Strain gradient plasticity: a Code_Aster trick

MFront user day

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Introduction: context

Improve representativeness of polycrystal models

- influence of dislocations accumulation at grain boundaries
- shear localization
- size effects
- $\rightarrow$ strain gradient plasticity, micromorphic model

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- enrich finite elements: extra DOFs
- modify stiffness matrix assemblage
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A Code_Aster trick [F. Latourte, 2017]

- micromorphic model with 1 scalar extra DOF [Ling *et al.*, IJSS, 2018]
- creative use of heat equation solver

Classical crystal plasticity model

Finite strain framework

Kinematics

- $\boldsymbol{F} = \boldsymbol{E} \cdot \boldsymbol{P}$ deformation gradient
- $\boldsymbol{E}^e_{GL} = (\boldsymbol{E}^{\mathrm{t}} \cdot \boldsymbol{E} - \mathbf{1})/2$ Green-Lagrange strain tensor
- $\boldsymbol{L}^p = \dot{\boldsymbol{P}} \cdot \boldsymbol{P}^{-1}$ plastic strain rate

Stresses

- $\boldsymbol{\sigma}$ Cauchy stress tensor
- $\boldsymbol{\Pi}^e = \det(\boldsymbol{E})\boldsymbol{E}^{-1} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{E}^{-\mathrm{t}}$ second Piola-Kirchhoff stress tensor
- $\boldsymbol{M} = \det(\boldsymbol{E})\boldsymbol{E}^{\mathrm{t}} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{E}^{-\mathrm{t}}$ Mandel stress tensor

Elasticity

- $\boldsymbol{\Pi}^e = \mathbb{C} : \boldsymbol{E}^e_{GL}$

Plastic flow rule; slip systems $s = 1..N$, $\boldsymbol{N}^s = \underline{m}^s \otimes \underline{n}^s$ Schmid tensor

- $\tau^s = \boldsymbol{M} : \boldsymbol{N}^s$ resolved shear stress
- $\phi^s = |\tau^s| - \tau^s_c$ yield function (τ^s_c critical resolved shear stress)
- $\dot{\gamma}^s = \langle \phi^s / K \rangle^n \operatorname{sgn}(\tau^s)$ plastic slip rate
- $\boldsymbol{L}^p = \sum_s \dot{\gamma}^s \boldsymbol{N}^s$ plastic strain rate

Reduced micromorphic crystal plasticity model

Single additional DOF: microslip [Ling *et al.*, IJSS, 2018]
Modifications wrt. classical crystal plasticity model:

DOFs

- $\underline{u}$ displacement
- γ_χ microslip

Gradient

$\underline{K} = \underline{\mathrm{Grad}}_{\underline{X}}(\gamma_\chi)$ microslip gradient vector

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Generalized stresses

- S dual of γ_χ
- $\underline{M}$ dual of $\underline{K}$

Equilibrium and BC

- $\mathrm{Div}_{\underline{X}}(\underline{M}) - S = 0$ in bulk
- $\underline{M} \cdot \underline{n}_0 = M$ on boundary

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Constitutive relations

- $S = -H_\chi e$ with H_χ penalty modulus
- $\underline{M} = \boldsymbol{A} \cdot \underline{K}$ with $\boldsymbol{A}$ high order moduli

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Additional variables

- $\gamma_{cum} = \int_0^t \sum_s |\dot{\gamma}^s| \,\mathrm{d}u$ cumulative total slip
- $e = \gamma_{cum} - \gamma_\chi$ relative plastic slip

Simplification

Extra relations reduce to

- $\phi^s = |\tau^s| - \langle \tau_c^s - S \rangle$ yield function
- $\gamma_{cum} = \int_0^t \sum_s |\dot{\gamma}^s| \, \mathrm{d}u$ cumulative total slip
- $S = \mathrm{Div}_{\underline{X}}(\boldsymbol{A} \cdot \underline{\mathrm{Grad}}_{\underline{X}}(\gamma_\chi)) = H_\chi(\gamma_\chi - \gamma_{cum})$ field equation on γ_χ

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Main idea [F. Latourte, 2017]

- field equation on γ_χ is similar to heat equation!
  $\rho C_p \dot{T} = \mathrm{div}\left(\boldsymbol{\lambda} \cdot \underline{\mathrm{grad}}\,(T)\right) + q_s$
- staggered resolution
  $\gamma_\chi \rightarrow$ mechanics $\rightarrow \gamma_{cum} \rightarrow$ thermics $\rightarrow \gamma_\chi \rightarrow \ldots$

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First prototype in the framework of infinitesimal strain theory

Mechanics implementation

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

Elastic part $\quad \boldsymbol{\sigma} = \mathbb{C} : \varepsilon^e$

Plastic part

$\boldsymbol{N}^s = (\underline{m}^s \otimes \underline{n}^s)^{\mathrm{sym}}$	for $s = 1..N$ slip systems
$\tau^s = \boldsymbol{\sigma} : \boldsymbol{N}^s$	resolved shear stress
$S = H_\chi(\gamma_\chi - \gamma_{cum})$	generalized stress
$\phi^s = \lvert\tau^s\rvert - \langle \tau_c^s - S \rangle$	yield function
$\dot{\gamma}^s = \langle \phi^s / K \rangle^n \operatorname{sgn}(\tau^s)$	plastic slip rate
$\dot{\varepsilon}^p = \sum_s \dot{\gamma}^s \boldsymbol{N}^s$	plastic strain rate
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MFront implementation

