A variational approach to gradient plasticity

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Joint work with R. March (Rome), G. Del Piero (Ferrara), G. Zitti (Ancona), T. Yalcinkaya (Ankara), A. Cocks (Oxford)

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Workshop «Variational Models of Fracture»

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**Variational Model**

- **Evolution of the plastic deformation**
  - Hardening (diffuse plasticity)
  - Yielding plateau (plastic waves)
  - Softening (strain localization)

- Fracture: material instability occurring at the end of the strain localization process

- **Tensile steel bar**

- Rate-independent
- Non-convex totally dissipative plastic energy
- Non-local energy, depending on the plastic strain gradient
- Evolution of the deformation -> Incremental energy minimization

**References**
- Del Piero, Lancioni, March, JMMS, 2013
- Lancioni, J. Elasticity, 2015
Modeling assumptions

i. Kinematics

\[ u'(x) = \varepsilon(x) + \gamma(x) \]

\( u'(x) \) is total strain, \( \varepsilon(x) \) is elastic strain, \( \gamma(x) \) is plastic strain.

\[ 1D \text{ Pb.} \]

\[ u(l) = d_t l \]

ii. Energy

**internal variable** \( e = e(\gamma) \). In isotropic gradient plasticity

\[
E(u, \gamma, e) = \int_0^l \left( \frac{1}{2} E(u'-\gamma)^2 + \theta(e) + \frac{1}{2} \alpha(e)e^2 \right) dx
\]

\( E(u, \gamma, e) \) = stored elastic energy + dissipative plastic energy + non-local stored plastic energy

- **stored elastic energy**
- **dissipative plastic energy**
- **non-local stored plastic energy**

\[ \theta(e) = \theta'(e) \dot{e} \geq 0 \]

\( \theta(e) \) = strictly increasing for increasing strain rate \( \dot{e} \)

\( \alpha(e) \) = not increasing for increasing strain \( e \)

iii. Dissipation

\[
\frac{d}{dt} \theta(e) = \theta'(e) \dot{e} \geq 0
\]
Comparisons with non-local variational approaches in literature

**Damage energy** [Bourdin, Francfort, Marigo, 2000], …

\[
E(u, \alpha) = \int_0^l \left( \frac{1}{2} E(\alpha) u'^2 + \theta(\alpha) + \frac{1}{2} A \alpha'^2 \right) dx
\]

**Damage and plasticity energy**

[Ambrosio, Lemenant, Royer-Carfagni, 2013], [Freddi, Royer-Carfagni, 2014]

\[
E(u, \alpha) = \int_0^l \left( \frac{1}{2} E(\alpha) u'^2 + \theta(\alpha) + \frac{1}{2} A \alpha'^2 + \sigma_0 \alpha^2 |u'| \right) dx
\]

[yielding stress]

[Alessi, Marigo, Vidoli, 2014, 2015]

\[
E(u, \alpha, \gamma, e) = \int_0^l \left( \frac{1}{2} E(\alpha)(u' - \gamma)^2 + \theta(\alpha) + \frac{1}{2} A \alpha'^2 + \sigma_\rho(\alpha)e \right) dx
\]

Damage + von Mises plasticity
Equilibrium

\[ \delta E(u, \gamma, e; \delta u, \delta \gamma, |\delta \gamma|) \geq 0 \]

\[ \sigma' = 0, \quad \text{with} \quad \sigma = E(u' - \gamma) \]

\[ |\sigma| \leq \sigma^c \quad \text{with} \quad \sigma^c = \theta' + \frac{1}{2} \alpha' e'^2 - \frac{d}{dx} (\alpha e') \]

Yield condition

\[ e(0) = e(l) = 0, \quad \text{or} \quad e'(0) \leq 0, \quad e'(l) \geq 0 \quad \text{b.c.} \]
Flow rule

\[ E_{t+t}(u_t, \dot{y}_t, \dot{e}_t) = E_t + \tau \dot{E}_t(u_t, \dot{y}_t, \dot{e}_t), \]

with \( \dot{E}_t = \int_0^l (-\text{sign}(\dot{y}_t)\sigma_t + \sigma_c^c)\dot{e} \, dx \)

