Mathematical modeling of dislocation dynamics

Régis Monneau

Thursday 13th, December 2007

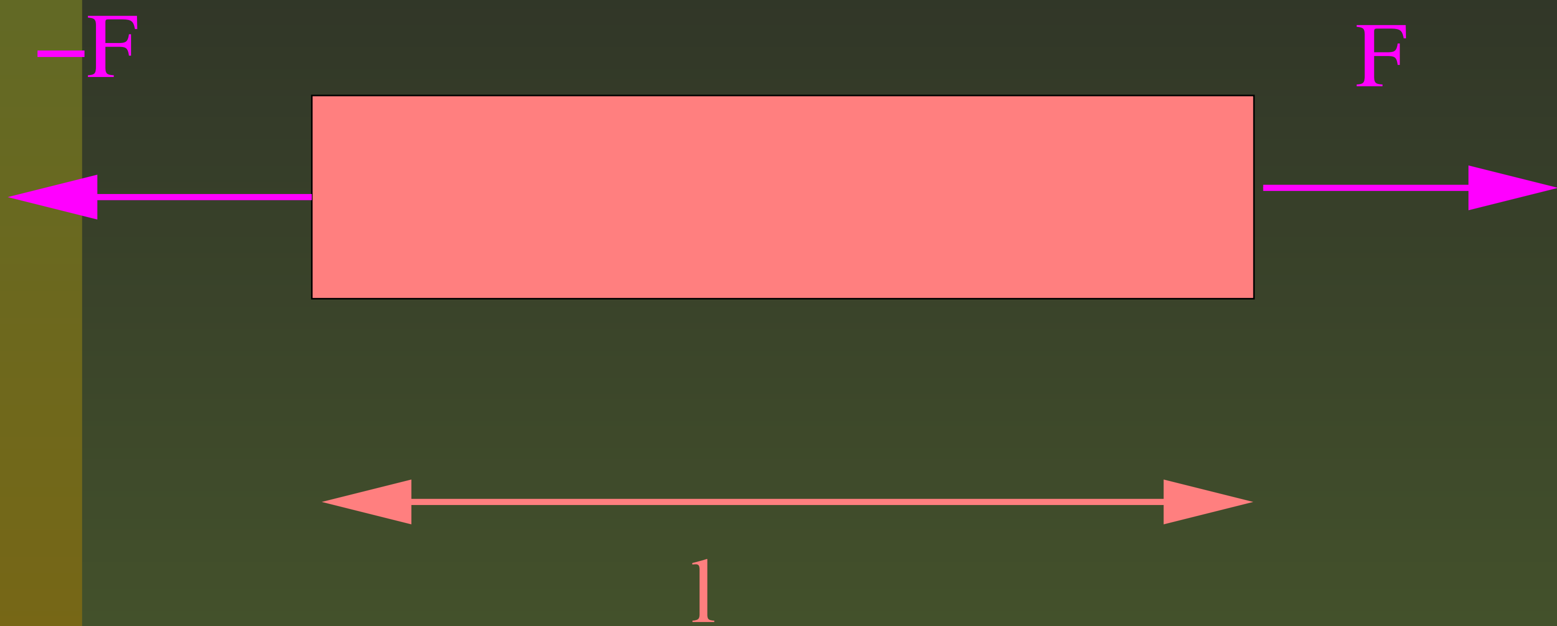
CERMICS-ENPC

Plan of the talk

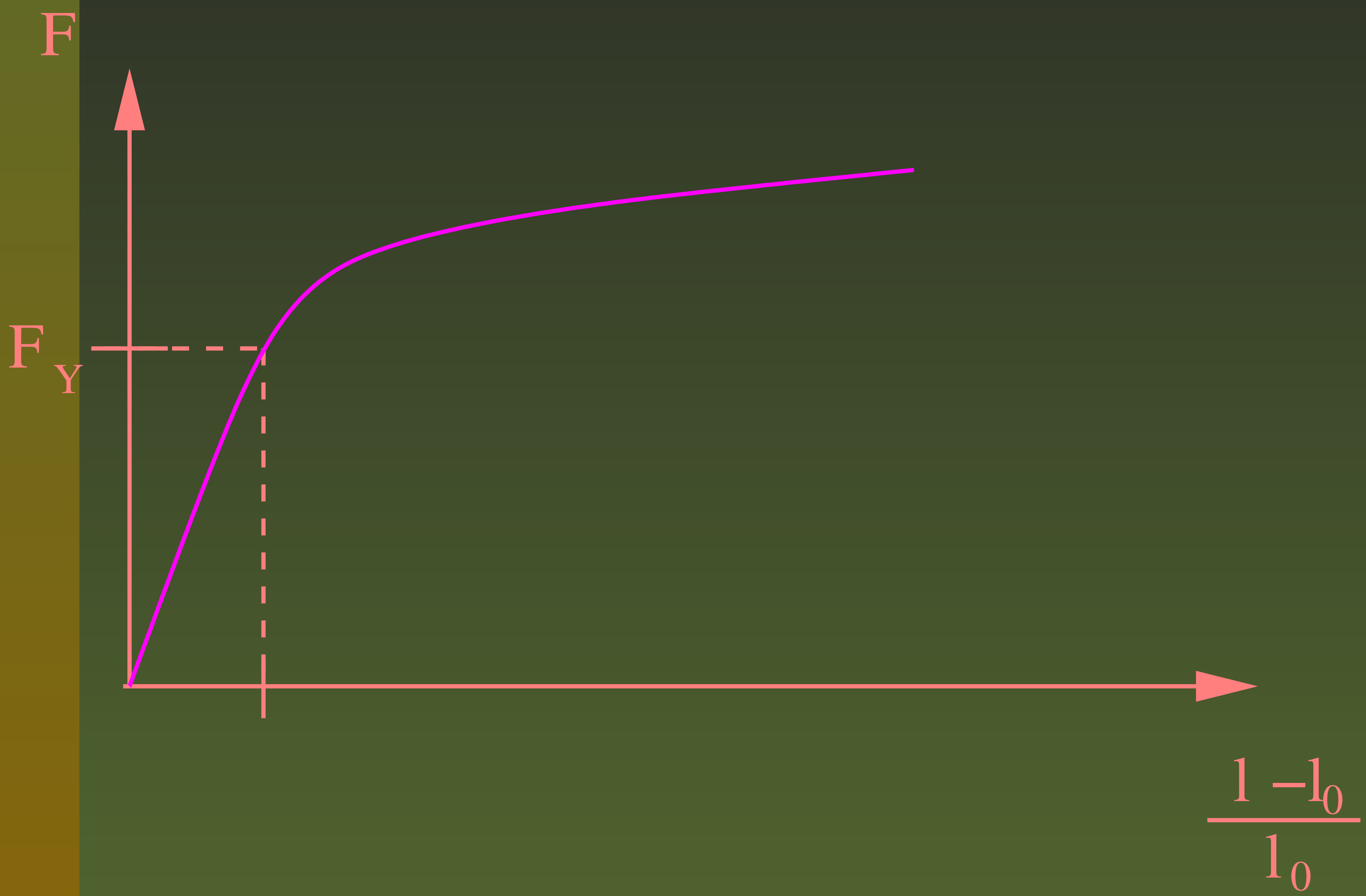
- Introduction to dislocations
- Sharp interface modeling
- Mathematical results for the dynamics
- Link with MCM

Introduction to dislocations

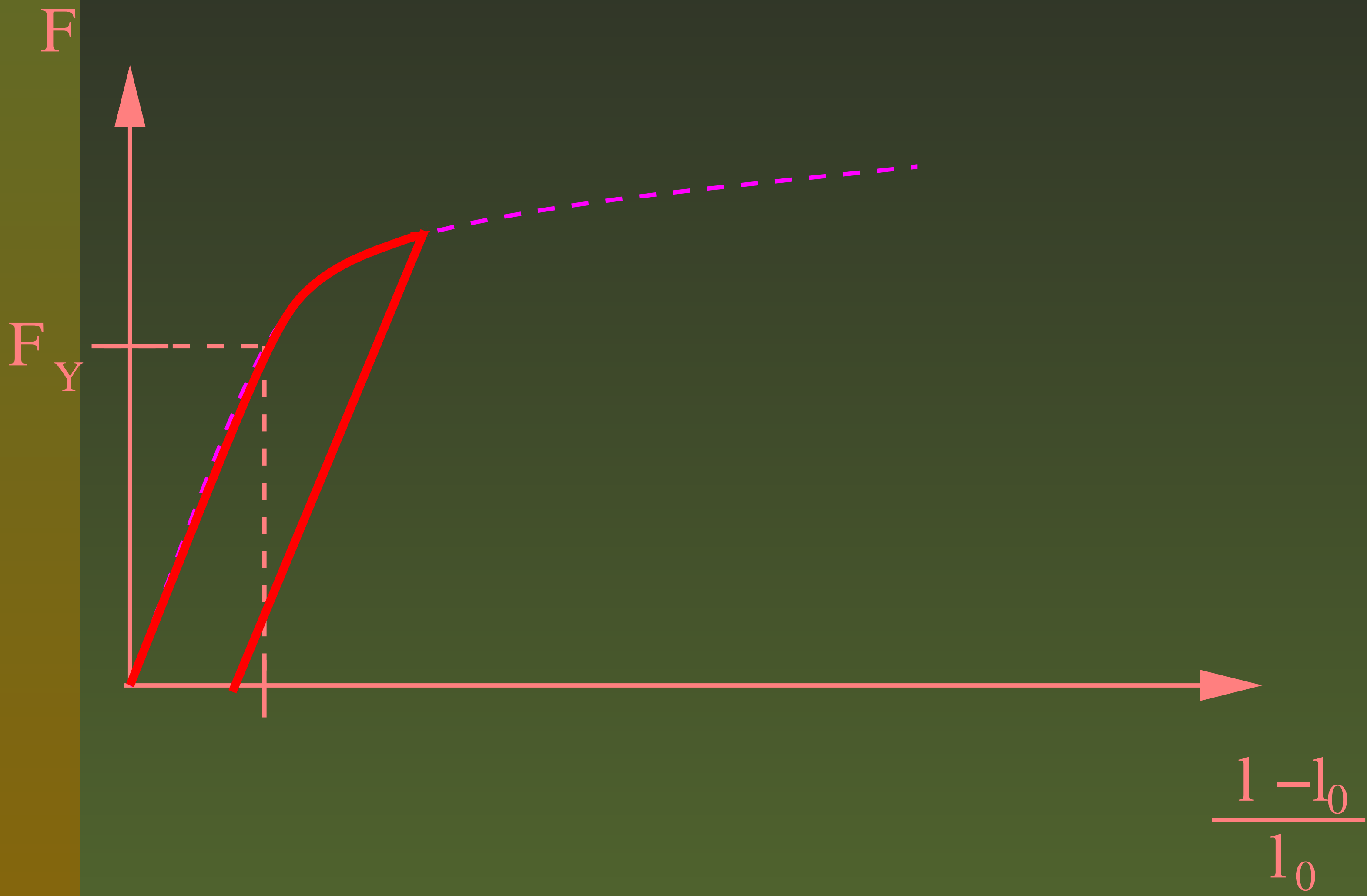
Traction of a sample



Plasticity



Persistent plastic strain



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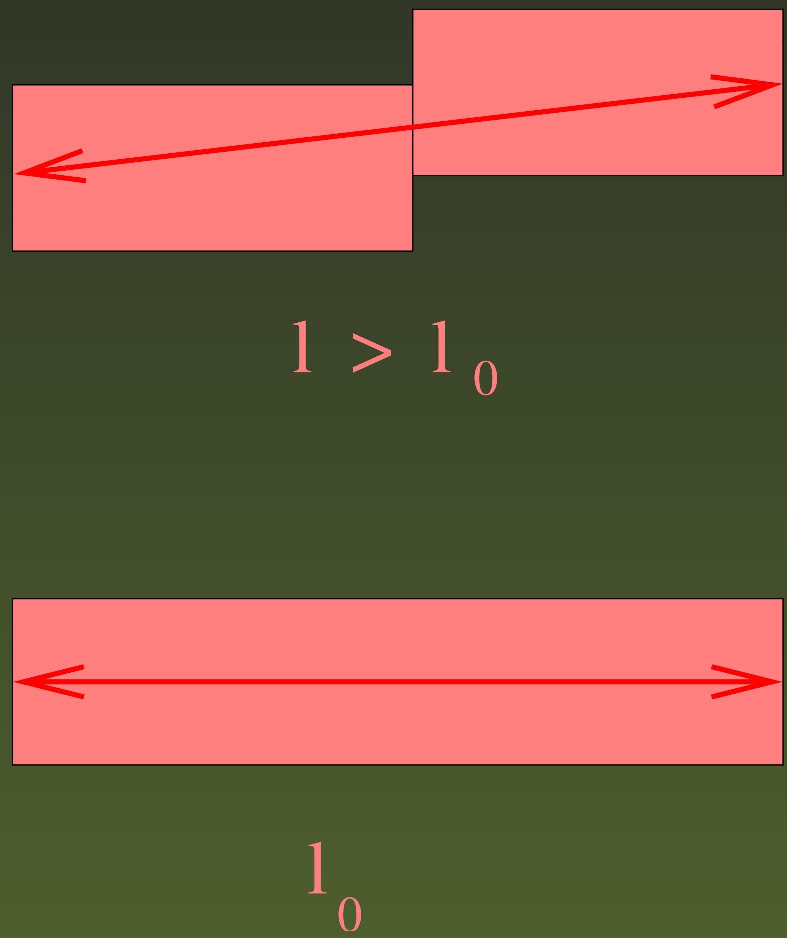
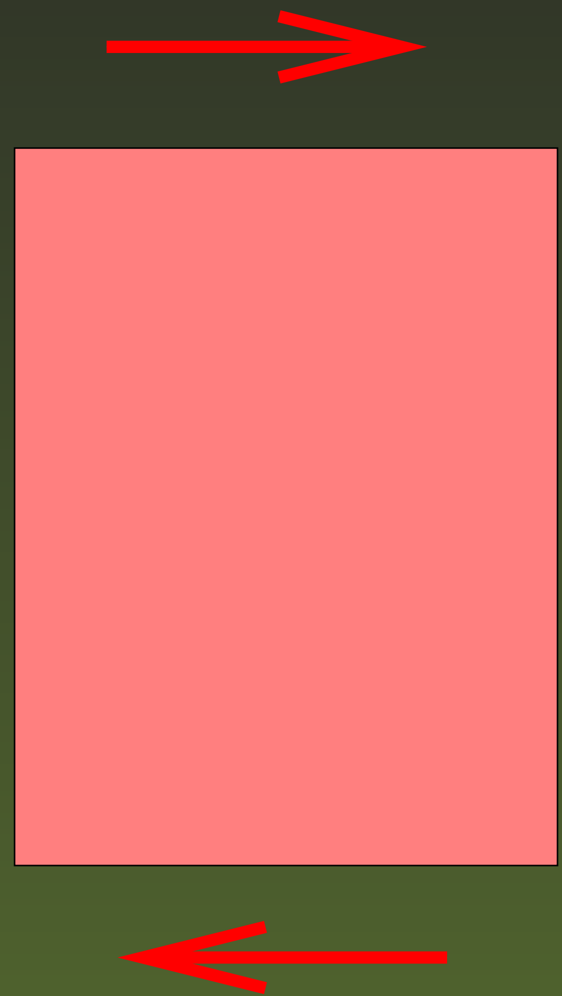