Modification of any crystal viscoplastic constitutive behaviour

- add state variable γ_{cum}
- get γ_χ through T field (Code_Aster VARC)
- compute $S, \ldots, \dot{\varepsilon}^p$
- update γ_{cum}

Thermics implementation

$$\boldsymbol{A} = A\mathbf{1}, \qquad A\Delta\gamma_\chi = H_\chi(\gamma_\chi - \gamma_{cum}) \quad \Leftrightarrow \quad \rho C_p \dot{T} = \lambda \Delta T + q_s$$

First idea: transient linear heat equation

ad hoc solution $T = \gamma_\chi t$

$\rightarrow$ failed (poor convergence)

$$\rho C_p = H_\chi t$$
$$\lambda = A$$
$$q_s = H_\chi \gamma_{cum} t$$

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Second idea: steady state non linear heat equation

ad hoc solution $T = \gamma_\chi$

$\rightarrow$ OK: $\gamma_{cum} \rightarrow \gamma_\chi$

$$\dot{T} = 0$$
$$\lambda = A$$
$$q_s = H_\chi(\gamma_{cum} - T)$$

Thermics implementation

$$\boldsymbol{A} = A\mathbf{1}, \qquad A\Delta\gamma_\chi = H_\chi(\gamma_\chi - \gamma_{cum}) \quad \Leftrightarrow \quad \rho C_p \dot{T} = \lambda \Delta T + q_s$$

First idea: transient linear heat equation

ad hoc solution $T = \gamma_\chi t$ $\qquad \rho C_p = H_\chi t$

$\lambda = A$

→ failed (poor convergence) $\qquad q_s = H_\chi \gamma_{cum} t$

Second idea: steady state non linear heat equation

ad hoc solution $T = \gamma_\chi$ $\qquad \dot{T} = 0$

$\lambda = A$

→ OK: $\gamma_{cum} \to \gamma_\chi$ $\qquad q_s = H_\chi(\gamma_{cum} - T)$

Code_Aster resolution

THER_NON_LINE with non linear source term field

- field part $(H_\chi \gamma_{cum})$ from
  AFFE_CHAR_THER / SOURCE / SOUR_CALCULEE
- non linear part $(-H_\chi T)$ from
  AFFE_CHAR_THER_F / SOUR_NL / SOUR

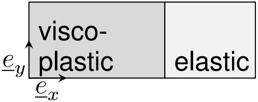
Staggered resolution

$\gamma_\chi \to$ mechanics $\to \gamma_{cum} \to$ thermics $\to \gamma_\chi \to \dots$

Python loop in Code_Aster ".comm" file

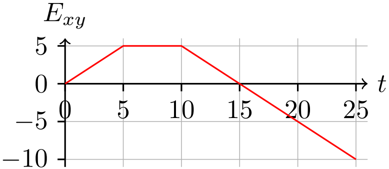
- γ_χ field is known at t
- AFFE_VARC: γ_χ as T field
- one STAT_NON_LINE step (calling MFront behaviour)
  $\to$ fields at $t + \Delta t$: $\underline{u}$, $\boldsymbol{\sigma}$, γ_{cum} (as internal variable)
- extract γ_{cum} field, compute source term
- THER_NON_LINE
  $\to$ field at $t + \Delta t$: γ_χ (as T)
- γ_χ field is known at $t + \Delta t$: iterate...

Verification: periodic bi-crystal



periodic BC, average strain

$$\boldsymbol{E} = E_{xy}(\underline{e}_x \otimes \underline{e}_y + \underline{e}_y \otimes \underline{e}_x)$$



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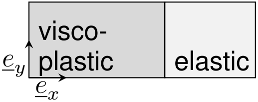

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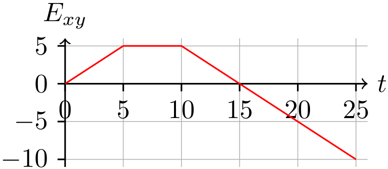

Prototype implementation Code_Aster + MFront (from scratch)

- one slip system: $N = 1$, $\underline{m}^s = \underline{e}_x$, $\underline{n}^s = \underline{e}_y$
- τ_c^s constant
- BC at crystal boundaries: $\gamma_\chi = 0$

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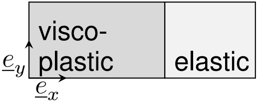

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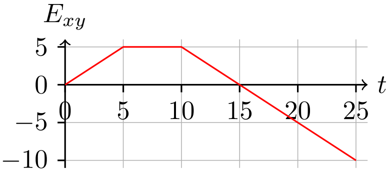

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Input data (arbitrary units!)

