leftrightarrow |\sigma| < \sigma_y$

$\dot{\varepsilon}_p \neq 0 \Leftrightarrow |\sigma| = \sigma_y$

$\sigma = \sigma_y \operatorname{sgn}(\dot{\varepsilon}_p)$

Admissible stress range

$f(\sigma) = |\sigma| - \sigma_y \leq 0$

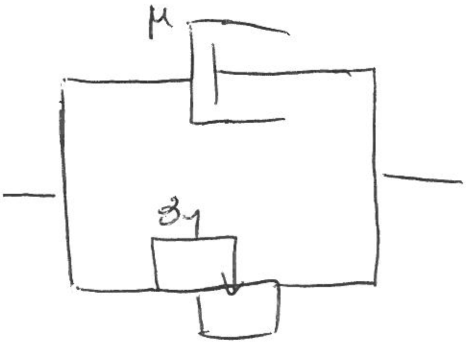
strain rate in direction of applied stress

$\dot{\varepsilon}^p = \gamma \operatorname{sgn}(\sigma)$, $\gamma \geq 0$

LOADING/UNLOADING.

$\gamma \cdot f(\sigma) = 0$

example



visco-plastic

$\sigma = \sigma_v + \sigma_p$

$\varepsilon = \varepsilon_p = \varepsilon_e$

$\sigma = \mu\dot{\varepsilon} + \sigma_y \operatorname{sgn}\dot{\varepsilon}$

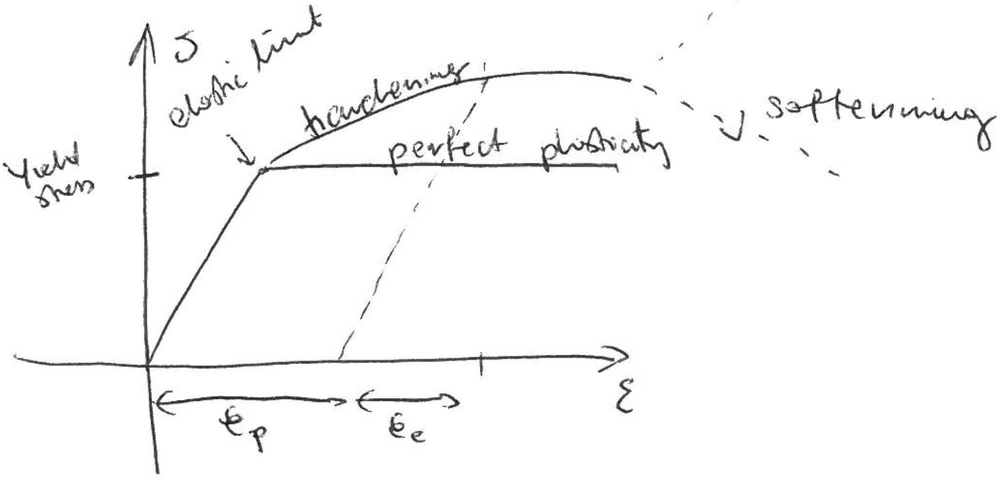
BINGHAM.

Kuhn-Tucker conditions.