Scenario 1



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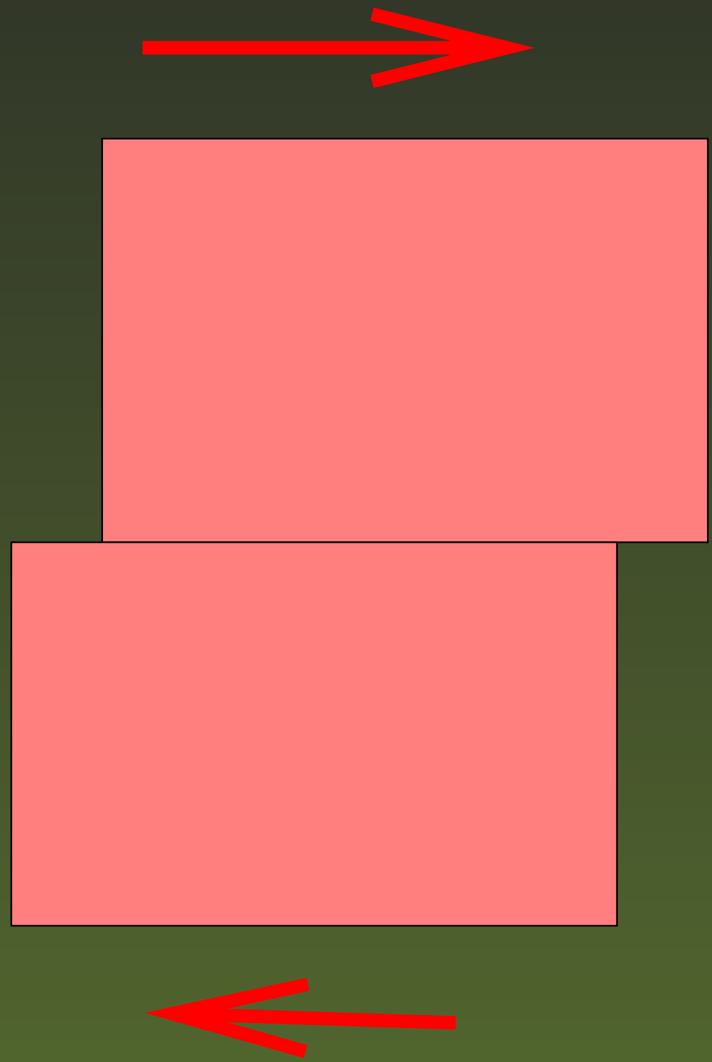

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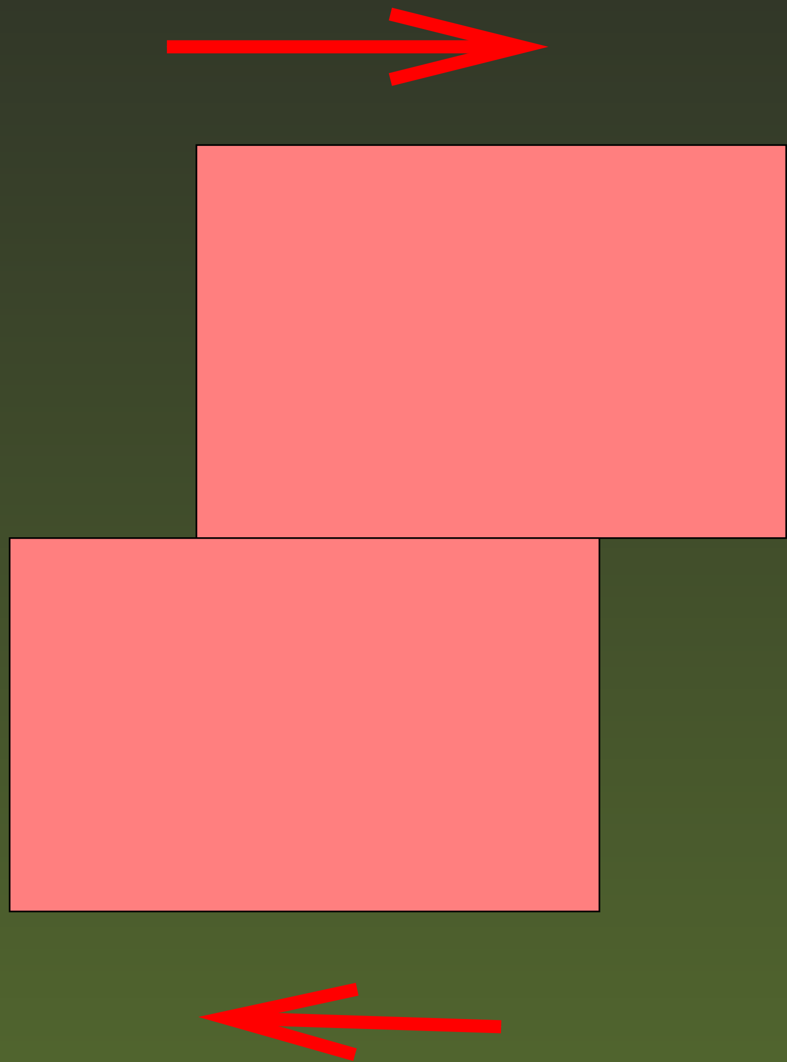

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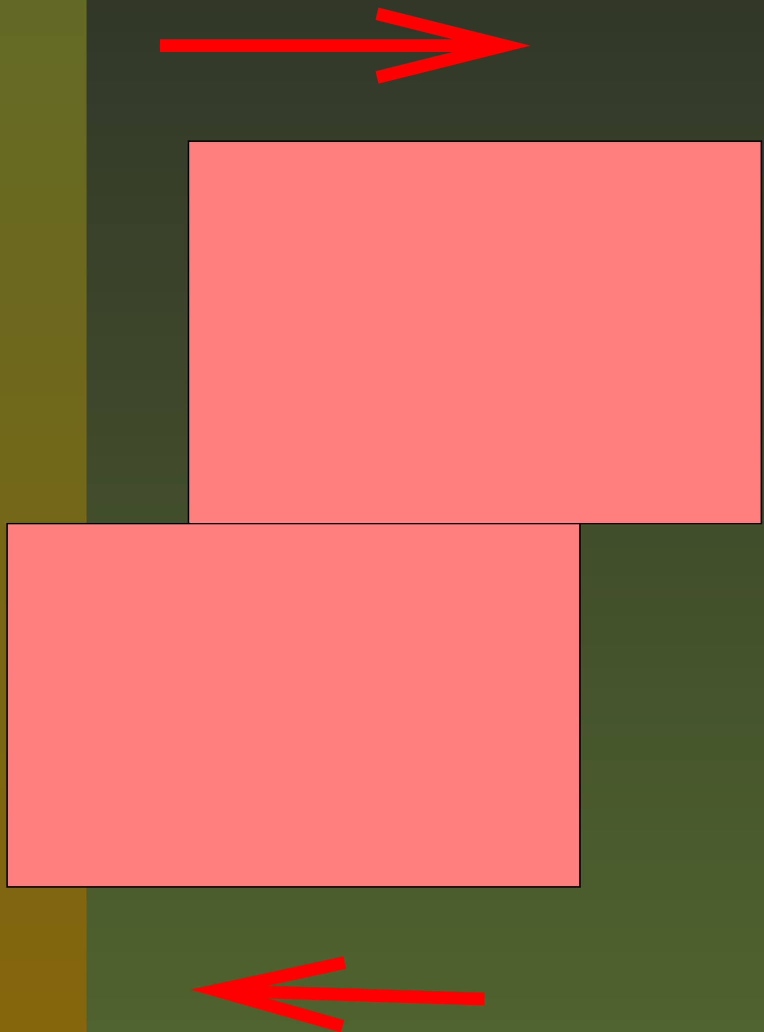
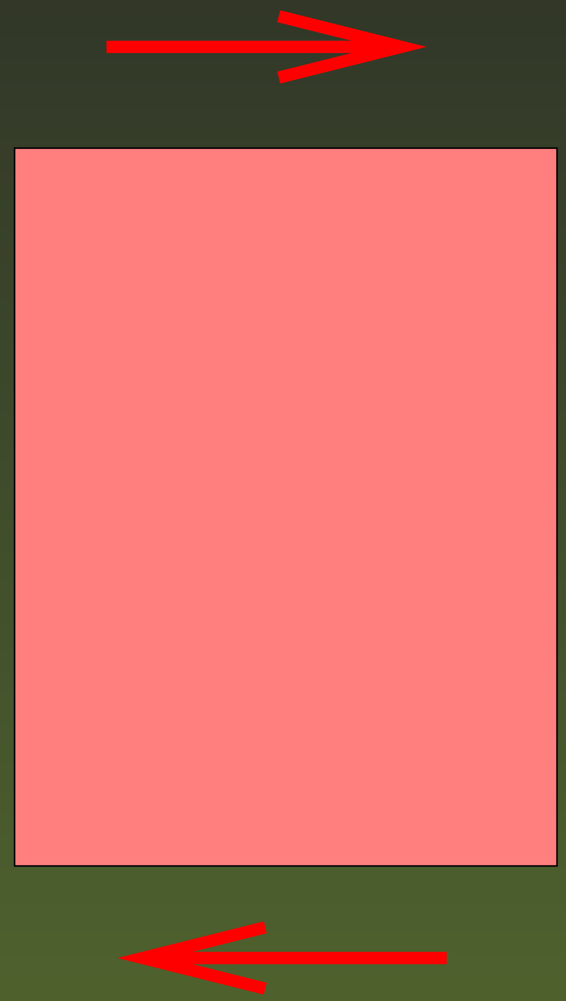
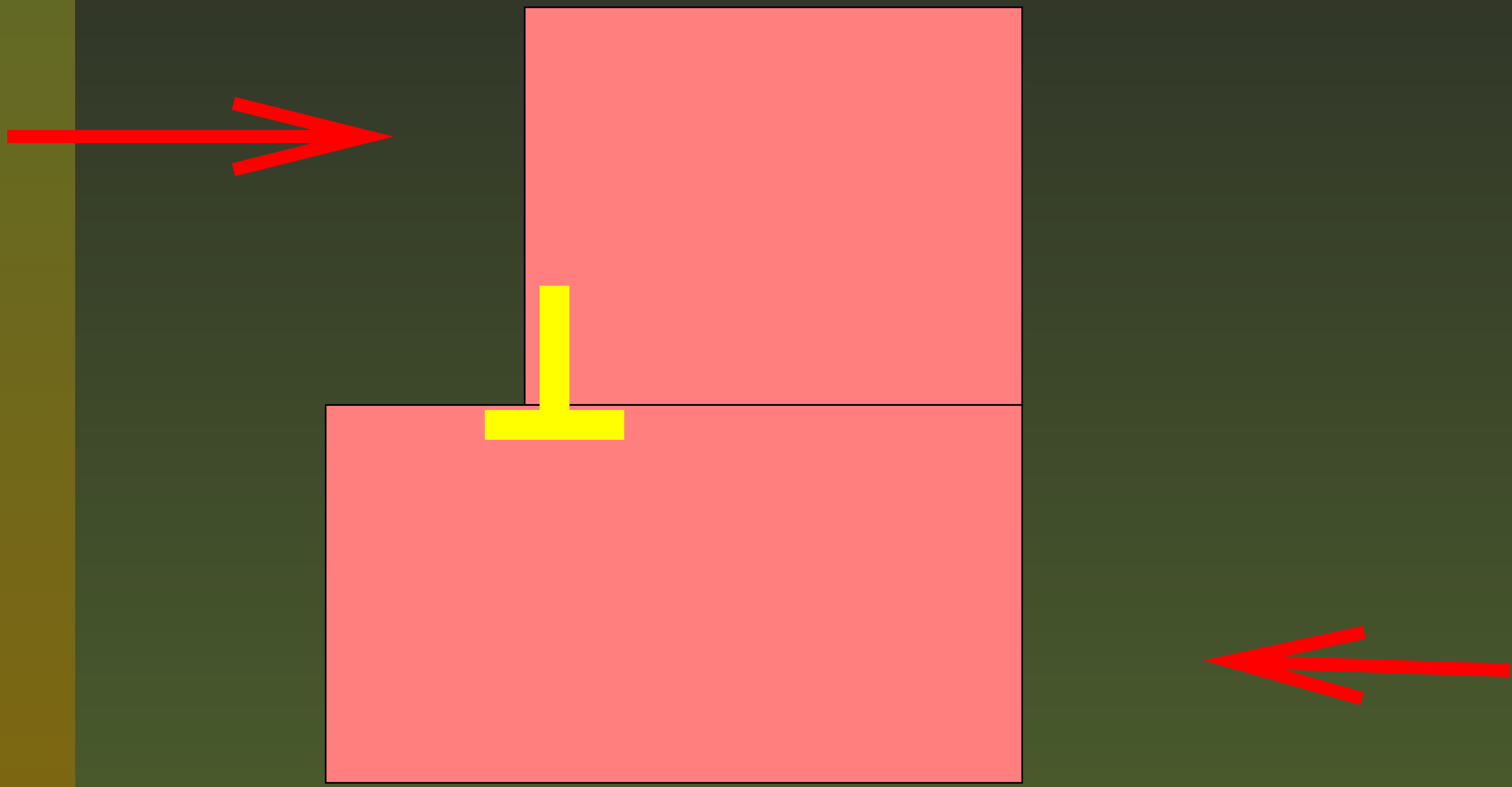


IMPOSSIBLE !!