Elasto-viscoplastic crystal

$f = 0.6$, $E = 3$, $\nu = 0.1$

$n = 3$, $K = 1.4$, $\tau_c^s = 2.3$

$H_\chi = 3.1$, $A = 0.17$

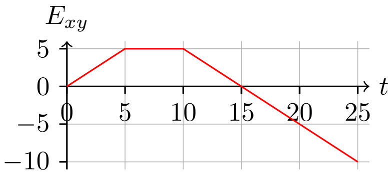
Elastic crystal

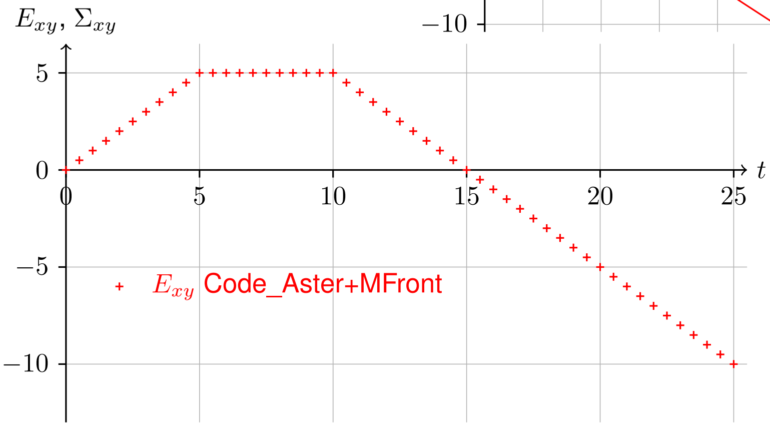
$f = 0.4$, $E = 1$, $\nu = 0.3$

Reference “analytical” computation

direct resolution of PDE system over time and 1D spatial domain

Evolution of average strain, stress





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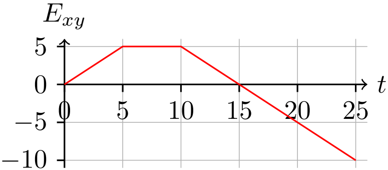

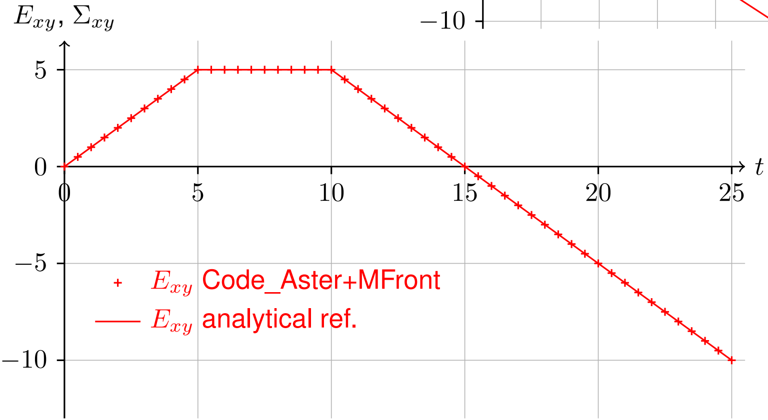

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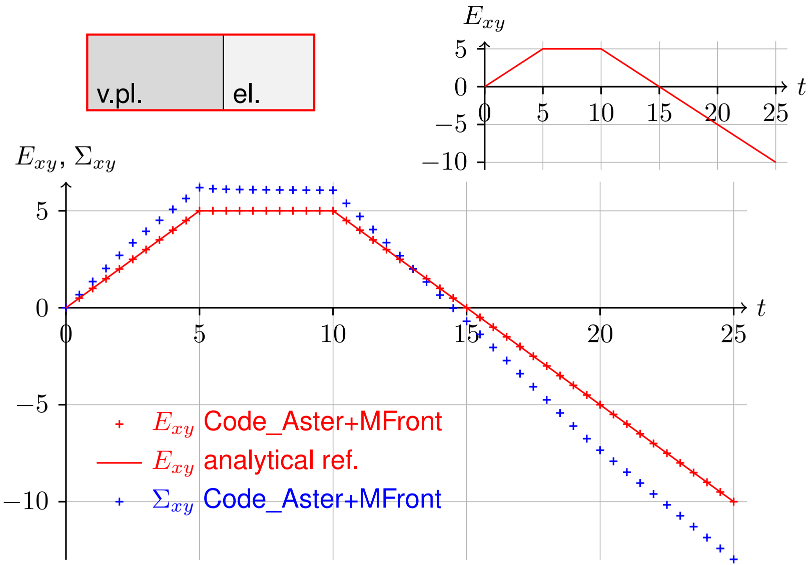