$\gamma \cdot \dot{f}(\sigma) = 0$

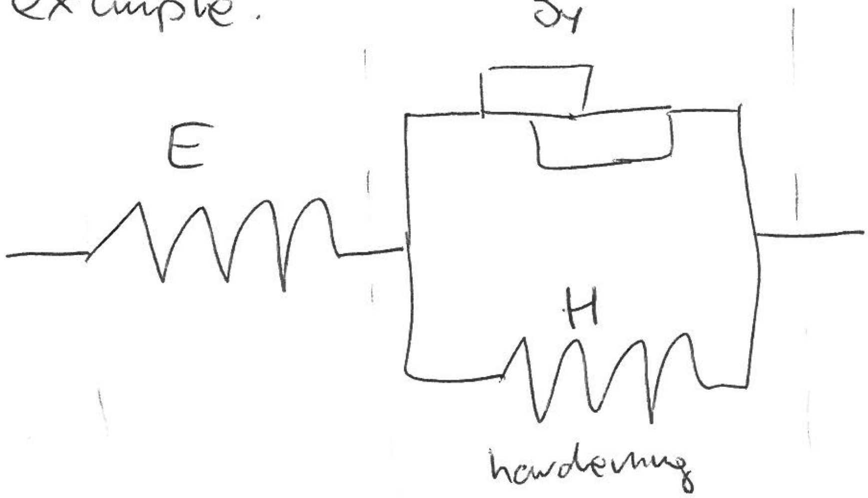
consistency conditions

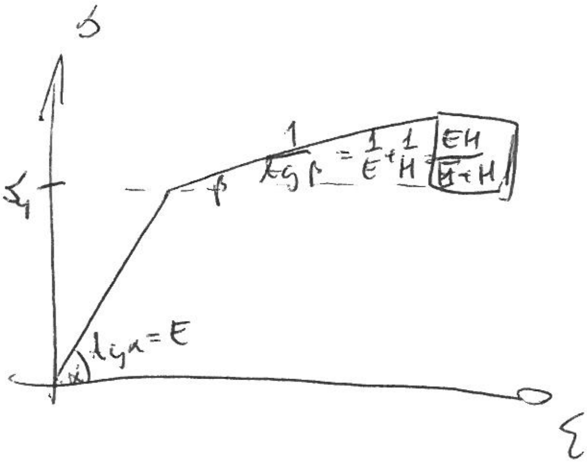
② Stress - Strain Curve



example:

Strain hardening



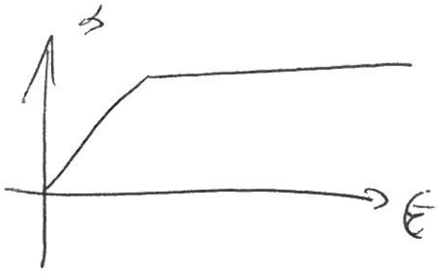


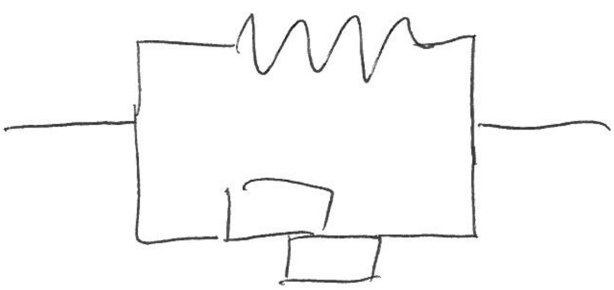
$$\overbrace{\varepsilon \quad = \quad \varepsilon_e}\quad + \quad \overbrace{\varepsilon_p = \varepsilon_H}$$

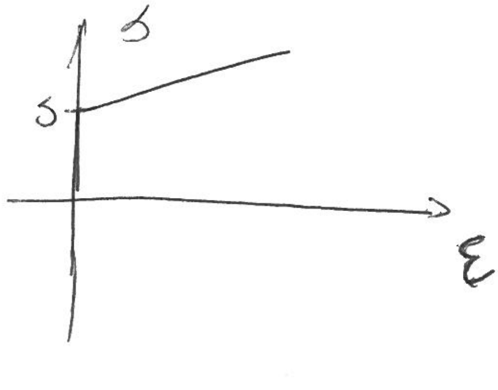
$$\sigma = \sigma_e = \sigma_{pH} + \sigma_H$$