**Necessary condition** for a minimum

\[ \delta \dot{E}_t(u_t, \dot{y}_t, \dot{e}_t; 0, 0, \delta e) \geq 0, \forall \delta e : \dot{e}_t + \delta e \geq 0 \]

\[ \dot{e}_t \geq 0, \quad -\text{sign}(\dot{y}_t)\sigma_t + \sigma_c^c \geq 0, \quad \left(-\text{sign}(\dot{y}_t)\sigma_t + \sigma_c^c\right)\dot{e}_t = 0 \]

\[ \dot{y}_t = \frac{\sigma_t}{\sigma_c} \dot{e}_t \quad \text{Flow rule} \]
Tensile test

Assume  \( d_t \geq 0 \)

\( \sigma_t \geq 0 \)  \( \Rightarrow \)  \( \dot{\gamma} = \dot{\varepsilon} \)

\[
E(u, \gamma) = \int_0^l \left( \frac{1}{2} E(u' - \gamma)^2 + \theta(\gamma) + \frac{1}{2} \alpha(\gamma) \gamma'^2 \right) dx
\]

Dissipation inequality  \( \dot{\gamma} \geq 0 \)
Quasi-static evolution

**Incremental minimum problem**

\((u_t, \gamma_t) \rightarrow (u_{t+\tau}, \gamma_{t+\tau}), \quad \varepsilon_{t+\tau} = u'_{t+\tau} - \gamma_{t+\tau}\)

\(u_{t+\tau} = u_t + \alpha \dot{u}_t,\)

\(\gamma_{t+\tau} = \gamma_t + \tau \dot{\gamma}_t\)

\(E(u_{t+\tau}, \gamma_{t+\tau}) \approx E(u_t, \gamma_t) + \tau \dot{E}(u_t, \gamma_t) + \frac{1}{2} \tau^2 \ddot{E}(u_t, \gamma_t) = E(u_t, \gamma_t) + \tau F(u_t, \gamma_t; \dot{u}_t, \dot{\gamma}_t)\)

\((\dot{u}_t, \dot{\gamma}_t) = \arg \min \{F(u_t, \gamma_t; \dot{u}_t, \dot{\gamma}_t), \ \dot{\gamma} \geq 0, \ \text{b.c.}\}\)

**Constrained quadratic programming pb.**
**Necessary condition** for a minimum

\[
\delta F(u_t, \dot{\gamma}_t, \delta u, \delta \dot{\gamma}) \geq 0
\]

\[
\dot{\gamma}_t + \delta \gamma \geq 0
\]

\[
\dot{\sigma}' = 0,
\]

**Kuhn-Tucker conditions (flow rule)**

\[
\begin{align*}
\dot{\gamma}_t & \geq 0, \\
\sigma_t + \tau \dot{\sigma}_t & \leq \sigma_t^c + \tau \dot{\sigma}_t^c, \\
[\sigma_t + \tau \dot{\sigma}_t - (\sigma_t^c + \tau \dot{\sigma}_t^c)] & \dot{\gamma}_t = 0
\end{align*}
\]

**consistency condition**

(the yield function maintains equal to zero when \(\gamma\) grows)
Elastic evolution

1. Elastic regime \( 0 < d_t \leq d_e = \theta'(0)/E \)

\[
\sigma_e = \theta'(0) \\
\sigma_t = Ed_t \\
u_t = xd_t, \\
\gamma_t = 0, \\
d_e = \theta'(0)/E
\]

2. Elastic unloading \( \dot{d}_t < 0, \quad d_t \geq 0 \)

\[
\dot{\gamma}_t = 0, \\
\dot{\sigma}_t = E\dot{d}_t < 0
\]
Evolution of plastic def. from homogeneous configurations

\[ u_t = \text{const}, \quad \gamma_t = \text{const}, \quad \sigma_t = \sigma_t^c, \quad \text{bc: } \frac{\dot{\gamma}_t}{\gamma_t}(0) = 0, \quad \frac{\dot{\gamma}_t}{\gamma_t}(l) = 0 \]

\[ \dot{u}_t(0) = 0, \quad \dot{u}_t(l) = \dot{d}_t l \]

Evolution pb.

\[
\begin{align*}
\dot{\gamma}_t &\geq 0, \\
\dot{\sigma}_t &\leq \dot{\sigma}_t^c, \text{ with } \dot{\sigma}_t = E(\dot{d}_t - \frac{1}{l} \int_0^l \dot{\gamma}_t dx) \\
[\dot{\sigma}_t - \dot{\sigma}_t^c] \dot{\gamma}_t &= 0
\end{align*}
\]

\[ \dot{\varepsilon}_t = \dot{d}_t - \frac{1}{l} \int_0^l \dot{\gamma}_t dx \]
\( \dot{\gamma}_t \) depends on \( \theta(\gamma_t), \alpha(\gamma_t), l \) and \( E \)