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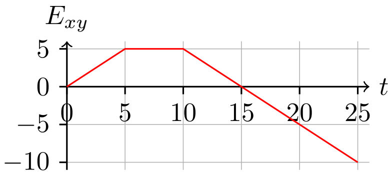
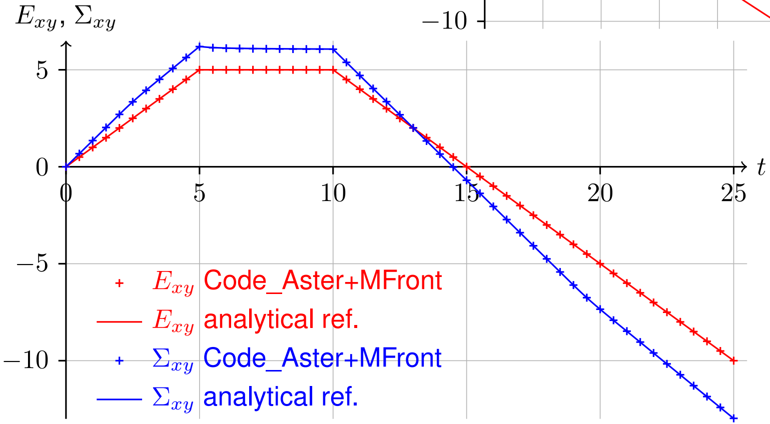
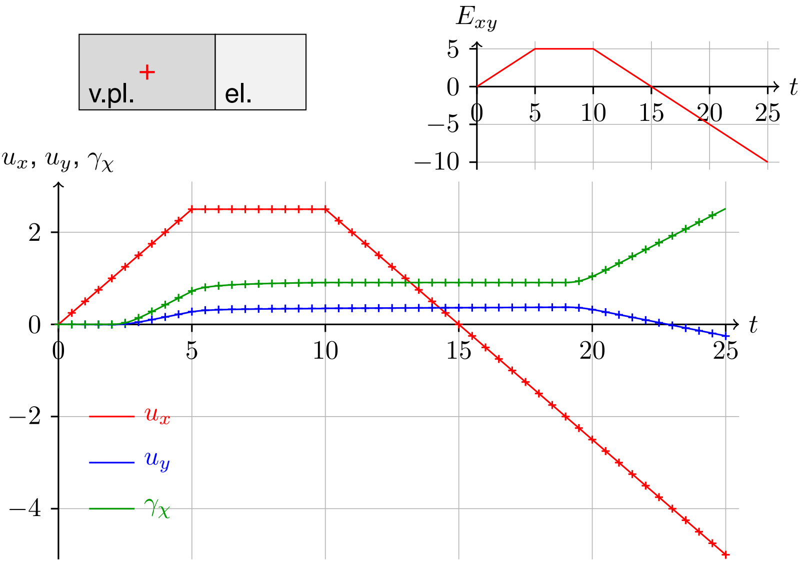
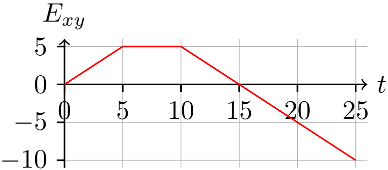


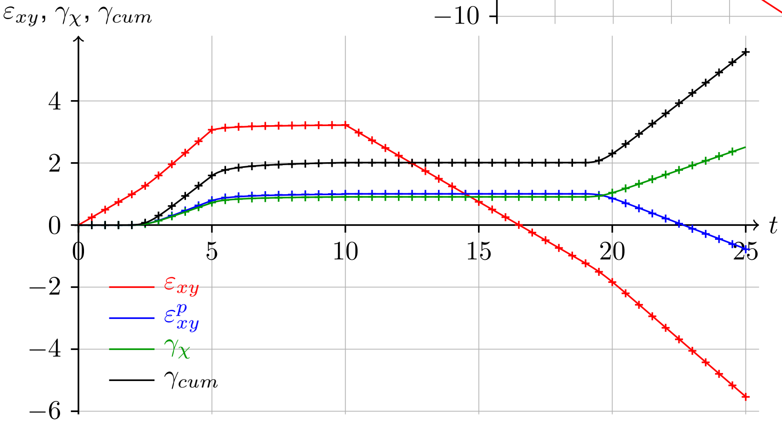


Evolution of DOFs at center of viscoplastic phase

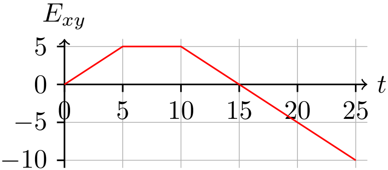


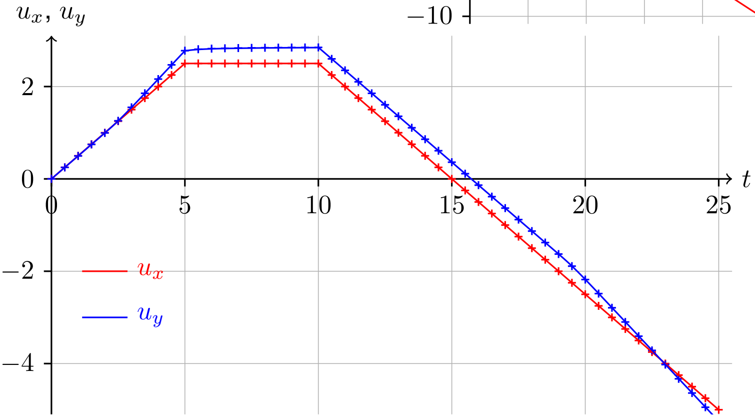
Evolution of strains at center of viscoplastic phase