Scenario 2



Scenario 2



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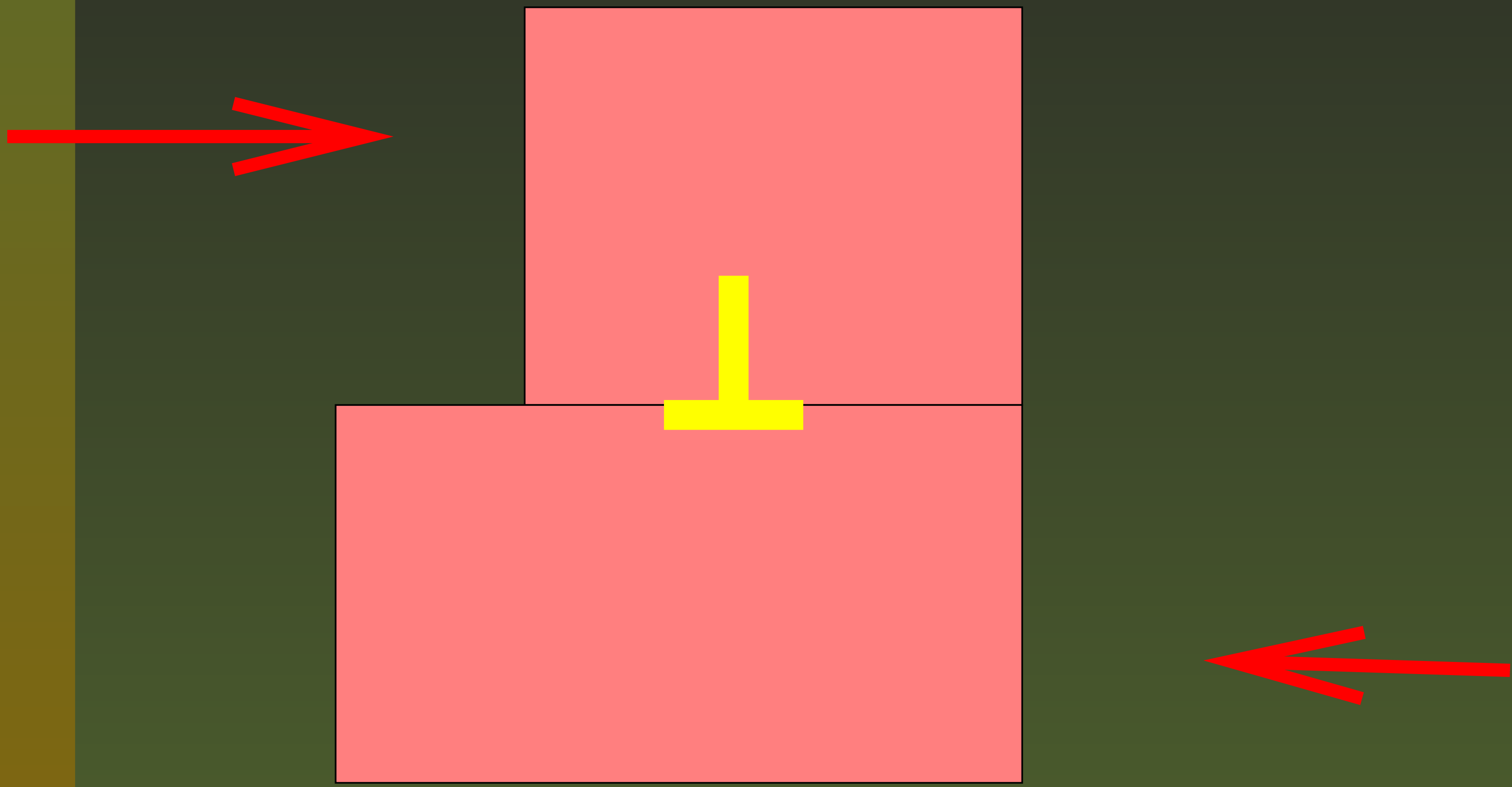
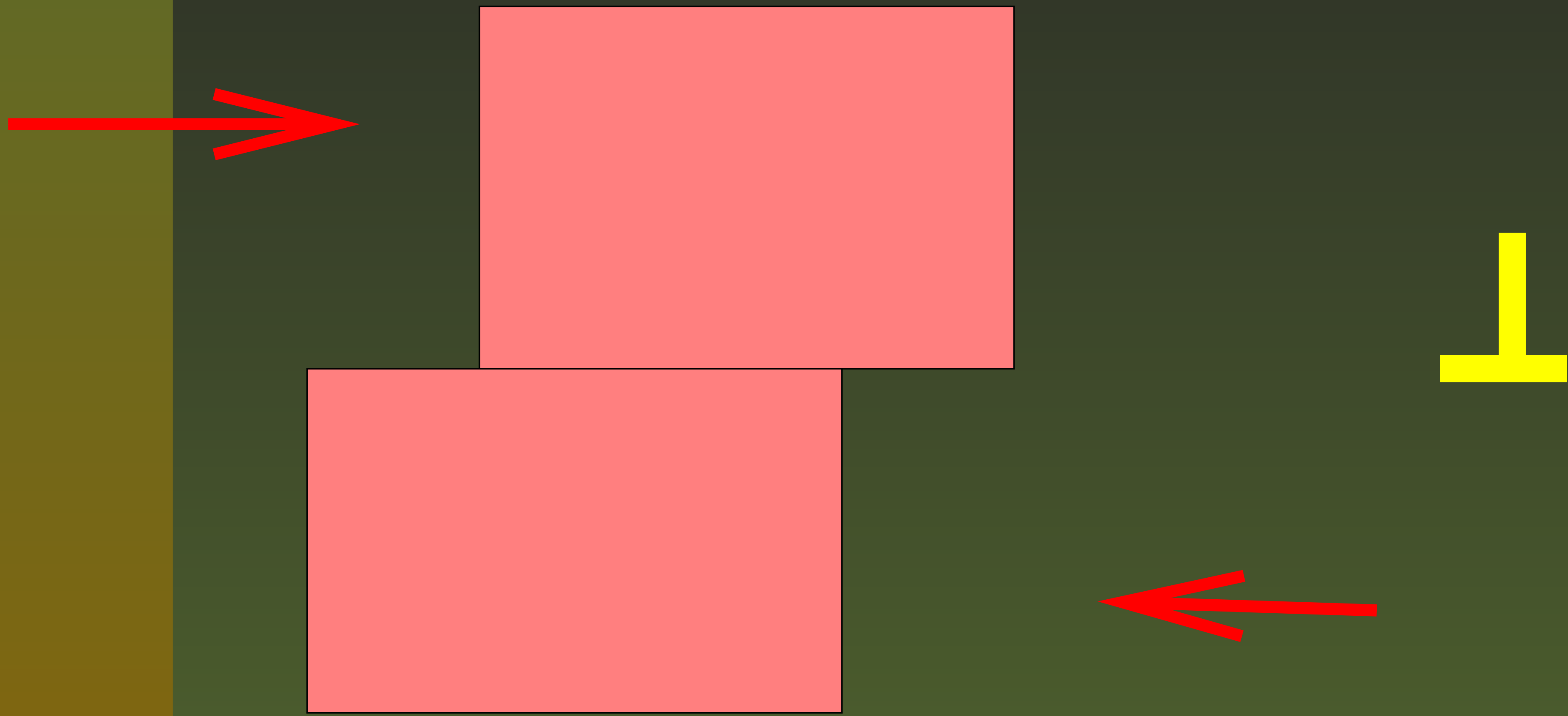


Concept of dislocation (1934): Orowan; Polanyi; Taylor

Scenario 2



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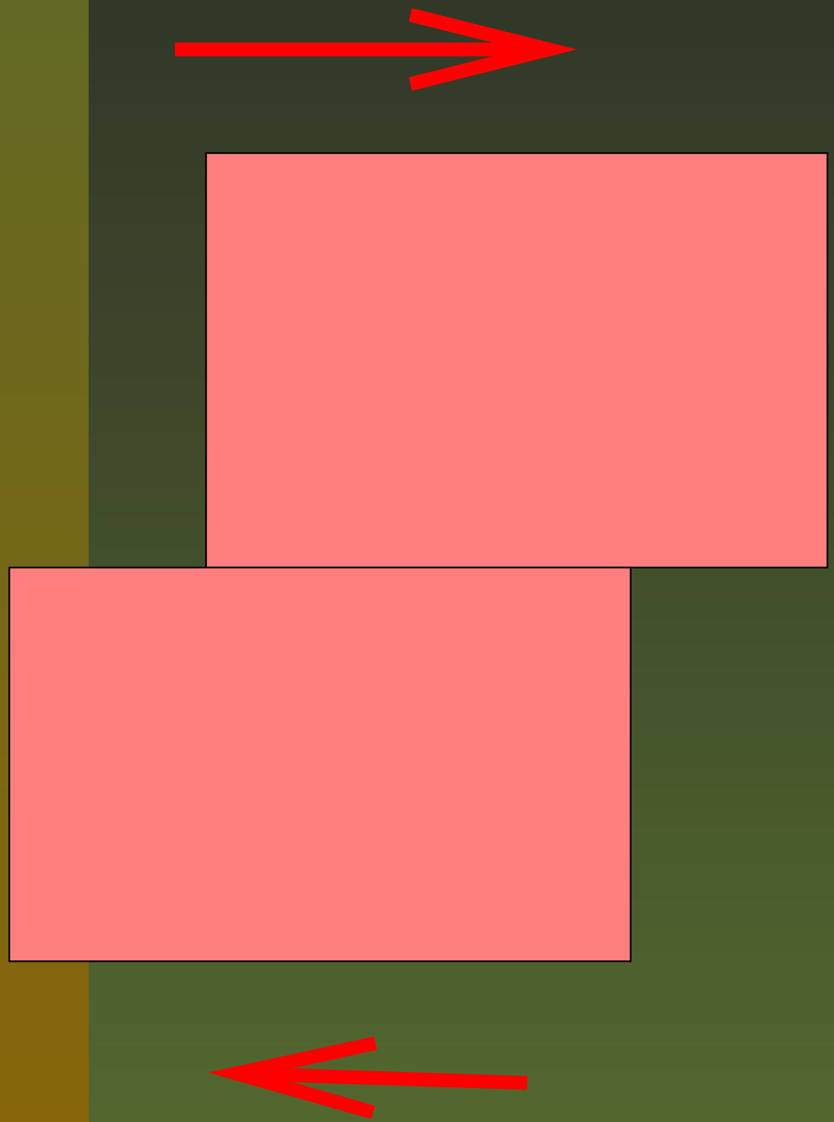
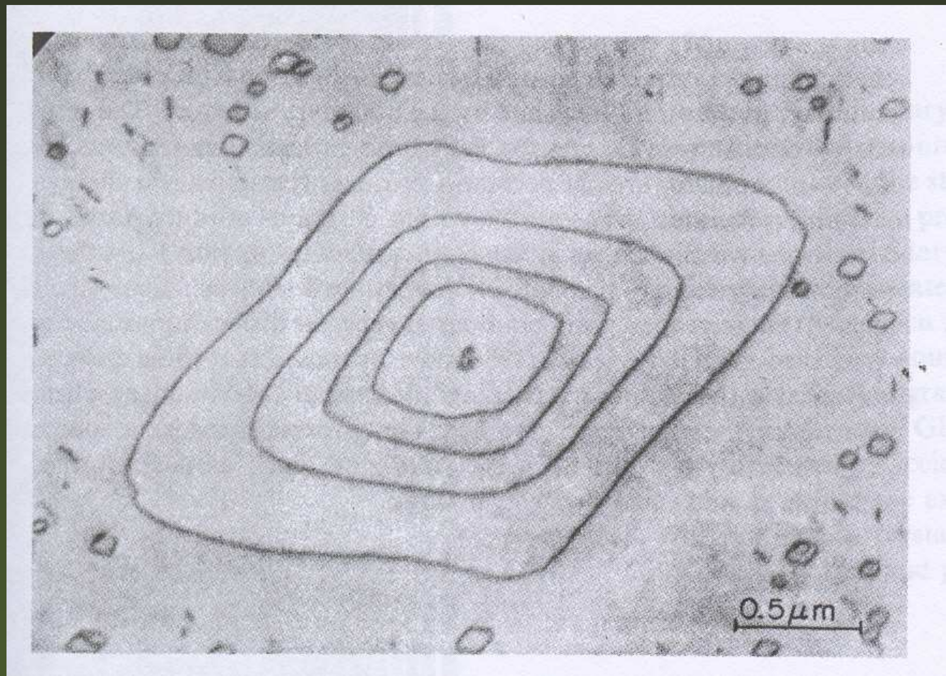


POSSIBLE !!

Description of dislocations

Observation of dislocations

Dislocations in metallic alloys Al-Mg



Observation of dislocations

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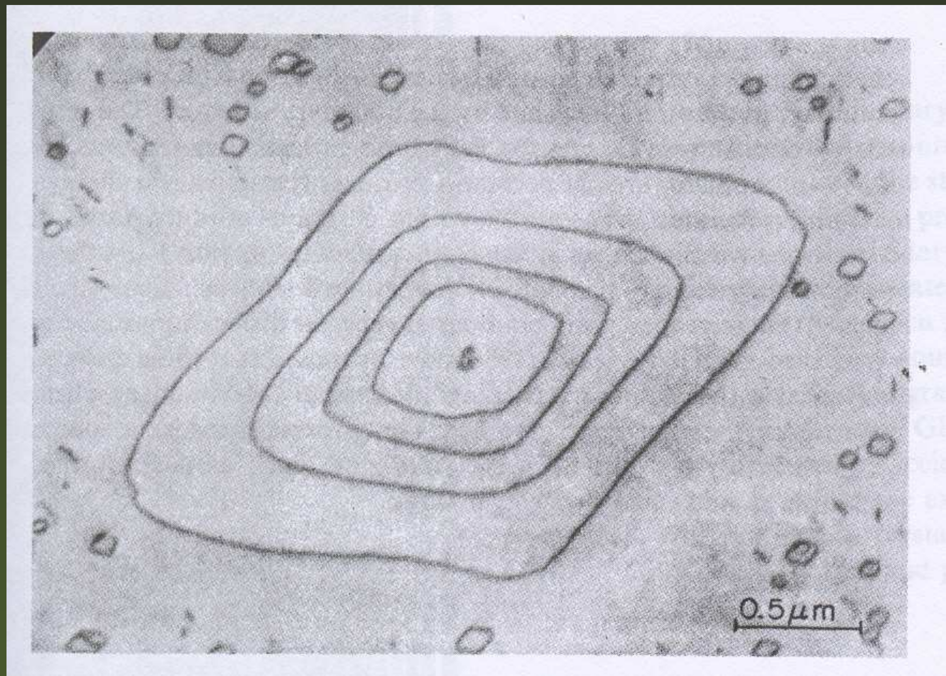

Definition: a dislocation is a line of crystal defects.