**\( \theta-\alpha \) map**

- Localized solution (\( \dot{\gamma} \) trigonometric)
- Full-size solution (\( \dot{\gamma} \) hyperbolic)

Internal length: 
\[
l_i = 2\pi \sqrt{\frac{\alpha}{|\theta''|}}
\]

\[
l \leq l_i \implies \text{full size sol.}
\]
\[
l > l_i \implies \text{localized sol.}
\]

manifestation of the size-effect
Instability and fracture

**Sufficient condition** for a minimum:

\[ \delta F \geq 0, \text{ and } \delta^2 F \geq 0 \text{ for all perturbations for which } \delta F = 0 \]

\[ \delta^2 F(\dot{\gamma}_t, \delta \dot{\gamma}) = \int_0^l \left( (\theta''(\gamma_t)) \delta \dot{\gamma}^2 + E \delta\ddot{\gamma}^2 + \alpha \delta \dot{\gamma}^2 \right) dx \geq 0, \text{ for all } \delta \dot{\gamma} \text{ in the plastic zone,} \]

where \( \sigma_t = \sigma_t^c \) and \( \delta F = 0 \)

The smallest eigenvalue \( \rho_1 \) of the eigenvalue pb

\[ \int_0^l \left( (\theta''(\gamma_t)) \delta \dot{\gamma}^2 + E \delta\ddot{\gamma}^2 + \alpha \delta \dot{\gamma}^2 \right) dx = \rho_1 \int_0^l \delta \dot{\gamma}^2 dx \]

is positive

\[ \rho_1 \geq 0 \iff s(\theta'', \alpha) = \psi \left( l \sqrt{-\theta''/\alpha} \right) + \theta''/E \geq 0 \]

If \( s < 0 \), \( F \) can attain unlimited negative values for perturbations concentrated on intervals of sufficiently small length. This situation variationally characterizes fractured configurations.
Which shapes to $\theta(\gamma)$ and $\alpha(\gamma)$? ... hints from the analytical solution
Stress-hardening

Full size solution
Stress-softening
Full size solution
Stress-softening

Localized solution
Plastic energy $\theta$, piecewise cubic

Non-local coefficient $\alpha$
Lancioni, J. Elasticity, 2015

\( f \) [kN]

\( \Delta s \) [mm]

\( \gamma \) [s\(^{-1}\)]

\( u' \)

homogeneous deformation

SAMPLE

\( \Delta x_{meas} = 80 \text{ mm} \)

140 mm
Lancioni, J. Elasticity, 2015
Lancioni, J. Elasticity, 2015
Lancioni, J. Elasticity, 2015
Lancioni, J. Elasticity, 2015
Constitutive parameters setting [Lancioni, J. Elast., 2015]

$E = 210 \text{kN/mm}^2$,

$c_1 = \frac{f_0^c}{A}$

$\gamma_1 = \frac{\Delta s_{t_m} - f_{t_m}}{\Delta x} \frac{1}{EA}$

$c_2 = \frac{2}{A \gamma_1} \left( f_{t_m} - f_0^c \right)$

$\gamma_2 = 2 \frac{d_0 - d_f}{d_0}$

$f_{t_m} = 39.1 \text{kN}$

$f_0^c = 29.5 \text{kN}$

$\Delta s_{t_m} = 12.8 \text{mm}$

$d_f = 6.50 \text{mm}$

$\gamma_1 = 0.16$

$\gamma_2 = 0.7$

$c_1 = 0.375$

$c_2 = 1.5$
\( \theta \) concave-convex-concave
McReynolds’ slow plastic wave (1948)  

Maxwell line

[Froli, Royer-Carfagni, 1999]
Tensile response of a concrete specimen

\( E = 18 \text{ kN/mm}^2 \),
\( A = 50 \times 50 \text{ mm}^2 \),
\( \theta'(0) = 6.9 \text{ kN} \) (yielding force),
\( \alpha = 3500 \text{ kN mm}^2 \)
hardening (θ convex)

convex softening (θ concave)

 Localization and enlargement of the plastic zone (θ concave)

(D.A. Hordijk, 1992)
Multi-dimensional extensions

1D rate-dependent plasticity model
[Yalcinkaya, Brekelmans, Geers, JMPS, 2011]
Virtual work principle, dissipation inequality;
Nonconvex plastic potential;
Non-local gradient energy term.
Plastic deformation partially recoverable and partially dissipated through a viscous micro-stress