Example

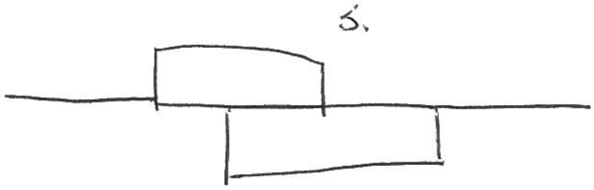
elastoplastic

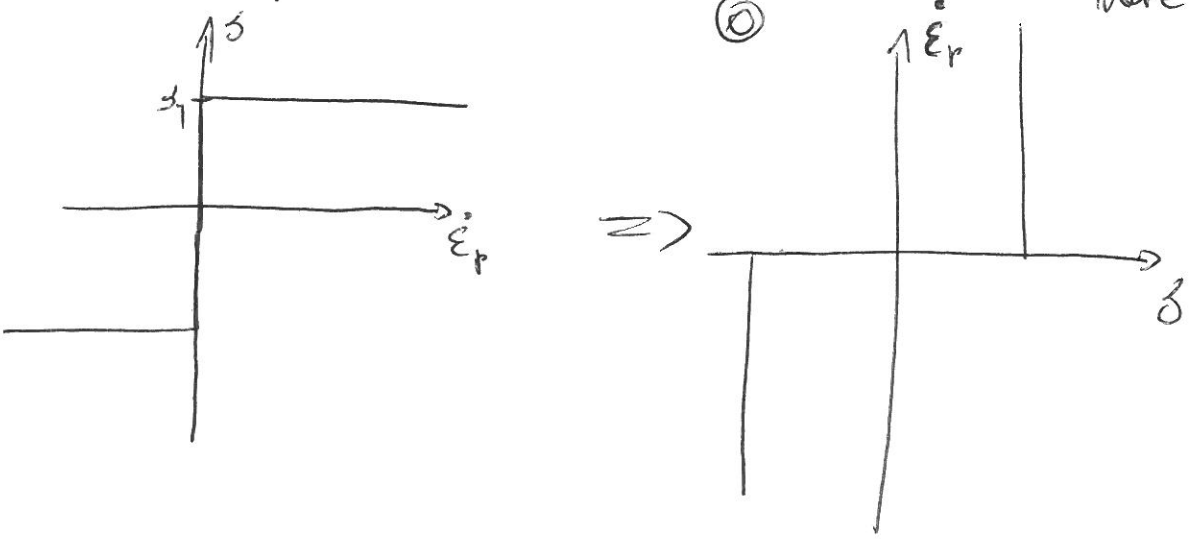




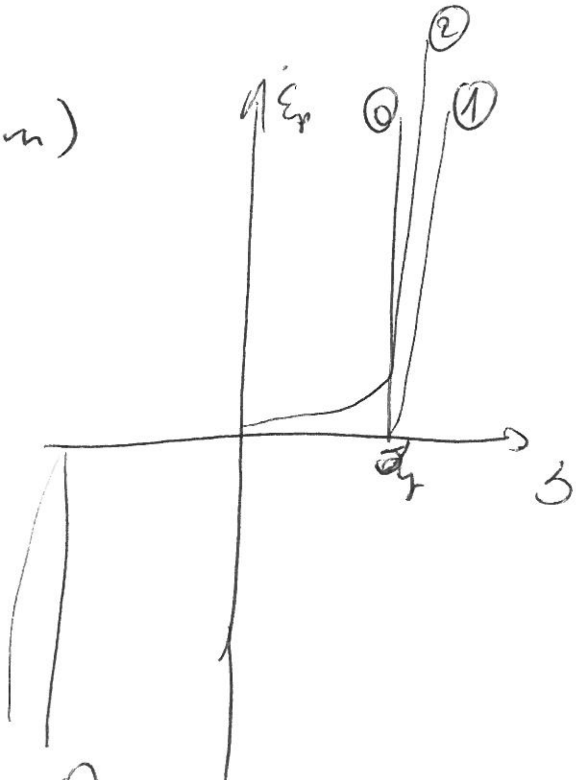


③



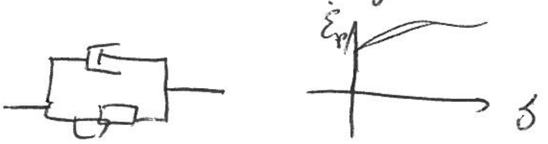


From stress we can not determine rate of strain !