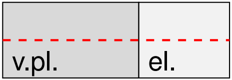


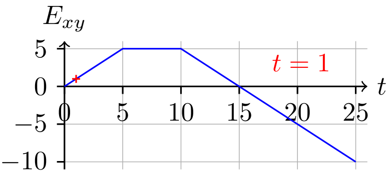
Evolution of DOFs at center of elastic phase

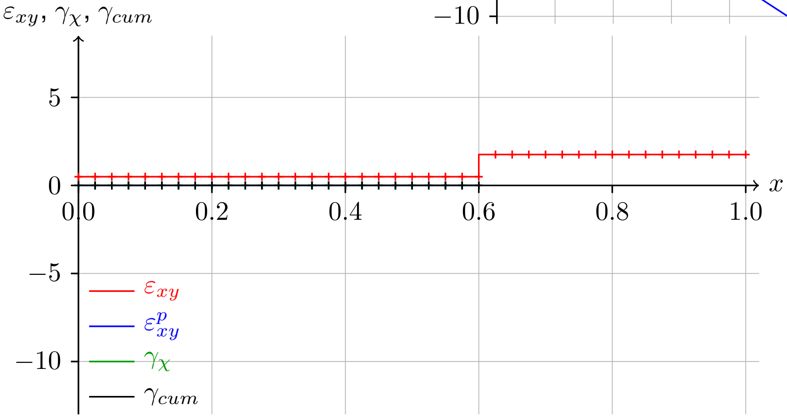




Profiles of strains







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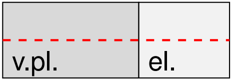

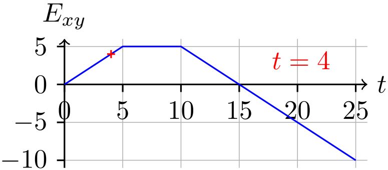

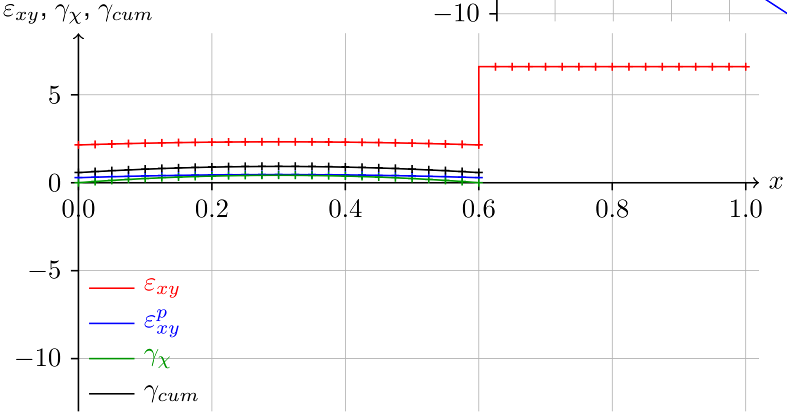

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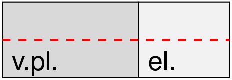

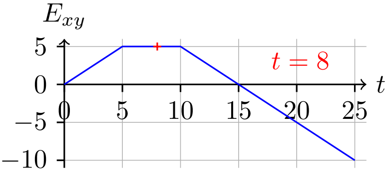

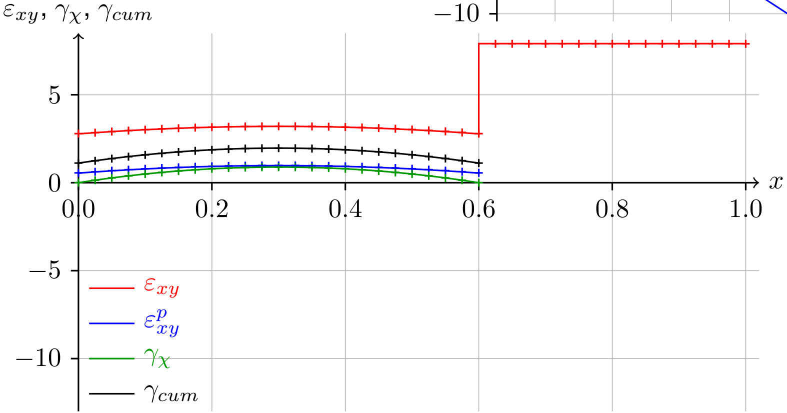

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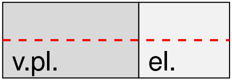