Extension to 2D single crystal plasticity

... joint work with Gianluca Zitti (PhD at Univpm)
Deformation

\[ \text{sym} \nabla \mathbf{u}(x) = \mathbf{E}^e(x) + \mathbf{E}^p(x) \]

- total def.
- elastic def.
- plastic def.

\[ \mathbf{E}^p(x) = \sum_{\alpha} \gamma^{\alpha}_{\text{sym}} (\mathbf{s}_{\alpha} \otimes \mathbf{n}_{\alpha}) \]

- plastic slip
- slip direction
- slip-plane normal

Single crystal

\[ \mathbf{u} = t \hat{\mathbf{u}} \text{ at } \partial \Omega_u \]

\[ \mathbf{u} = \text{traction free at } \partial \Omega_t \]
Energy

\[ E(u, \gamma_\alpha) = \int_\Omega \left( \psi_e(E^e) + \theta(|\gamma_\alpha|) + \psi_{\nabla \gamma}(\nabla \gamma_\alpha) \right) dx \]

- Elastic energy
- Plastic energy
- Non-local energy

Free energy density (stored)

\[ \psi(u, \gamma_\alpha) = \psi_e(E^e) + \psi_{\nabla \gamma}(\nabla \gamma_\alpha) \]

\[ \psi_e(E^e) = \frac{1}{2} C[E^e] \cdot E^e, \quad \psi_{\nabla \gamma}(\nabla \gamma_\alpha) = \frac{1}{2} \sum_\alpha A_\alpha [\nabla \gamma_\alpha] \cdot \nabla \gamma_\alpha \]

Dissipative plastic energy

\[ \frac{d}{dt} \theta(|\gamma_\alpha|) = \sum_\alpha \text{sign}(\gamma_\alpha) \frac{d\theta(|\gamma_\alpha|)}{d|\gamma_\alpha|} \dot{\gamma}_\alpha \geq 0 \]

Suppose that \( \theta(|\gamma_\alpha|) \) is strictly increasing in each variable \(|\gamma_\alpha|\),

the **dissipation condition** reduces to \( \text{sign}(\gamma_\alpha) \dot{\gamma}_\alpha \geq 0 \).
Equilibrium

\[ \delta E(u, \gamma_\alpha, \delta u, \delta \gamma_\alpha) \geq 0, \quad \text{sign}(\gamma_\alpha) \delta \gamma_\alpha \geq 0 \]

Macroscopic balance equation

\[ \text{div} T = 0, \text{ with } T = C[E^e] \]

Yield condition

\[ |Tn_\alpha \cdot t_\alpha| \leq \pi_\alpha - \text{sign}(\gamma_\alpha) \text{div} \xi_\alpha \]

resolved shear \quad yield limit

with \[ \pi_\alpha = \frac{d \theta(|\gamma_\alpha|)}{d |\gamma_\alpha|} \quad \text{and} \quad \xi_\alpha = \frac{d \psi_{\nabla \gamma}(\nabla \gamma_\alpha)}{d \nabla \gamma_\alpha} \]

microscopic stress power-conjugated to \( \nabla \dot{\gamma}_\alpha \)

microscopic stress power-conjugated to \( \dot{\gamma}_\alpha \)
Evolution Pb. \(\Leftrightarrow\) Incremental energy minimization

\[
(u_t, \gamma_{\alpha,t}) \rightarrow \begin{cases} 
  u_{t+\tau} = u_t + \tau \dot{u}_t & \text{Unknows} \\
  \gamma_{\alpha,t+\tau} = \gamma_{\alpha,t} + \tau \dot{\gamma}_{\alpha,t}
\end{cases}
\]

\[
E_{t+\tau}(\dot{u}, \dot{\gamma}_{\alpha}) \approx E_t + \tau \dot{E}_t(\dot{u}, \dot{\gamma}_\alpha) + \frac{1}{2} \tau^2 \ddot{E}_t(\dot{u}, \dot{\gamma}_\alpha) = E_t + \tau J_t(\dot{u}, \dot{\gamma}_\alpha)
\]

\[
(\dot{u}_t, \dot{\gamma}_{\alpha,t}) = \arg\min\{J_t(\dot{u}, \dot{\gamma}_\alpha), \ \text{sign}(\gamma_\alpha)\dot{\gamma}_\alpha \geq 0, \ b.c.\}
\]

Constrained quadratic programming pb.