What we can do

① Add viscosity (like Bingham)



② rate type approximation

$$\dot{\varepsilon}_p = \mathrm{sgn}(\sigma)\left(\frac{|\sigma|}{\sigma_y}\right)^{k}$$

③ Implicit (on the curve)

$$f\left(|\sigma|\,\dot{\varepsilon}_p - \varepsilon_p \sigma_y\right) + \left(|\sigma| + \sigma_y\right)_+ = 0$$

$f(x) = |x| \quad x^2 \quad \arctan x$

FRICTIONAL ELEMENT

σ - balance law

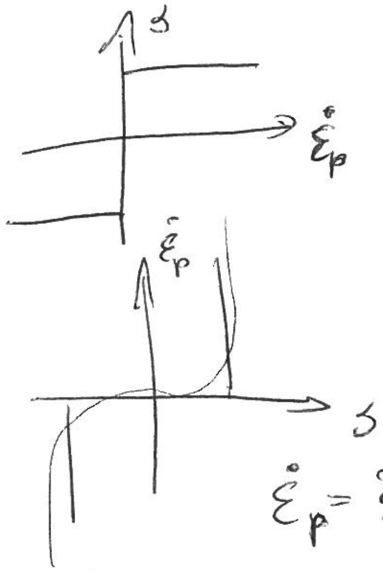
ε

$\dot\varepsilon_p = 0 \Rightarrow |\sigma| < \sigma_y$

$\dot\varepsilon_p \neq 0 \Rightarrow |\sigma| = \sigma_y$

$\sigma = \sigma_y \operatorname{sgn} \dot\varepsilon_p$

$\sigma = \sigma_e + \sigma_p$



$\sigma = E(\varepsilon - \varepsilon_p)$

↓ we need rate

$\dot\sigma = E(\dot\varepsilon - \dot\varepsilon_p)$

$\dot\varepsilon_p = ?$

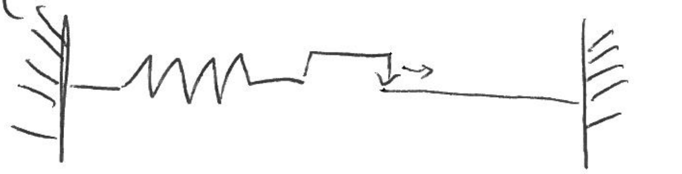
Implicitly (on the curve)

$$\| |\sigma| \dot\varepsilon_p - \varepsilon_p \sigma_y \| + (|\sigma| - \sigma_y)_+ = 0$$

if $\dot\varepsilon_p = \dot\gamma$

or $\dot\varepsilon_p = \operatorname{sgn}(\sigma)\, \sigma^\alpha$

+ BC



Topic of investigation

1D elastoplasticity

$\varepsilon = \varepsilon^e + \varepsilon^p$

$\sigma = E \varepsilon_e$

Yield $\phi(\sigma, \sigma_y) = |\sigma| - \sigma_y \leq 0$

Flow rule $\dot\varepsilon_p = \dot\gamma \operatorname{sgn}(\sigma)$

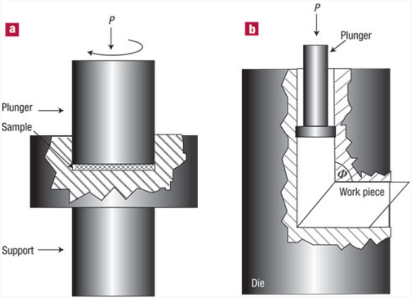
Hardening

loading / unloading $\dot\gamma\, \Phi \geq 0.$

Motivations

Severe plastic deformation:

- large proportion of shear during deformation
- large strains (torsion experiment with multiple rotations)
- no major changes of shape and cross section
- changes of internal properties by grain refinement (UFG)

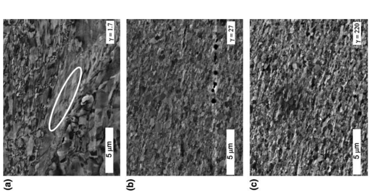


HPT / ECAE

Aims:

- formulate flow model of crystal plasticity (Eulerian coordinates)
- provide consistent thermodynamic description
- observe formation of shear bands, reach steady state micro-structure
- validate by comparison with experimental data