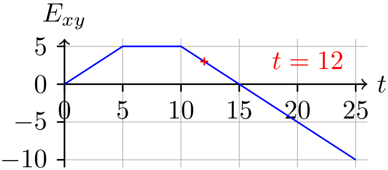

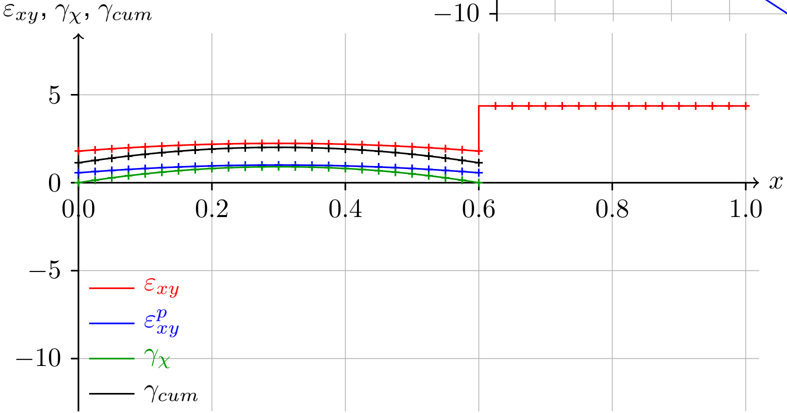

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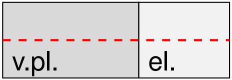

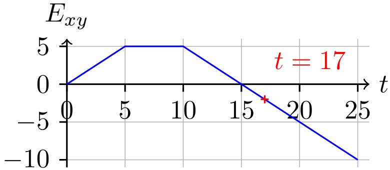

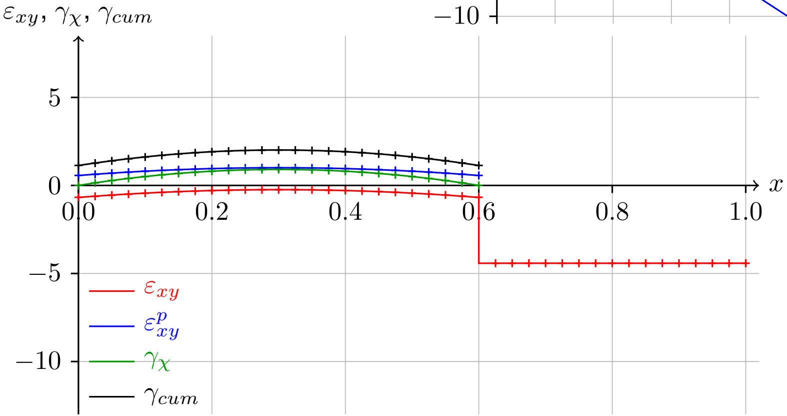

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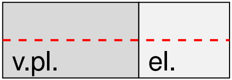
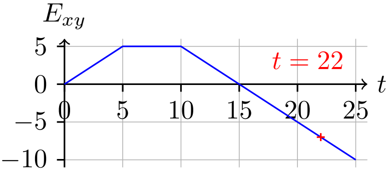
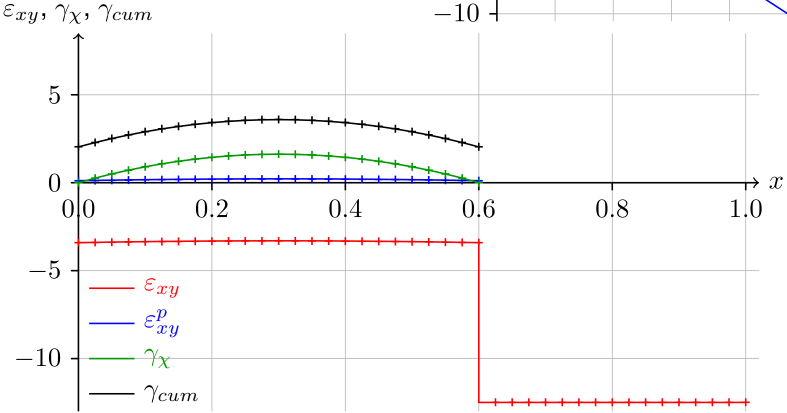
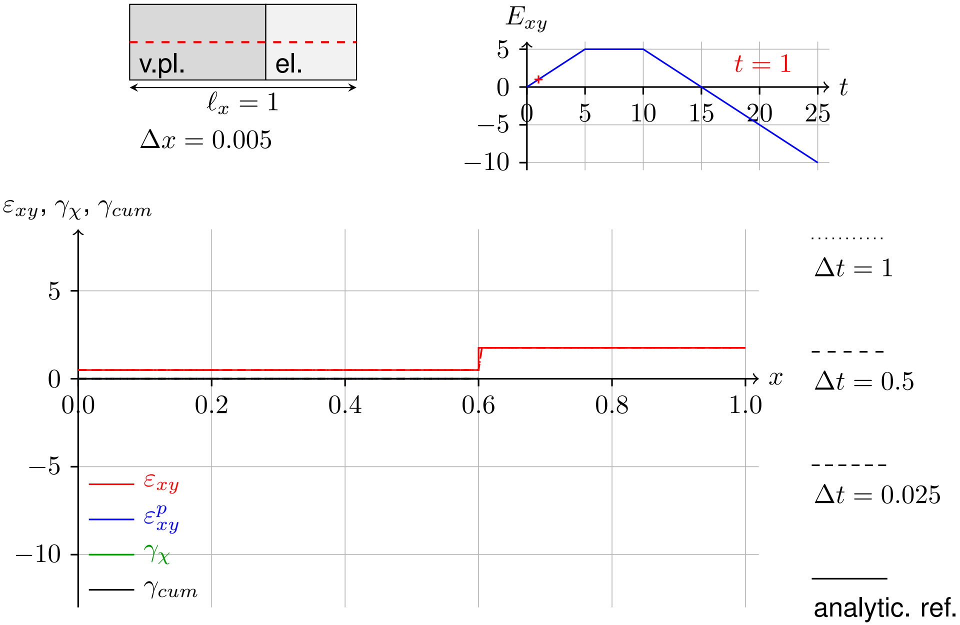