Observation of dislocations

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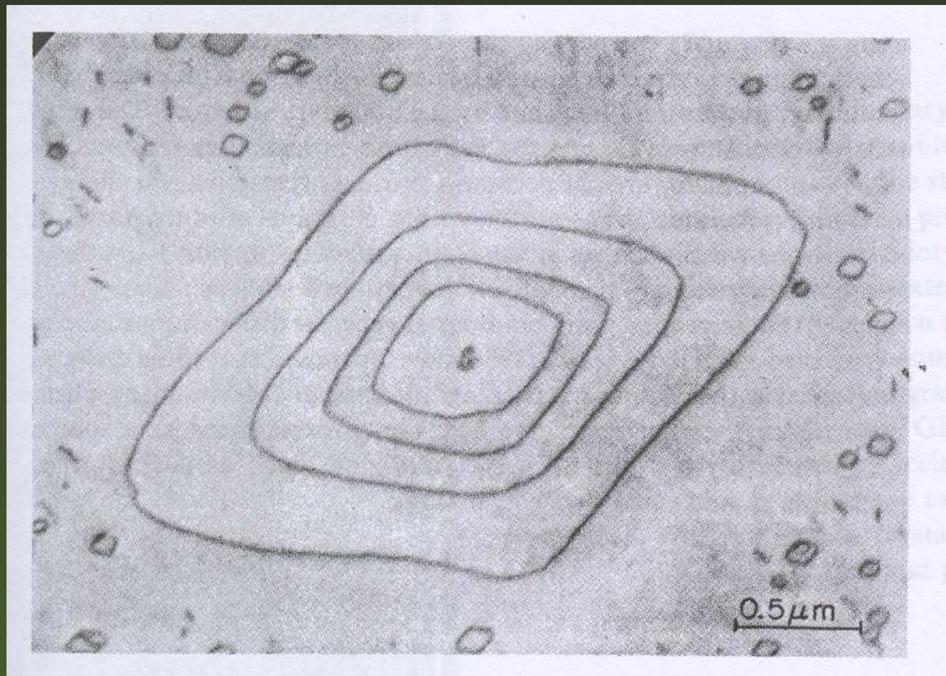

Definition: a dislocation is a line of crystal defects.

Length = $10^{-6}m$, Thickness = $10^{-9}m$.

A very brief summary of the history

- 1934: introdution of the concept of dislocation to explain plasticity [Orowan / Polanyi / Taylor]

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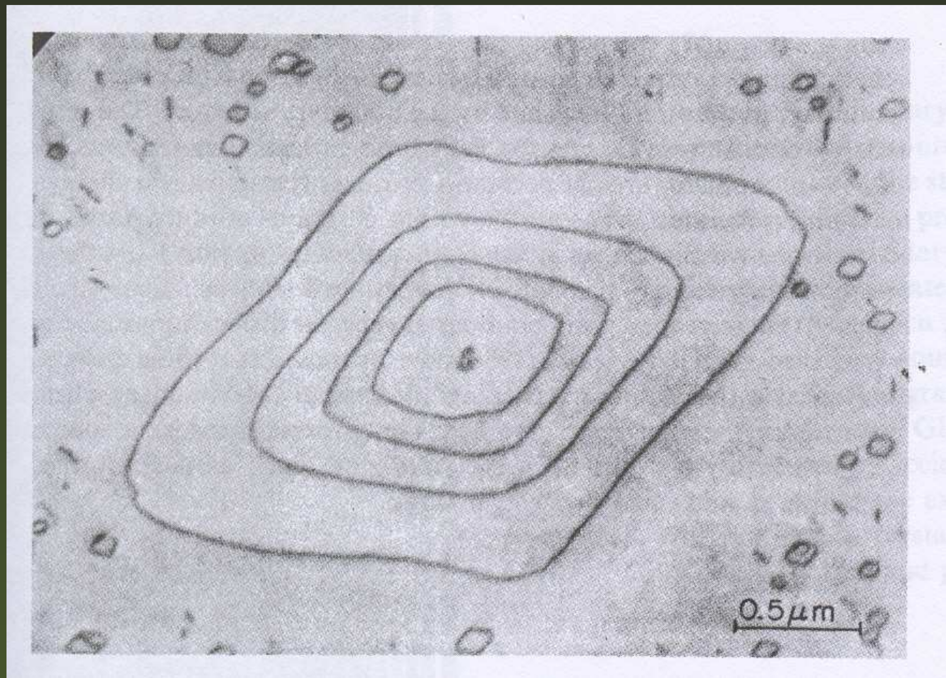
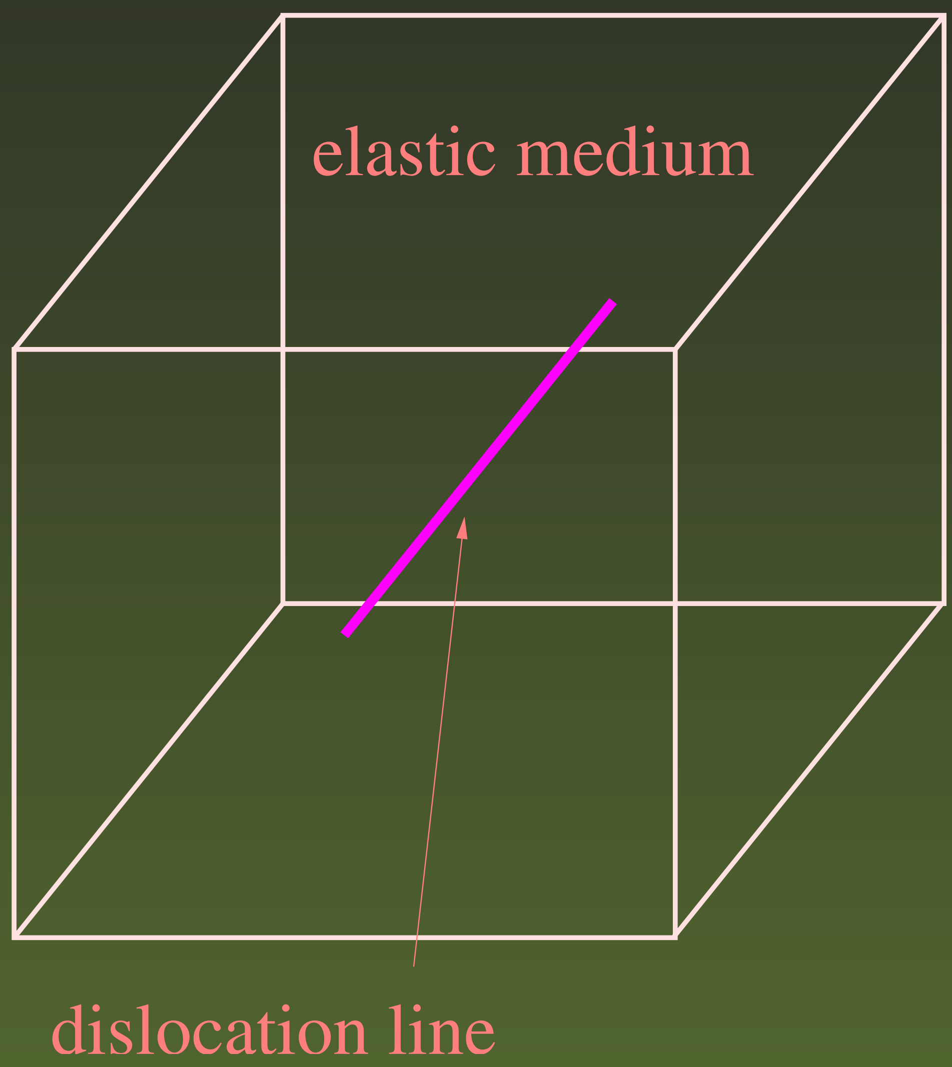
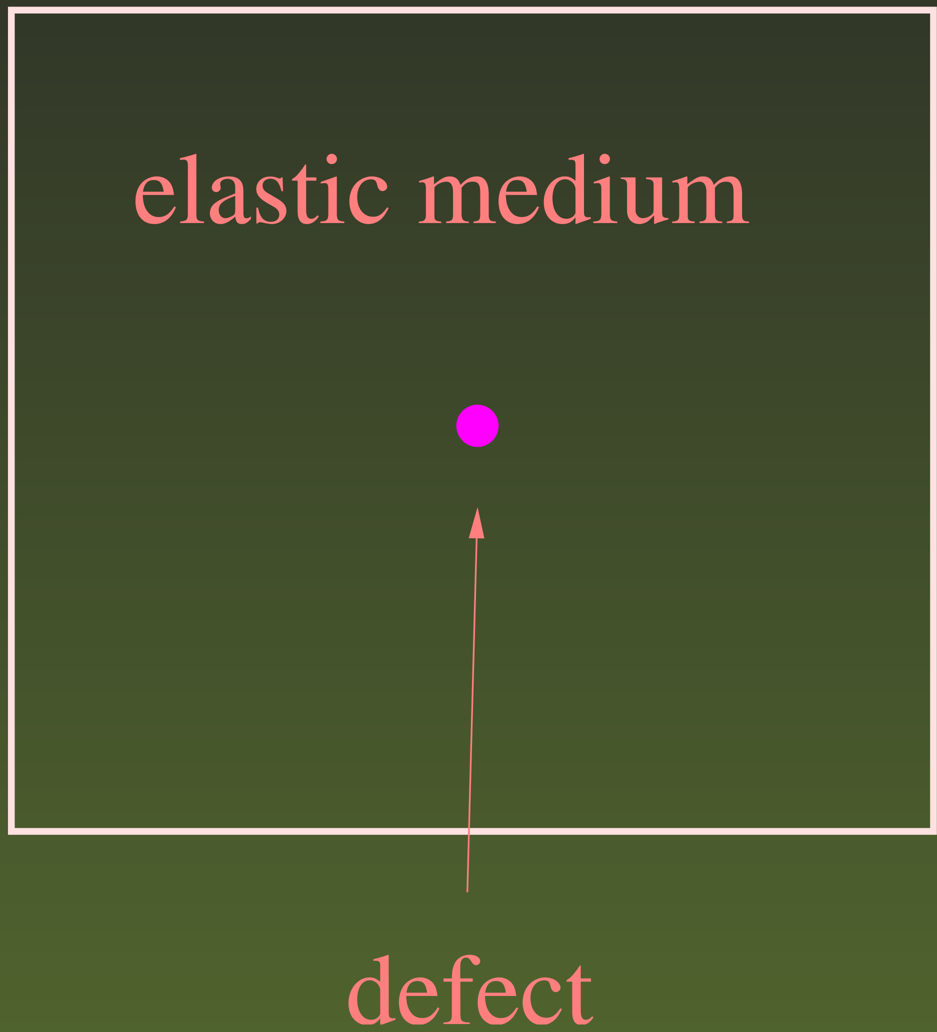
- 1934: introdution of the concept of dislocation to explain plasticity [Orowan / Polanyi / Taylor]
- 1956: first observation of dislocations
- $\sim$ 1970: treatises on dislocations equilibrium [Nabarro / Hirth &Lothe, ...]
- Since 1990: dislocations dynamics explored by computer simulations