ECAE



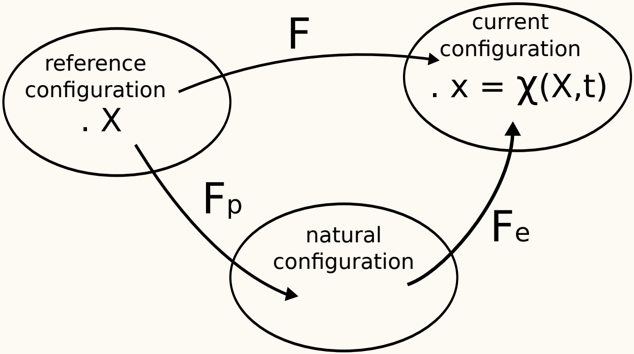
HPT

Large-deformation plasticity

Kröner decomposition

$$\mathbf{F} = \mathbf{F_e F_p}$$

- $\mathbf{F_e}$, the elastic distortion, stretch and rotation of the lattice
- $\mathbf{F_p}$, the plastic distortion distortion of the lattice due to formation of dislocations



The velocity gradient

In the virtue of Kröner decomposition

$$\nabla \mathbf{v} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{F}_\mathbf{e}}(\mathbf{F}_\mathbf{e})^{-1} + \mathbf{F}_\mathbf{e}(\dot{\mathbf{F}_\mathbf{p}}\left(\mathbf{F}_\mathbf{p}\right)^{-1})\left(\mathbf{F}_\mathbf{e}\right)^{-1}.$$

Let us denote by $\mathbf{L}_\mathbf{e}$ and $\mathbf{L}_\mathbf{p}$ elastic and plastic parts of velocity gradient (also called distortion-rate tensors)

$$\mathbf{L}_\mathbf{e} = \dot{\mathbf{F}_\mathbf{e}}\mathbf{F}_\mathbf{e}{}^{-1}, \quad \mathbf{L}_\mathbf{p} = \dot{\mathbf{F}_\mathbf{p}}(\mathbf{F}_\mathbf{p})^{-1}.$$

We have the decomposition

$$\nabla \mathbf{v} = \mathbf{L}_\mathbf{e} + \mathbf{F}_\mathbf{e}\mathbf{L}_\mathbf{p}(\mathbf{F}_\mathbf{e})^{-1}.$$

Moreover all the volumetric changes are assumed to result from elastic stretches in the lattice,

$$\det \mathbf{F}_\mathbf{p} = 1, \quad \det \mathbf{F} = \det \mathbf{F}_\mathbf{e} > 0.$$

Cauchy stress

Balance equation

Cauchy stress tensor $\mathbf{T}$ is divergence free

$$\operatorname{div} \mathbf{T} = 0$$

Jaumann rate of the Cauchy stress $\mathbf{T}$

$$\dot{\mathbf{T}} + \operatorname{div} \mathbf{v}\mathbf{T} - \mathbf{W}\mathbf{T} + \mathbf{T}\mathbf{W} = \mathcal{C} : \mathbf{D_e}$$

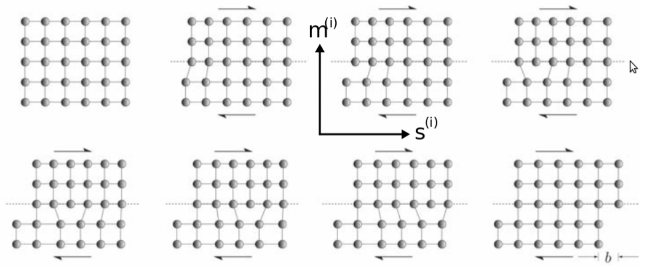
where $\mathbf{D} = \mathit{sym}(\mathbf{L})$, $\mathbf{W} = \mathit{skew}(\mathbf{L})$ and $\mathcal{C}$ is fourth order spatial elastic tensor

$$\mathcal{C} : \mathbf{D} = \lambda(\operatorname{tr} \mathbf{D})\mathbf{I} + 2\mu\mathbf{D}.$$

where λ and μ are Lame coefficients.