Profiles of strains: influence of time step



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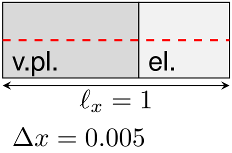

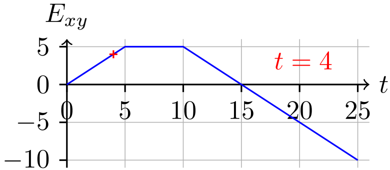

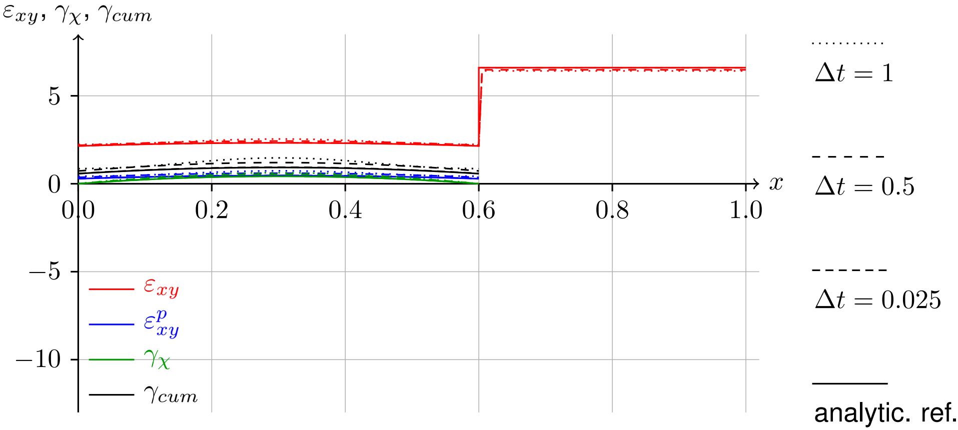

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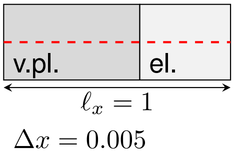

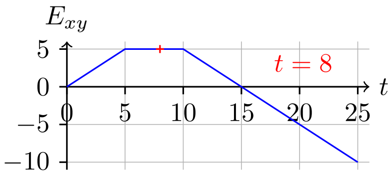

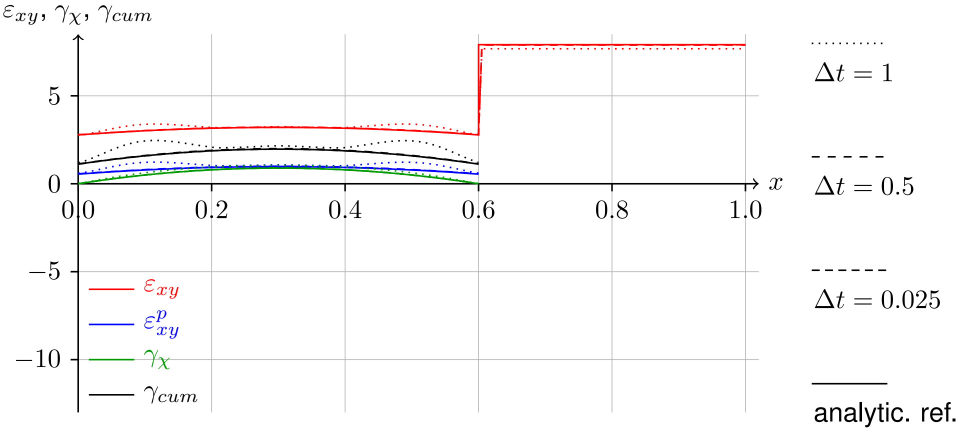

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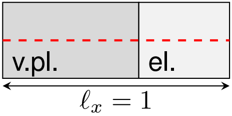
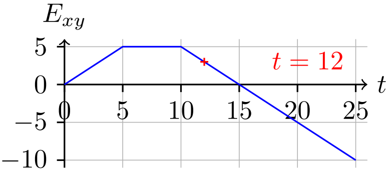
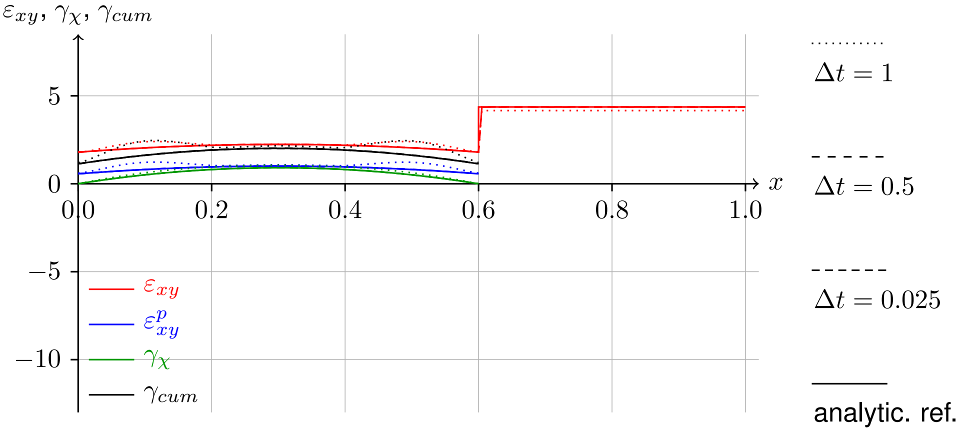