0.5μm

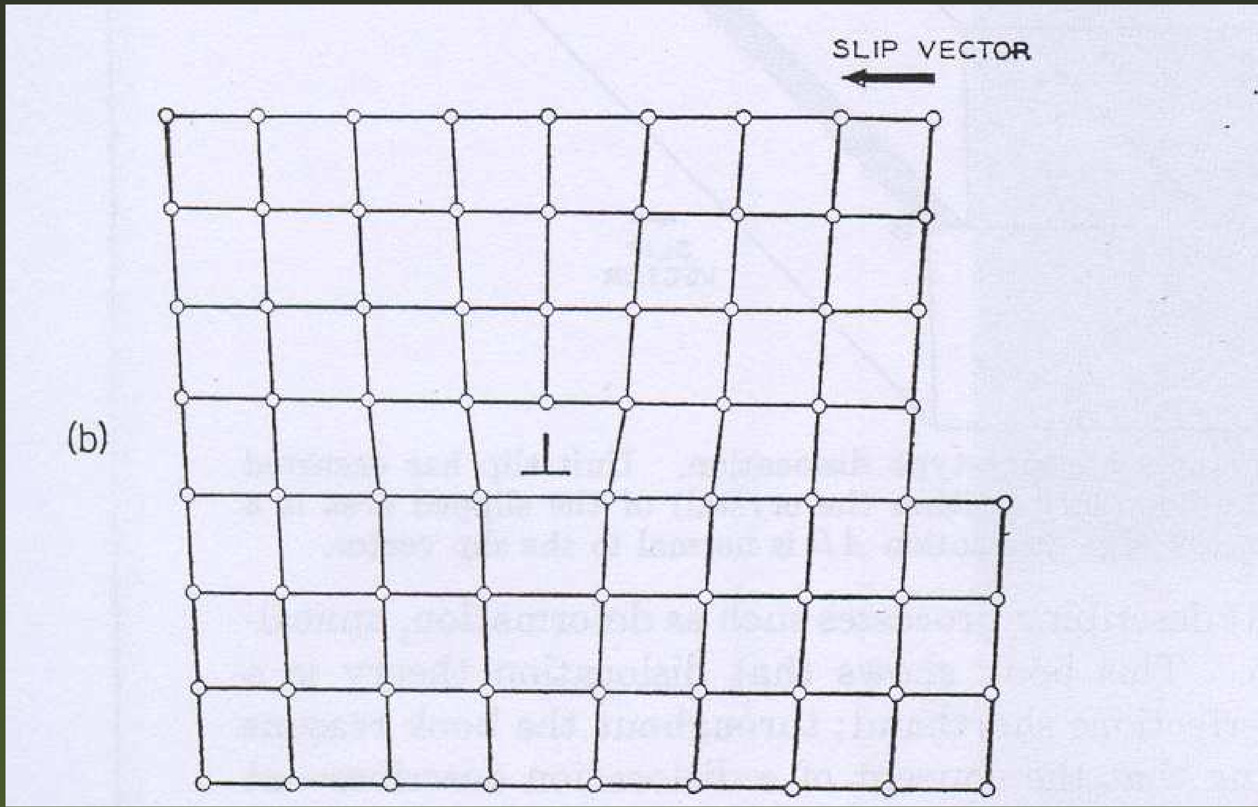
3D continuous model



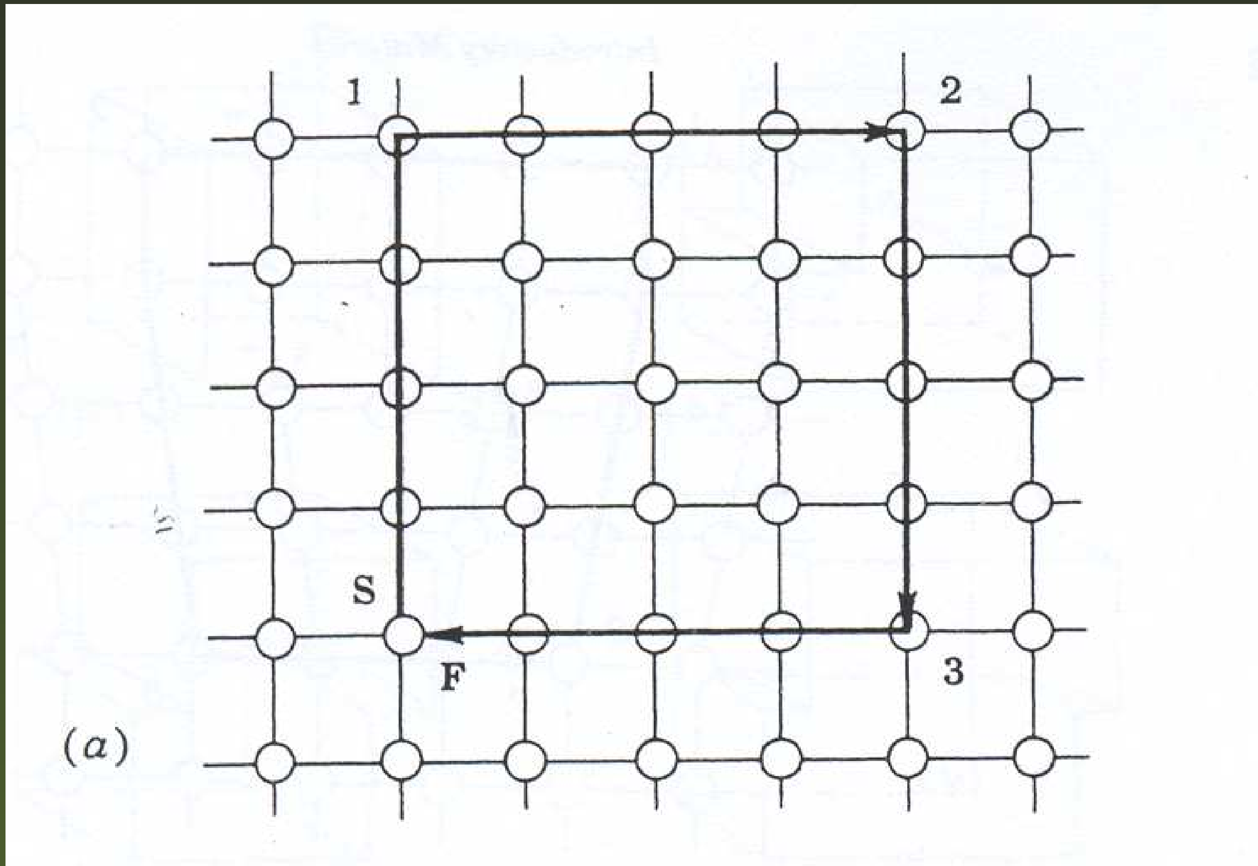
2D continuous model



2D atomic model



Perfect crystal



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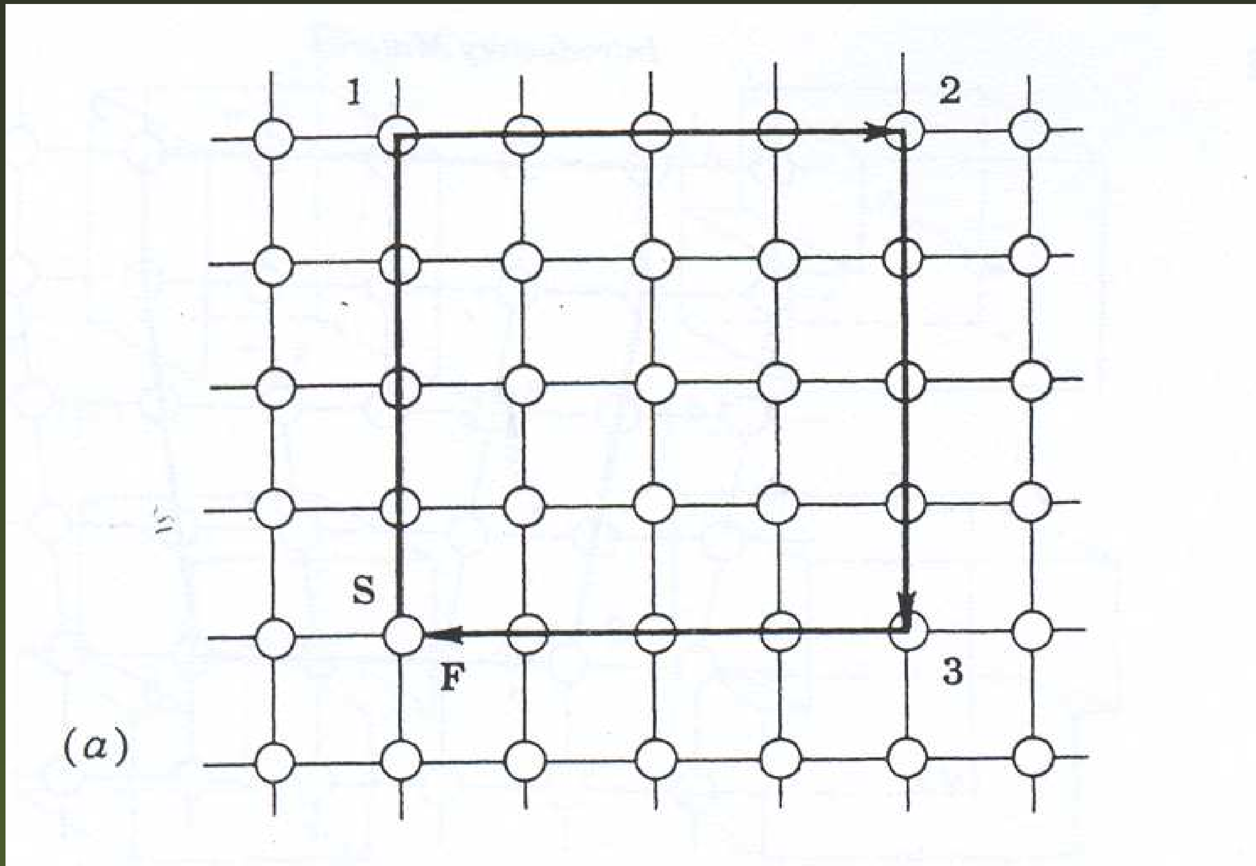
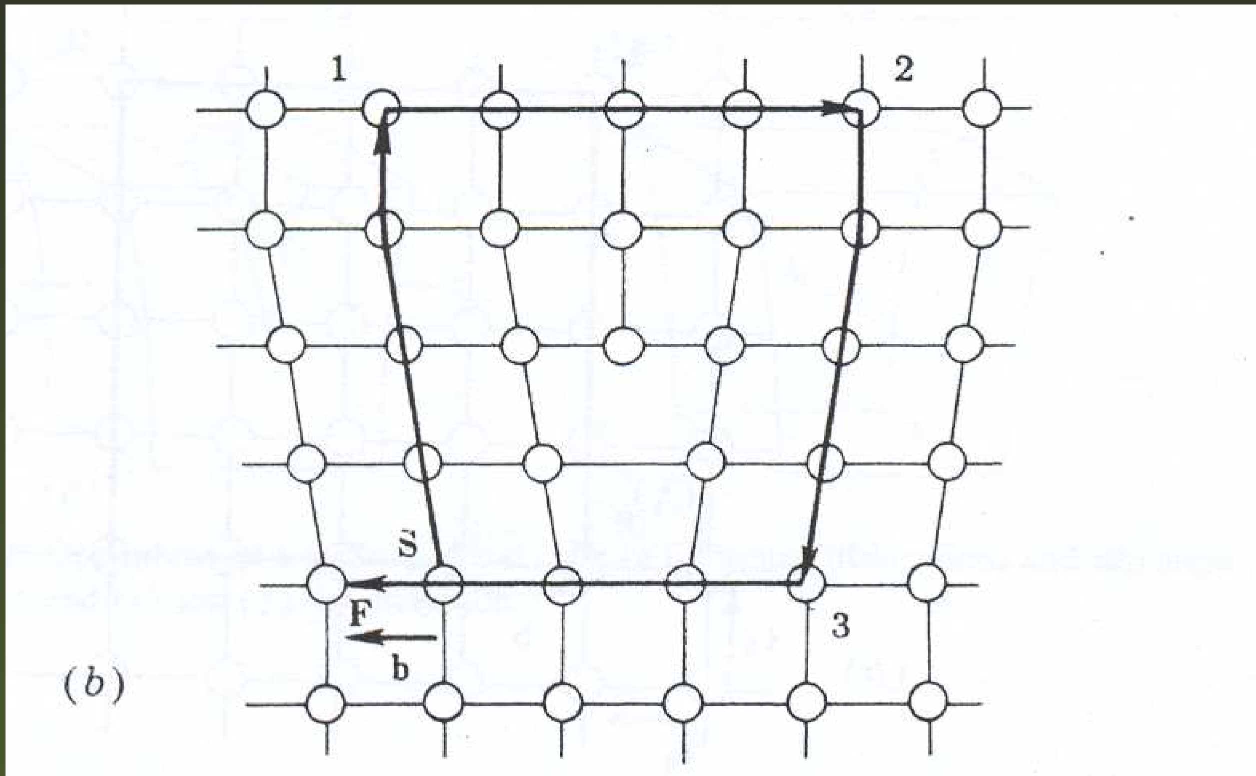