D. Peirce, R.J. Asaro, and A. Needleman. Material rate dependence and localized deformation in crystalline solids. Acta Metallurgica, 31(12):1951–1976, 1983

Resolved shear stress and slip systems

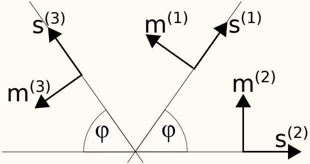


We define, resolved shear stress, the shear component of an applied stress resolved along a slip plane

$$\tau^{(i)} = \mathbf{s}^{(i)} \cdot \mathbf{T}\mathbf{m}^{(i)} = \mathbf{T} : \mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}.$$

Crystal plasticity assumption

$$
\begin{aligned}
\mathbf{L}_p &= \sum_{i=1}^{N} \nu^{(i)} \mathbf{s}_0^{(i)} \otimes \mathbf{m}_0^{(i)}, \\
\mathbf{D_p} &= \sum_{i=1}^{N} \nu^{(i)} \mathrm{sym}\left(\mathbf{s}_0^{(i)} \otimes \mathbf{m}_0^{(i)}\right)
\end{aligned}
$$



To complete the system, slip rates $\nu^{(i)}$ and hardening have to be specified,

$$
\nu^{(i)} = \nu_0 \mathrm{sgn}\left(\tau^{(i)}\right) \left(\frac{|\tau^{(i)}|}{\tau_c^{(i)}}\right)^{1/m},
$$

$$
\dot{\tau_c}^{(i)} = \sum_j H_{ij} |\nu^{(j)}|.
$$

The second law of thermodynamics is satisfied

$$
\xi = \mathbf{T} : \mathbf{D_p} = \sum_i \nu^{(i)} \mathbf{T} : \left(\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right) = \sum_{i=1}^{N} \nu^{(i)} \tau^{(i)} = \sum_i \nu_0 |\tau^{(i)}| \left(\frac{|\tau^{(i)}|}{\tau_c^{(i)}}\right)^{\frac{1}{m}}
$$

Evolution of slip systems

- Slip systems are changing with elastic stretches and rotations

$$\mathbf{s}^{(i)} = \mathbf{F_e}\mathbf{s}_0^{(i)} \quad \text{and} \quad \dot{\mathbf{F}}_\mathbf{e} = \left(\nabla\mathbf{v} - \sum_i \nu^{(i)}\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right)\mathbf{F_e}.$$

- Evolution of slip directions

$$\dot{\mathbf{s}^{(i)}} = \left(\nabla\mathbf{v} - \sum_i \nu^{(i)}\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right)\mathbf{s}^{(i)}.$$

- We reformulate vectorial equations in therms of scalar unknowns (ϕ, s_1, m_1, s_2, m_2, s_3, m_3),

$$\mathbf{s}^{(i)} = s_i(\cos\varphi_i, \sin\varphi_i), \quad \mathbf{m}^{(i)} = m_i(-\sin\varphi_i, \cos\varphi_i).$$

$$\begin{aligned}
\dot{\varphi} &= (-\sin\varphi, \cos\varphi)^T \left(\nabla\mathbf{v} - \sum_{i=1}^{3} \nu^{(i)}\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right) s_2(\cos\varphi, \sin\varphi), \\
\dot{s}_i &= (\cos\varphi_i, \sin\varphi_i)^T \left(\nabla\mathbf{v} - \sum_{i=1}^{3} \nu^{(i)}\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right) s_i(\cos\varphi_i, \sin\varphi_i), \\
\dot{m}_i &= (-\sin\varphi_i, \cos\varphi_i)^T \left(\nabla\mathbf{v} - \sum^{3} \nu^{(i)}\mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)}\right) m_i(-\sin\varphi_i, \cos\varphi_i).
\end{aligned}$$

Scaled model

- The unknowns are: velocity $\mathbf{v}$, Cauchy stress $\mathbf{T}$, density ϱ and slip directions $\mathbf{s}^{(i)}$,

$$
\begin{aligned}
&\varrho_{,t} + \operatorname{div}(\varrho \mathbf{v}) = 0,\\
&R_1 \varrho \dot{\mathbf{v}} + \operatorname{div} \mathbf{T} = 0,\\
&\dot{\mathbf{T}} + \mathbf{T} \operatorname{div} \mathbf{v} + \mathbf{WT} - \mathbf{TW} = \varrho \mathcal{C}(\mathbf{D} - \mathbf{D_p}),\\
&\dot{\varphi} = (-\sin\varphi, \cos\varphi)^T \left(\nabla \mathbf{v} - R_2 \sum_{i=1}^{3} \nu^{(i)} \mathbf{s}^{(i)} \otimes \mathbf{m}^{(i)} \right) s_2 (\cos\varphi, \sin\varphi)
\end{aligned}
$$