$\Delta x = 0.005$





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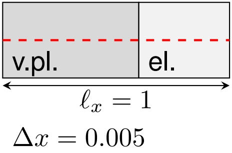

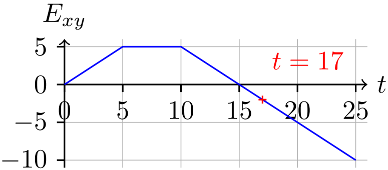

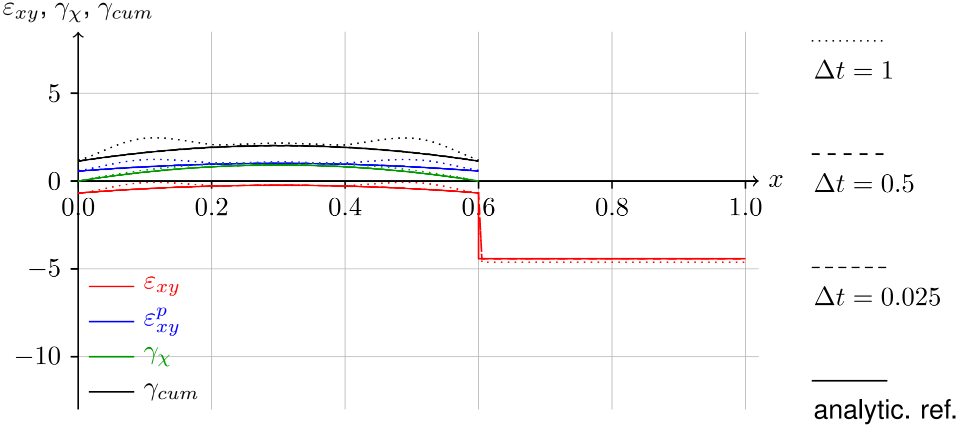

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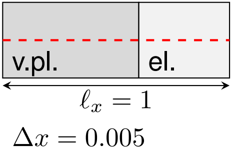

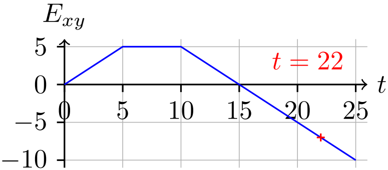

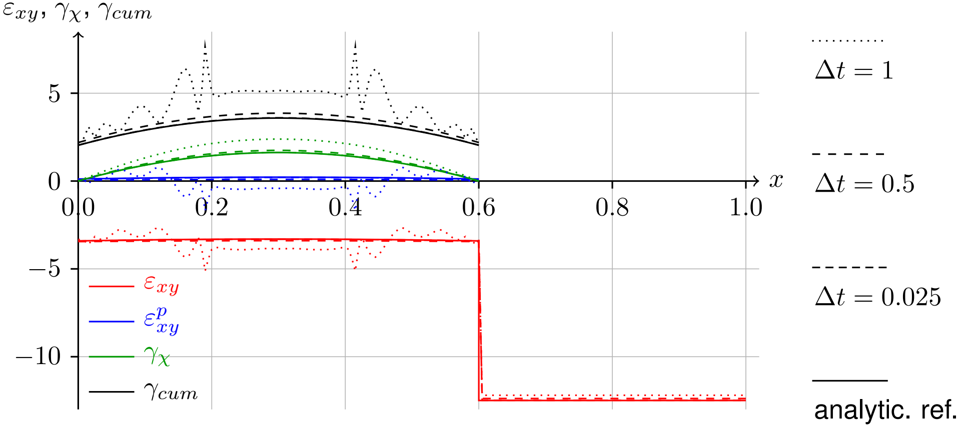

Conclusion, prospects

First prototype shows feasability

- infinitesimal strain theory
- one slip system
- constant critical resolved shear stress
- $\rightarrow$ verification on periodic bi-crystal

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- one slip system
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Next steps?

- non constant critical resolved shear stress: hardening/softening
- modify an existing MFront behaviour: several slip systems
- clean and optimize implementation
- polycristal applications:
  realistic input data + BC on microslip field at grain boundary
- finite strains
- direct Code_Aster/MFront management of
  enriched kinetics or strain gradient constitutive behaviors?
- ...