$\Longrightarrow$ elasticity at large scale

Singular deformation of the crystal



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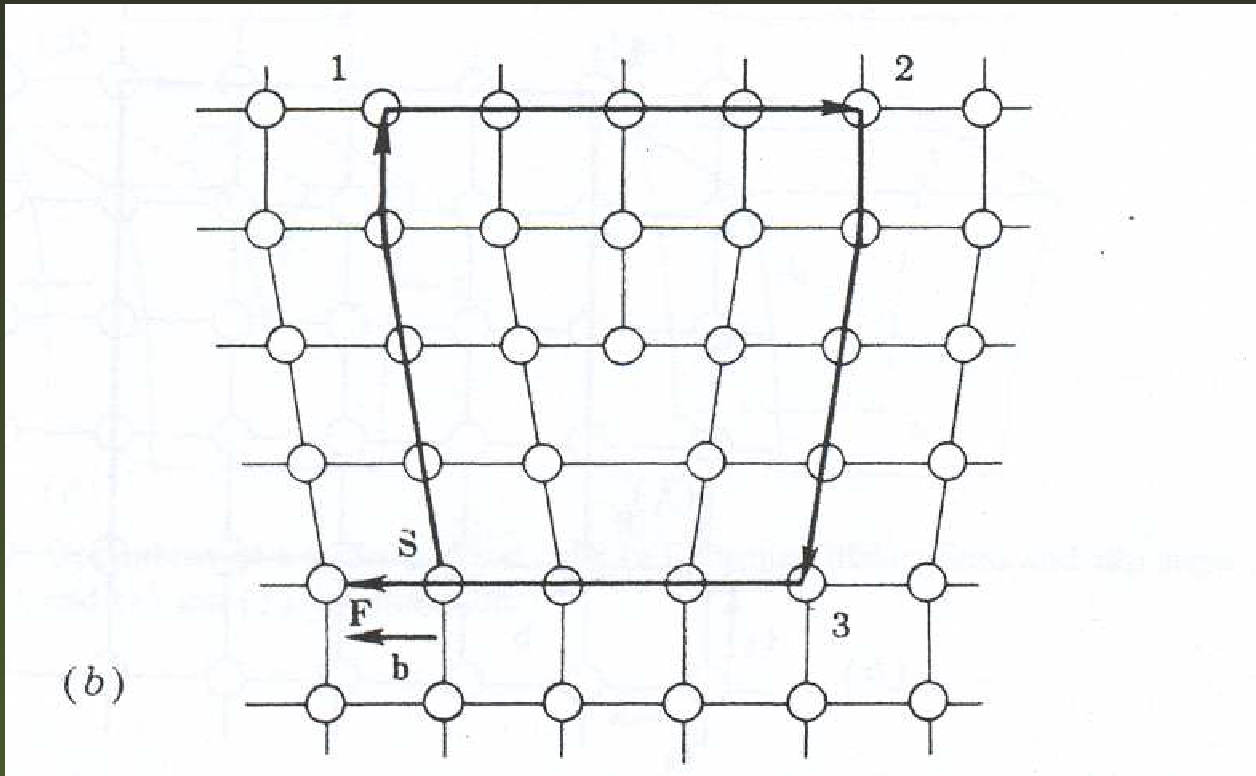
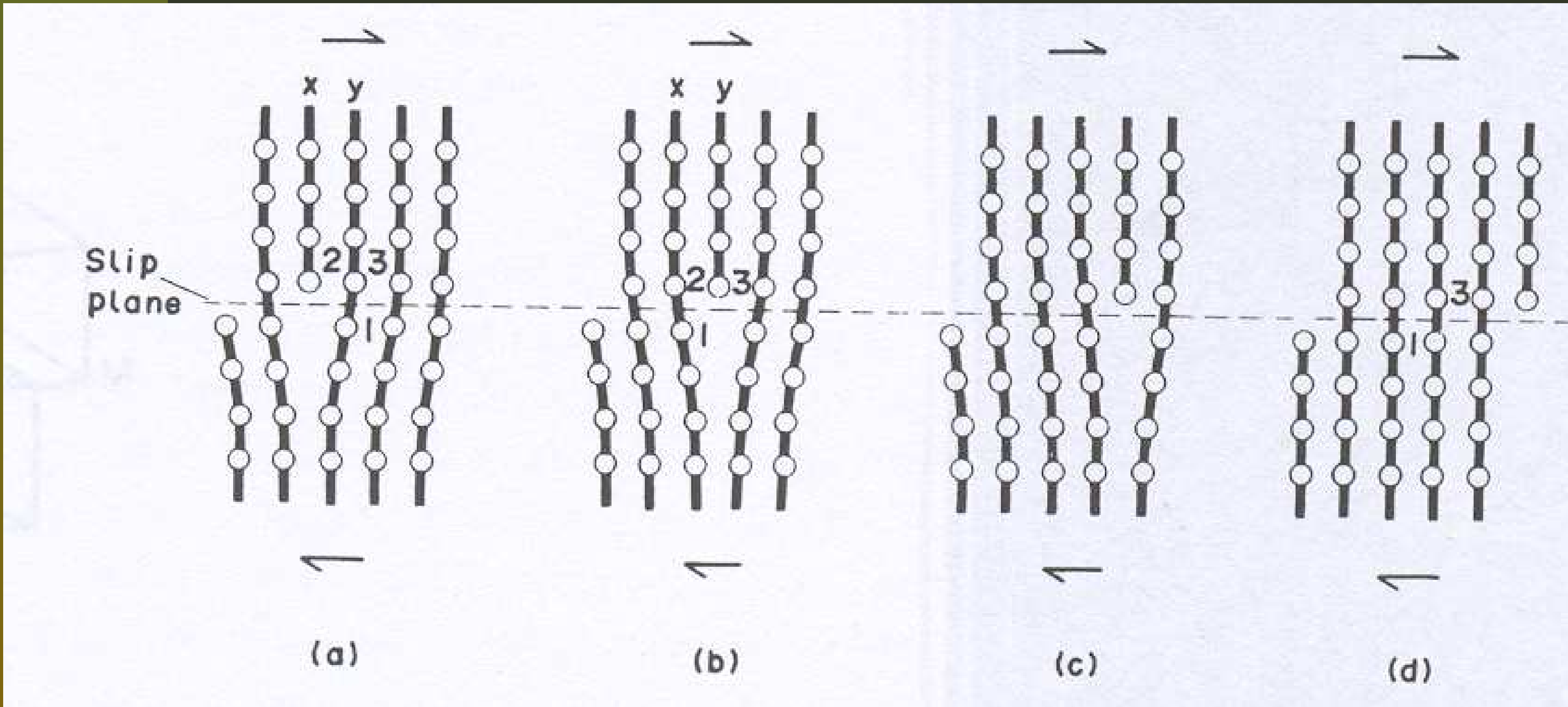


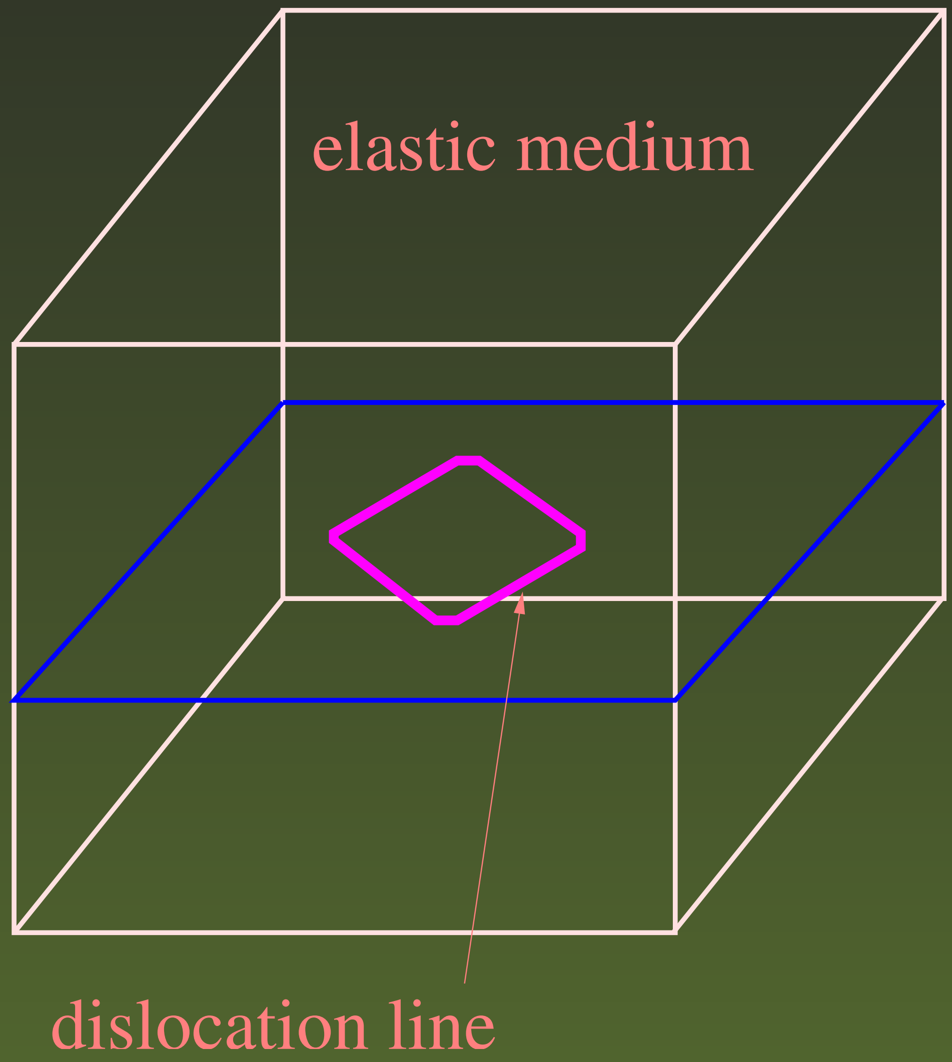
dislocation = topological defect

How do dislocations move ?

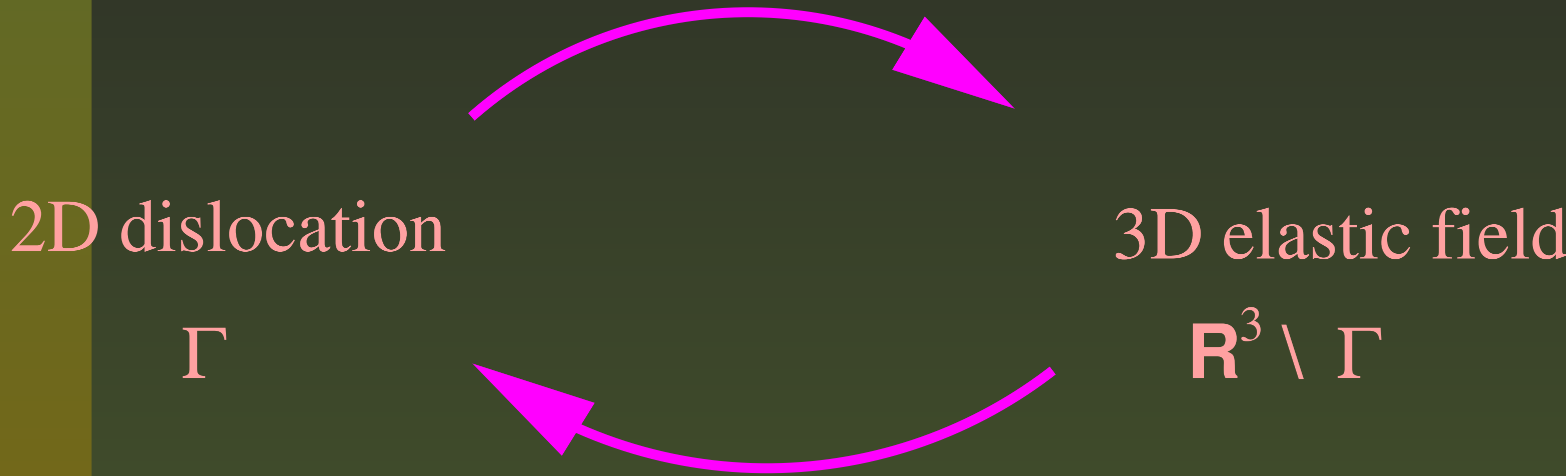


A sharp interface modeling of dislocation dynamics

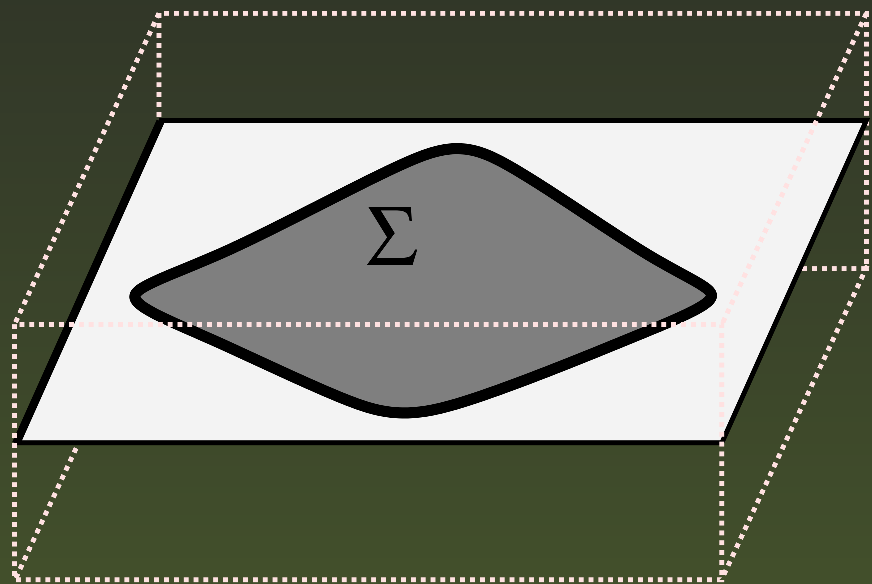
3D continuous model



2D-3D coupled system



Computation of the stress

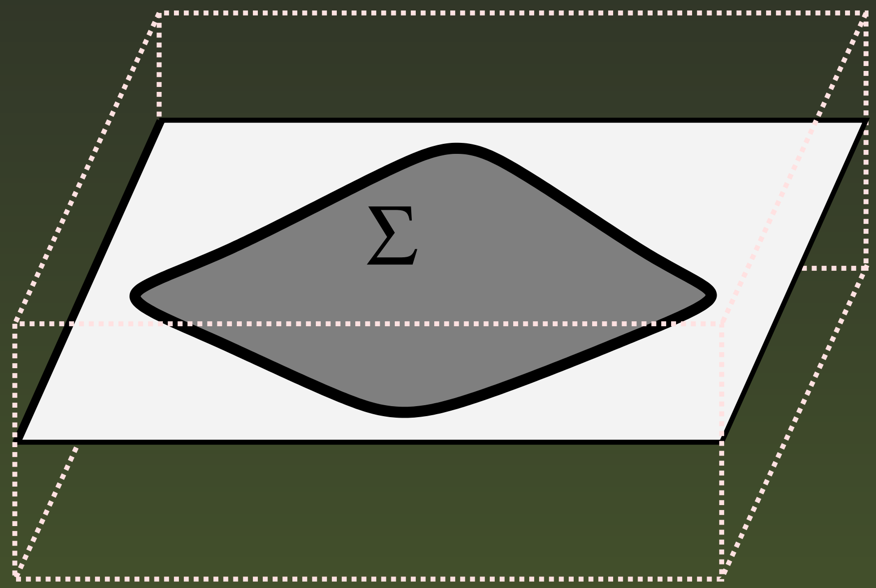


$$\text{div}\,\sigma = 0 \quad \text{with} \quad [u] = b \quad \text{on} \quad \Sigma$$

b : Burgers vector
σ : stress

[Volterra 1905]

Computation of the stress



$$\operatorname{div} \sigma = 0 \quad \text{with} \quad [u] = b \quad \text{on} \quad \Sigma$$

$$\sigma = \Lambda : e \quad \text{with} \quad e = \left(e(u) - \delta_\Sigma \cdot (b \otimes e_3)^{sym}\right)$$

$$e(u) = (\nabla u)^{sym} = \frac{1}{2}\left(\nabla u + {}^t\nabla u\right)$$

Dislocation dynamics

We define $E(\Gamma) = \int_{\mathbb{R}^3} \frac{1}{2} e : \Lambda : e$ with $e = e(\Gamma)$