**Necessary condition for a minimum**

\[
\delta J_t(\dot{u}, \dot{\gamma}_\alpha; \delta \dot{u}, \delta \dot{\gamma}_\alpha) \geq 0, \quad \dot{\gamma}_\alpha + \delta \dot{\gamma}_\alpha \geq 0
\]

\[\text{Balance of the macroscopic stress evolution} \]

\[\text{Kuhn-Tucker conditions (flow rule)}\]

\[
\text{sign}(\gamma_{\alpha_\text{t}})\dot{\gamma}_\alpha \geq 0, \quad |(T + \tau \dot{T})n_\alpha \cdot t_\alpha| \leq (\pi_\alpha + \tau \dot{\pi}_\alpha) - \text{sign}(\gamma_{\alpha_\text{t}}) \text{div}(\xi_\alpha + \dot{\xi}_\alpha) \]

\[
((\pi_\alpha + \tau \dot{\pi}_\alpha) - \text{sign}(\gamma_{\alpha_\text{t}}) \text{div}(\xi_\alpha + \dot{\xi}_\alpha) - |(T + \tau \dot{T})n_\alpha \cdot t_\alpha|)\dot{\gamma}_\alpha = 0
\]

**Consistency condition**

(the yield function maintains equal to zero when \(\gamma\) grows)
Numerical results – plane pure shear test

Single slip system

\[ E^p(x) = \gamma \text{ sym}(s \otimes n) \]

Orientations: \( \phi = 5^\circ; 15^\circ; 30^\circ \)

\( E = 210 \, \text{GPa}, \, \nu = 0,33, \)

\( A_s = 52,5 \, \text{kN}, \, A_n = 10,5 \, \text{kN} \)

Periodic b.c.

\[ u_x(l, y) = u_x(0, y); \, u_y(x, l) = u_y(x, 0); \]

\[ \gamma(x, l) = \gamma(x, 0); \, \gamma(l, y) = \gamma(0, y); \]
Double-well plastic energy

\[ \theta \text{ [GPa]} \]

\[ \gamma' = -\gamma \quad \gamma' = -\gamma \]

\[ \gamma_1 = 0.0072 \quad \gamma_2 = 0.0212 \]

Conclusions

The proposed model represents a variational approach to softening gradient plasticity (Aifantis-type model). Advantages:

i. the laws of classical plasticity are variationally deduced (and not given a priori);

ii. clear dependence of the response on the shape of the plastic energy $\theta(\gamma)$:

- $\theta(\gamma)$ convex $\rightarrow$ stress-hardening, diffuse plasticity
- $\theta(\gamma)$ concave $\rightarrow$ stress-softening, $\theta''(\gamma)$ decreasing $\rightarrow$ strain localization
- $\theta''(\gamma)$ increasing $\rightarrow$ localization zone enlargement
- $\theta(\gamma)$ double-wells $\rightarrow$ plastic wave propagation

Ductile failure is described as a bulk process of progressive strain localization, which concludes with a final material instability, variationally interpreting fracture.

Physical motivation: process zone, where strains localize, and only at the very end they coalesce in fracture surfaces.

The model presents as an alternative to classical cohesive fracture theories, which concentrate inelasticity on surfaces.

Perspectives

1. Extension to multi-dimension.
   Crystal plasticity: multiple slip systems

2. Find correlations between the covexity-concavity properties of $\theta$ and its derivatives and the microstructure of real materials.
   Crystal plasticity: non-convex energy proposed by Ortiz-Repetto (1999), accounting for latent hardening
Conclusions

Rate-Independent model based on incremental energy minimization;

Non-convex dissipative plastic energy ⇐⇒ - Irreversibility of plastic def.
- non-convexity leads to localization

Non-local energy ⇐⇒ - internal length scale (it makes possible to simulate phenomena at different scales)
- stabilizing effect (ductile failure; no brittle fracture)

Perspectives

- Simulations with multiple slip systems and plastic energy functions of different shapes;
- Find correlations between the covexity-concavity properties of $\theta$ and its derivatives and the microstructure of real materials → non-convex energy proposed by Ortiz-Repetto (1999), accounting for latent hardening
Numerical results

i. Slip patterning in an infinite long strip (1D Pb)

Single slip system

\[ \mathbf{E}^p(x) = \gamma \text{sym}(\mathbf{s} \otimes \mathbf{n}) \]

\[ E = 210 \text{ GPa}, \quad \nu = 0.33, \quad A_n = 147.29 \text{ N} \]
Soft boundary conditions $\gamma'(0)=0$, $\gamma'(l)=0$