- Characteristic values $\varrho_0 = 3000 \frac{kg}{m^3}$, $V = 10^{-5} \frac{m}{s}$, $L = 10^{-2} m$, $\nu_0 = 10^{-3} \frac{1}{s}$, $\Sigma = 70 MPa$

$$
R_1 = \frac{\varrho_0 V^2}{L \Sigma} \approx 10^{-12}, R_2 = \frac{L \nu_0}{V} = 1
$$

- Update of remaining variables

$$
m_i, \quad s_i, \quad \tau_c^{(i)}
$$

The elastic predictor/plastic corrector

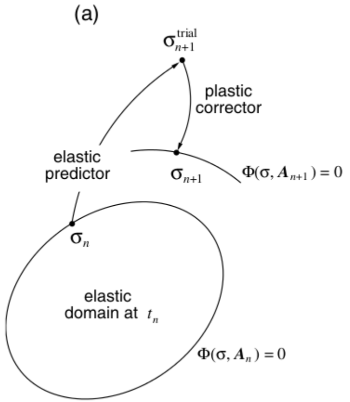


Figure 7.1. General return mapping schemes. Geometric interpretation: (a) hardening plasticity; and (b) perfect plasticity.

EA. de Souza Neto, D Perić, DRJ Owen, Computational Methods for Plasticity, Wiley 2008

Numerical treatment

- In time: One step finite difference
- In space: FE
  - $\mathrm{P}^1 - \textit{dis.}$: $\mathbf{T}$, $\nu^{(i)}$
  - P^2: $\mathbf{v}$
  - P^1: ϱ, φ, s_i, m_i
- Newton-Ralphson method, analytic jacobian by automatic differentiation (FEniCS)
- For now direct linear solver of the fully coupled discrete system
- Boundary conditions by Nitsche's method
  $(\mathbf{Z_T}\mathbf{n}\cdot\mathbf{n}, \mathbf{v}\cdot\mathbf{n})_{\Gamma_2} + (\mathbf{T}\mathbf{n}\cdot\mathbf{n}, \mathbf{z_v}\cdot\mathbf{n})_{\Gamma_2} + \frac{\beta}{h}(\mathbf{v}\cdot\mathbf{n}, \mathbf{z_v}\cdot\mathbf{n})_{\Gamma_2}$ with $\beta = 10$

Main obstacles

proper finite elements, power law with large exponent, boundary conditions

Discrete formulation

$$
\begin{aligned}
\mathbb{V}_h &= \{v_h \in W^{1,2}(\Omega;\mathbb{R}^2);\ \mathbf{v}|_{\Gamma_1} = (0,-1),\ \mathbf{v}\cdot\mathbf{n}|_{\Gamma_2} = 0,\ \mathbf{v}|_K \in \mathcal{P}_2(K)^2\ \forall K \in \mathcal{T}_h\},\\
\mathbb{R}_h &= \{\varrho_h \in W^{1,2}(\Omega;\mathbb{R});\ \varrho_h|_{\Gamma_1} = 1,\ \varrho_h|_K \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\},\\
\mathbb{T}_h &= \{\mathbf{T}_h \in W^{1,2}(\Omega;\mathbb{R}^{2\times 2}_{sym}); \mathbf{T}_h|_K \in \mathcal{P}_1(K)^{2\times 2}\ \forall K \in \mathcal{T}_h\},\\
\mathbb{N}_h &= \{\nu_h \in L^2(\mathbb{R}); \nu_h|_1 \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\},\\
\mathbb{A}_h &= \{\varphi_h \in W^{1,2}(\Omega;\mathbb{R});\ \varphi_h|_{\Gamma_1} = 0,\ \varphi_h|_K \in \mathcal{P}_1(K)\ \forall K \in \mathcal{T}_h\}.
\end{aligned}
$$