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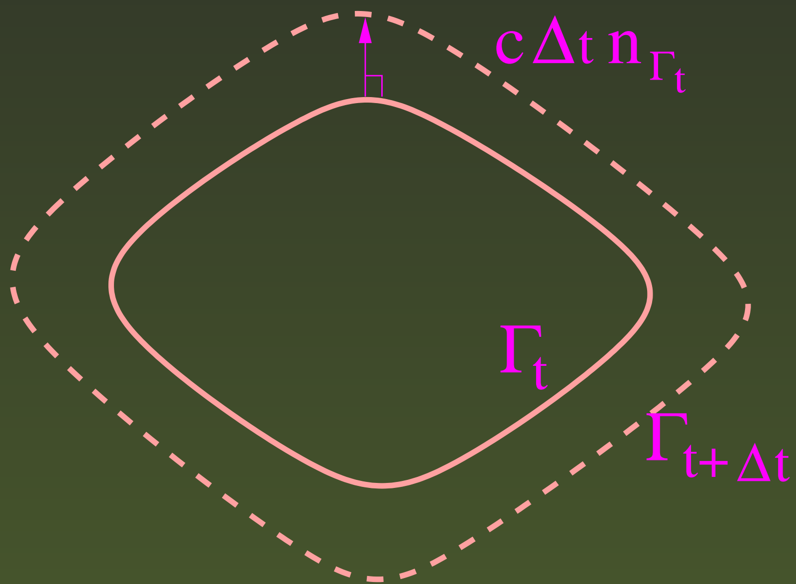

$$\frac{d\Gamma_t}{dt} = c\, n_{\Gamma_t}$$

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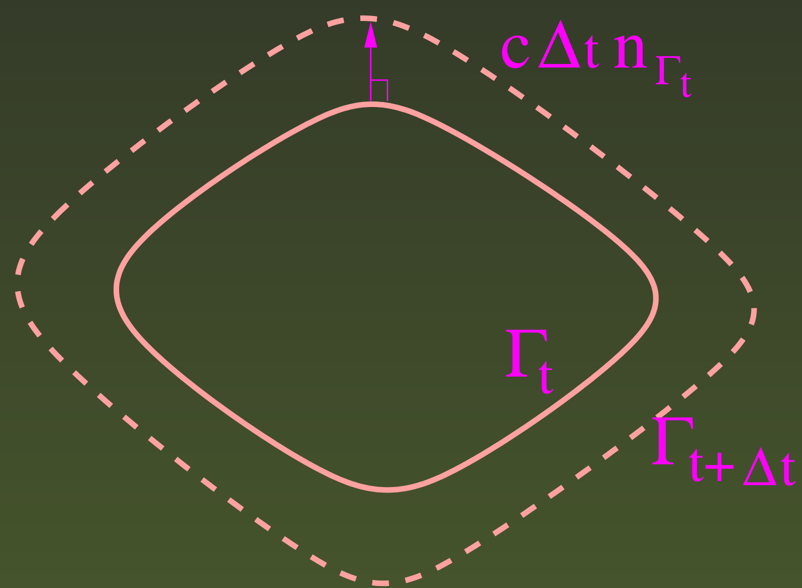
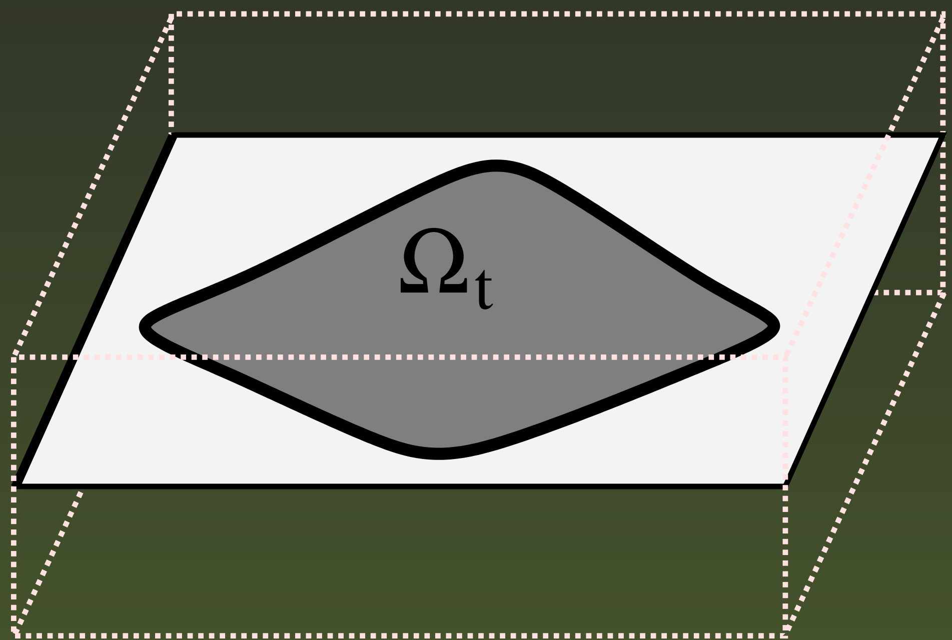


$$\frac{d\Gamma_t}{dt} = c\, n_{\Gamma_t} \quad \text{with} \quad c = \text{“} - \nabla_\Gamma E(\Gamma_t)\text{''} = \sigma : (b \otimes e_3)$$

A sharp interface modeling



$$\rho(t, x_1, x_2) = \begin{cases} 1 & \text{if} \quad (x_1, x_2) \in \Omega_t \\ 0 & \text{otherwise} \end{cases}$$

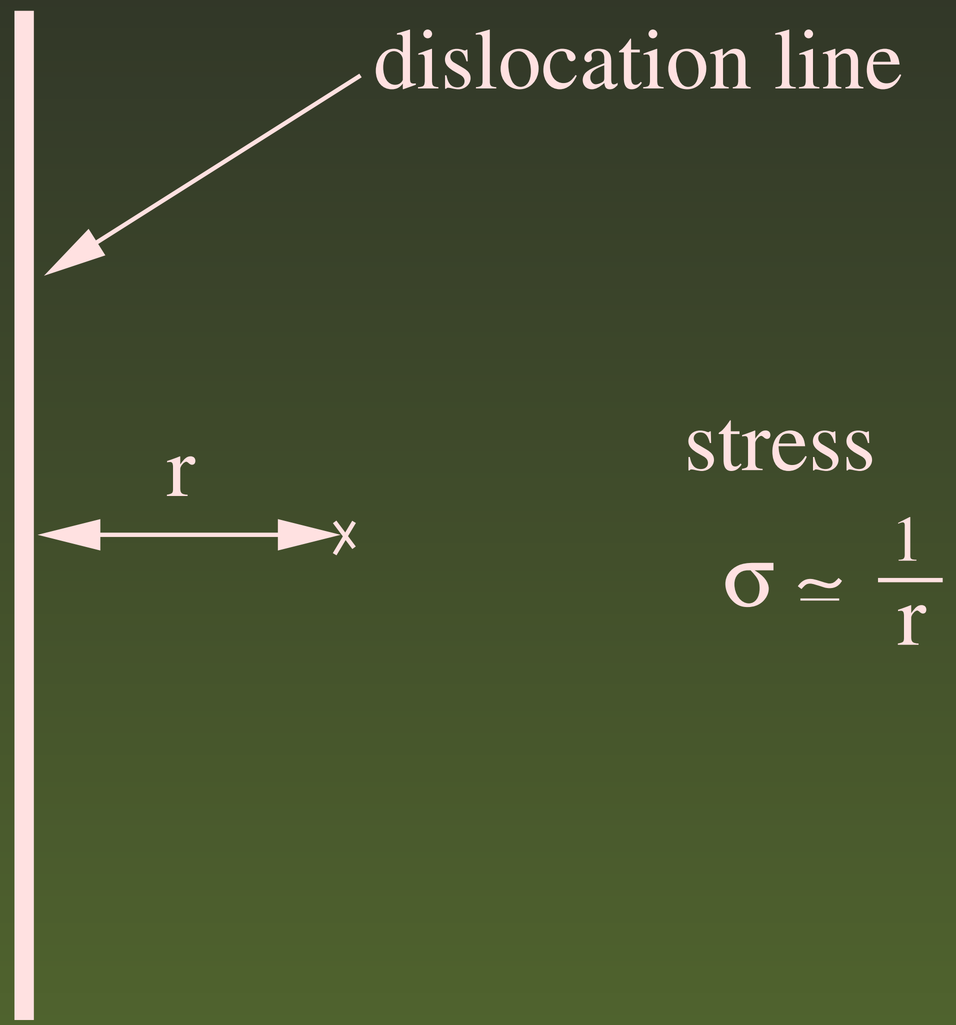
and

$$\Gamma_t = \partial \Omega_t$$

A sharp interface modeling

$$\frac{d\Gamma_t}{dt} = c\, n_{\Gamma_t} \quad \text{with} \quad c = c(\rho) = -(-\Delta)^{\frac{1}{2}}\rho$$

A difficulty of the classical theory



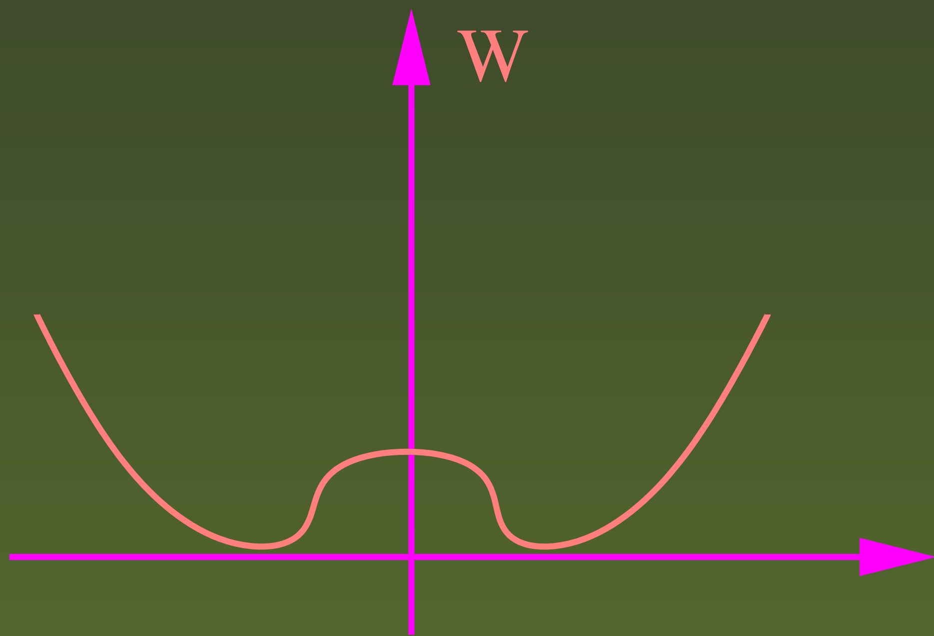
Regularization

Peierls-Nabarro model

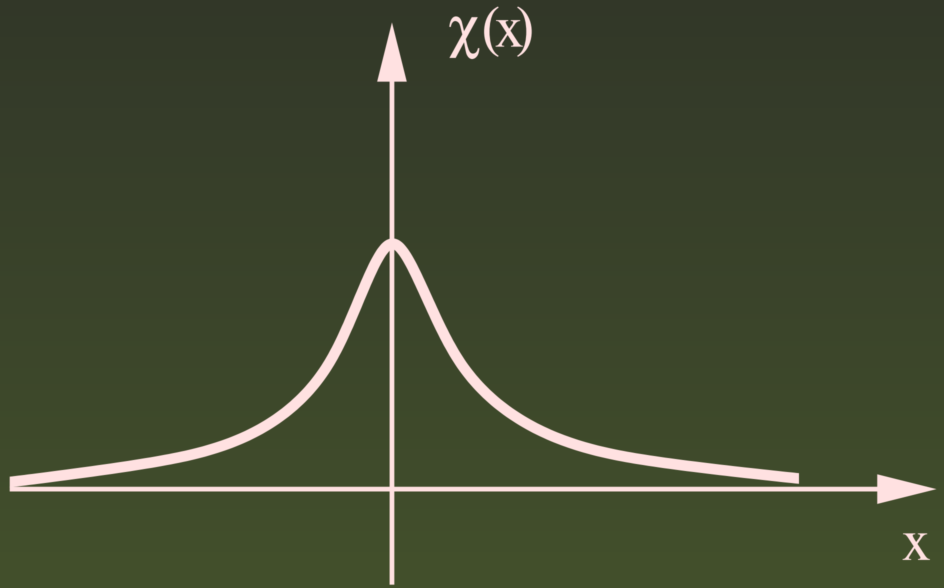
Replace the energy by

$$E(\rho) + \int_{\mathbb{R}^2} W(\rho)$$

with



Notion of core function



We consider

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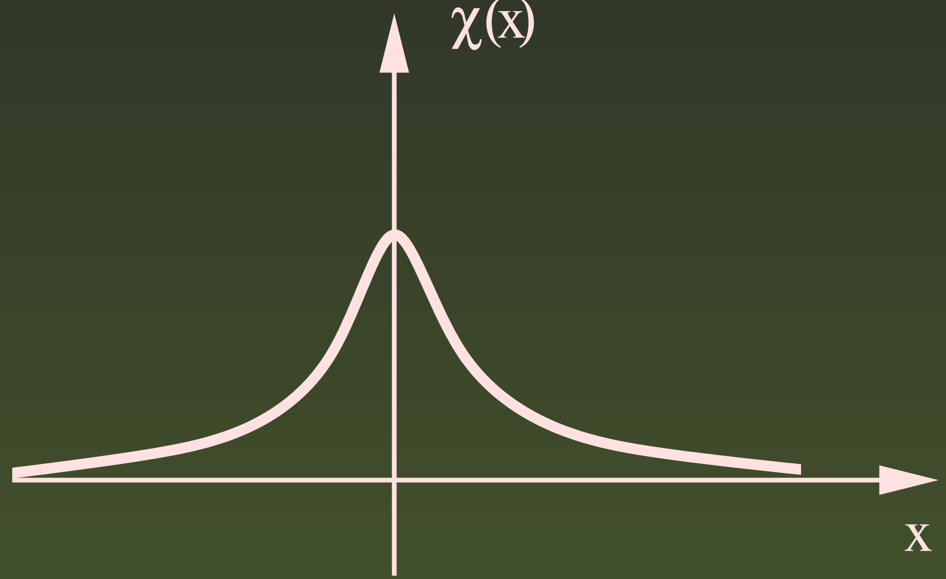

We consider

$$\text{regularized stress} = \chi \star (\text{classical stress})$$

$$c = c_0 \star \rho \quad \text{with} \quad c_0 = -(-\Delta)^{\frac{1}{2}} \chi$$