Find $(\mathbf{v}_h, \varrho_h, \mathbf{T}_h, \nu_{1h}, \nu_{2h}, \nu_{3h}, \varphi_h) \in \mathbb{V}_h \times \mathbb{R}_h \times \mathbb{T}_h \times \mathbb{N}_h \times \mathbb{N}_h \times \mathbb{N}_h \times \mathbb{A}_h$, s.t.

$$
\begin{aligned}
&(\varrho_{h,t}\,, z_\varrho) + (\mathbf{v}_h \nabla \varrho_h, z_\varrho) + (\varrho_h \operatorname{div}(\mathbf{v}_h), z_\varrho) = 0 \quad \forall z_\varrho \in \mathbb{R}_{h0},\\
&R_1\,(\varrho_h \dot{\mathbf{v}}_h, \mathbf{z_v}) + (\mathbf{T}_h, \nabla(\mathbf{z_v})) + (\mathbf{T}_h\mathbf{n}\cdot\mathbf{n}, \mathbf{z_v}\cdot\mathbf{n})_{\Gamma_2} + \frac{\beta}{h}(\mathbf{v}_h\cdot\mathbf{n}, \mathbf{z_v}\cdot\mathbf{n})_{\Gamma_2} = 0 \quad \forall \mathbf{z_v} \in \mathbb{V}_{h0},\\
&\left(\dot{\mathbf{T}}_h + \mathbf{T}_h \operatorname{div}\mathbf{v}_h + \mathbf{W}_h\mathbf{T}_h - \mathbf{T}_h\mathbf{W}_h, \mathbf{Z_T}\right) - (\varrho\mathcal{C}(\mathbf{D}_h - \mathbf{D_p}_h), \mathbf{Z_T}) + (\mathbf{Z_T}\mathbf{n}\cdot\mathbf{n}, \mathbf{v}_h\cdot\mathbf{n})_{\Gamma_2} = 0\\
&\left(\nu_h^{(i)} - \operatorname{sgn}(\mathbf{T}_h : \mathbf{s}_h^{(i)} \otimes \mathbf{m}_h^{(i)}) \left(\frac{|\mathbf{T}_h : \mathbf{s}_h^{(i)} \otimes \mathbf{m}_h^{(i)}|}{\tau_c^{(i)}}\right)^{20}, z_{\nu i}\right) = 0 \quad \forall z_{\nu i} \in \mathbb{N}_h \text{ and } i \in \{1,\\
&\left(\dot{\varphi}_h - (-\sin\varphi_h, \cos\varphi_h)^T \left(\nabla \mathbf{v}_h - R_2 \sum_{i=1}^{3} \nu_h^{(i)} \mathbf{s}_h^{(i)} \otimes \mathbf{m}_h^{(i)}\right) s_{2h}(\cos\varphi_h, \sin\varphi_h), z_\varphi\right) = 0
\end{aligned}
\tag{1}
$$

Let's dive into code

File Edit Tools Syntax Buffers Window Help

```python
"""Piotr Minakowski
ale
"""

from dolfin import *

import os, sys
from math import pi, cosh
#from math import pi

from numpy import array
from numpy import linalg as lin
from datetime import datetime, time

label = str(sys.argv[0]) + str(datetime.now()) #+ str(r_) + str(var_)

#scaling constanrs
R1_ = 2e-10
R2_ = 1.0  #float(sys.argv[1])
R3_ = 1.0  #float(sys.argv[1])

parameters["form_compiler"]["cpp_optimize"] = True
parameters["form_compiler"]["quadrature_degree"] = 8

ffc_options = {"optimize": True, \
                           "eliminate_zeros": True, \
                           "quadrature_degree": 8  ,\
                           "precompute_basis_const": True, \
                           "precompute_ip_const": True
                           }
#set_log_level(ERROR)
#set_log_level(PROGRESS)
#set_log_level(DEBUG)

#############
### domain ##
#############

height = 1.0
```

Summary

Conclusions

- Eulerian formulation of crystal plasticity for large strain problems
- Consistent thermodynamic derivation of the model
- Finite element discretization method for fully coupled problem
- Numerical tools available to solve such systems

Further investigation

- adaptivity (time, space)
- stability conditions
- pass to rate independent (perfect plastic) limit
- mathematical properties (sequential stability result)
- ...

Thank you for your attention.