Core function

For the Peierls-Nabarro model we have

$$W(\rho) = \frac{1}{\zeta}(1 - \cos(2\pi\rho))$$

with

$$\hat{\chi}(\xi_1, \xi_2) = e^{-\zeta\sqrt{\xi_1^2 + \xi_2^2}}$$

$\zeta > 0$: Peierls-Nabarro parameter

Dynamics of a single dislocation

$$\frac{d\Gamma_t}{dt} = c\, n_{\Gamma_t} \quad \text{with} \quad c = c(\rho) = c_0 \star \rho$$

where $c_0(x_1, x_2)$ is a fixed kernel

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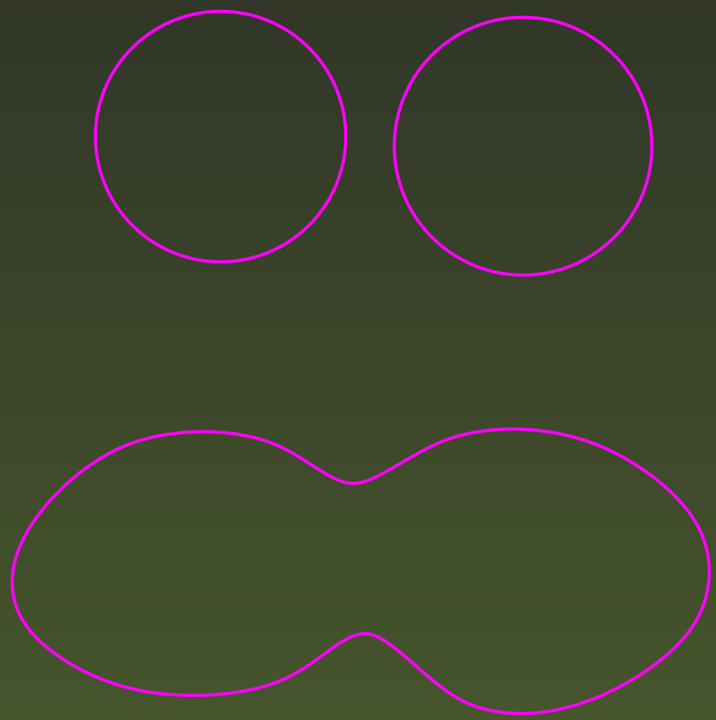
Under an exterior stress field c_1, we get

$$\frac{\partial \rho}{\partial t} = (c_1 + c_0 \star \rho)\, |\nabla \rho| \text{ on } \mathbb{R}^2$$

Mathematical studies of the dynamics

Mathematical difficulty

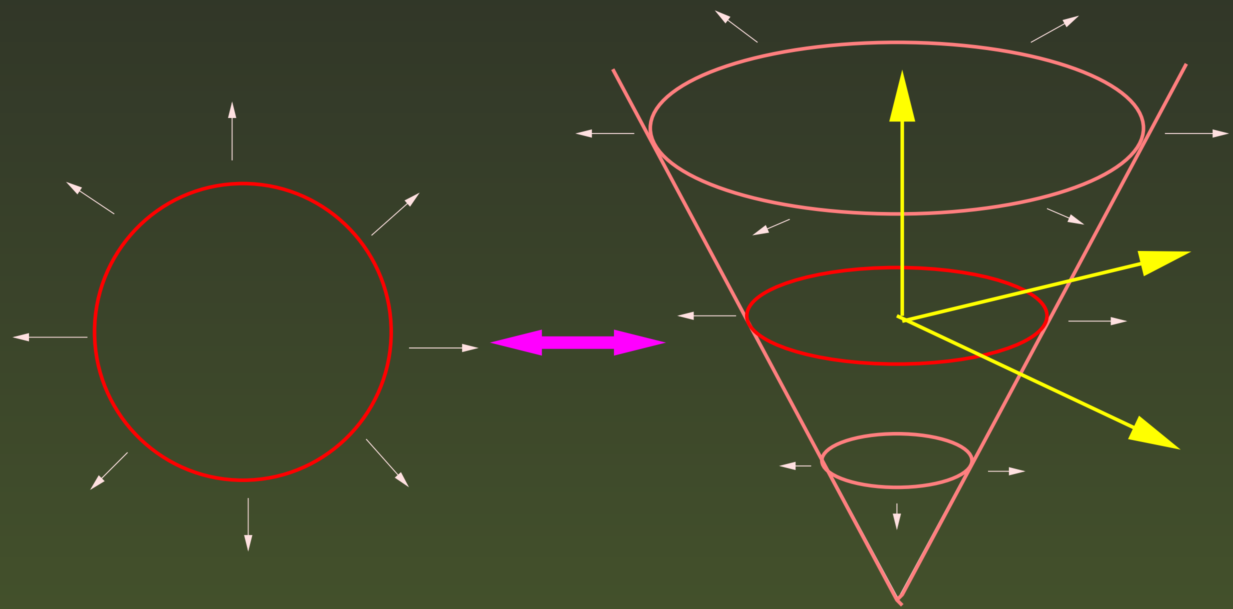


How to define the evolution
with the change of topology ?

Mathematical difficulty !

Change of topology = you can be affraid !

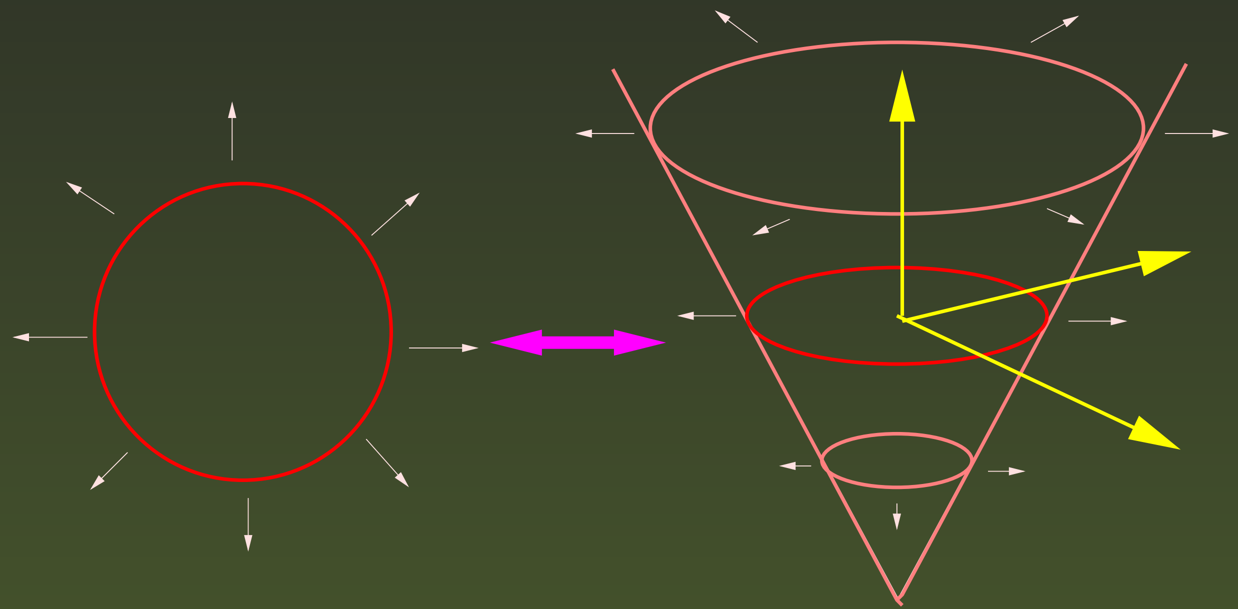
Level Sets method



Front in the plan xy

Front = intersection of the surface
with the plan xy

Level Sets method



Front in the plan xy

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Level Sets equation: $$\frac{\partial f}{\partial t} = c(x,t)|\nabla f|$$

Notion of solution

$$\frac{\partial \rho}{\partial t} = (c_1 + c_0 \star \rho) \, |\nabla \rho| \text{ on } \mathbb{R}^2$$

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Viscosity solutions (introduced by Crandall and Lions) for Hamilton-Jacobi equations.

Known results (general c_0)

- Short time existence, uniqueness
  [Alvarez, Hoch, Le Bouar, M.], [Forcadel]
- Convergent schemes
  [Alvarez, Carlini, M., Rouy], [Ghorbel, M.]
- Fast Marching schemes
  [Carlini, Cristiani, Forcadel], [Carlini, Falcone, Forcadel, M.]

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  [Alvarez, Cardaliaguet, M.], [Barles, Ley], [Cardaliaguet, Marchi], [Cannarsa, Cardaliaguet]
- Long time (general c)
  [Barles, Cardaliaguet, Ley, Monneau]

Main difficulty

Physics $\Longrightarrow$ $\int_{\mathbb{R}^2} c_0 = 0$ and $c_0(-x) = c_0(x)$.

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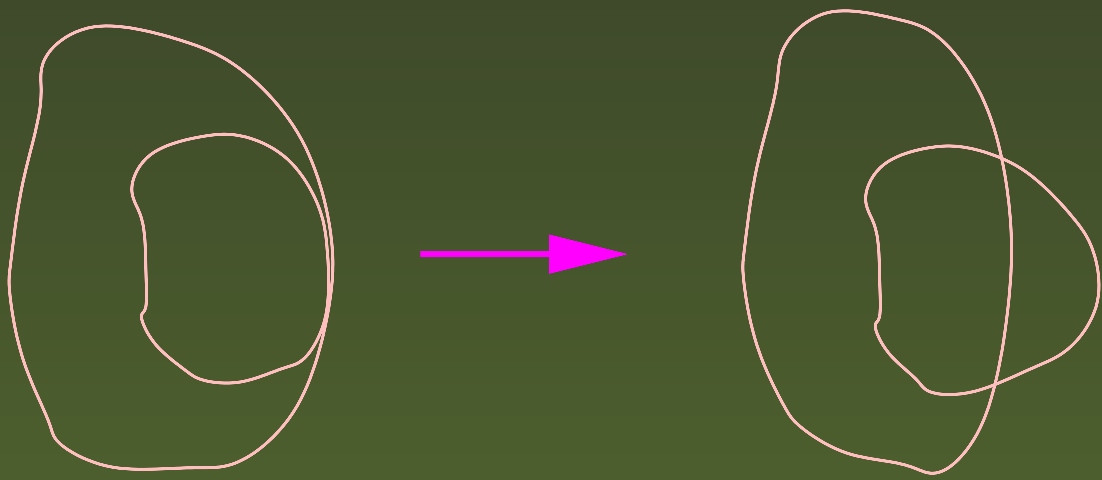
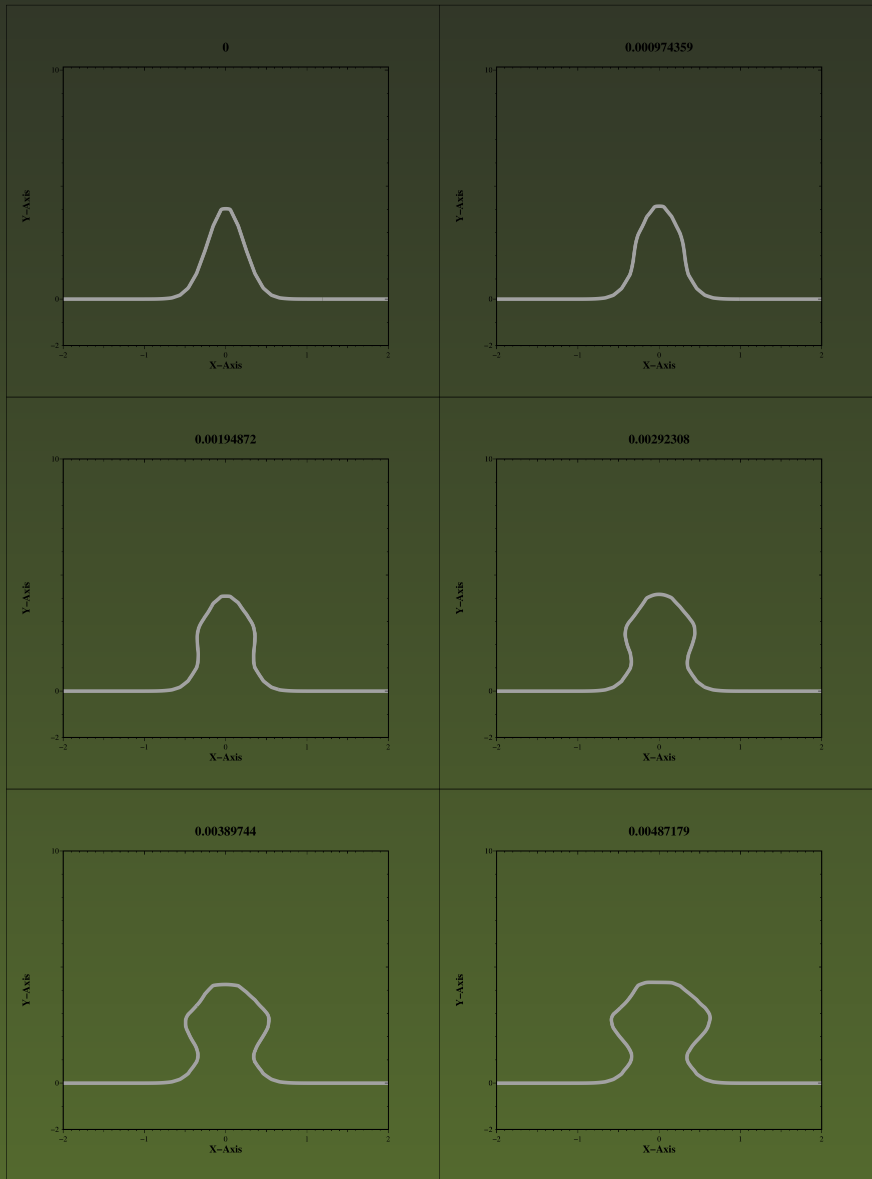
$\Longrightarrow$ no inclusion principle



Loosing the graph in finite time



Link with MCM

particular kernels

Let $x \in \mathbb{R}^n$, and

$$J(-x) = J(x) = \frac{1}{|x|^{n+1}} g\left(\frac{x}{|x|}\right) 1_{\{|x| \geq 1\}} \geq 0$$

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$$J(-x) = J(x) = \frac{1}{|x|^{n+1}} g\left(\frac{x}{|x|}\right) 1_{\{|x| \geq 1\}} \geq 0$$

We define

$$c_0 = J - \left(\int_{\mathbb{R}^n} J\right) \delta_0$$

Rescaling

$$\frac{\partial \rho}{\partial t} = (c_0 \star \rho)\, |\nabla \rho| \quad \text{on} \quad \mathbb{R}^n$$

For $\varepsilon > 0$, we define

$$\rho^\varepsilon(x,t) = \rho\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2 |\ln \varepsilon|}\right)$$

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$$\rho^\varepsilon(x,t) = \rho\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2 |\ln \varepsilon|}\right)$$

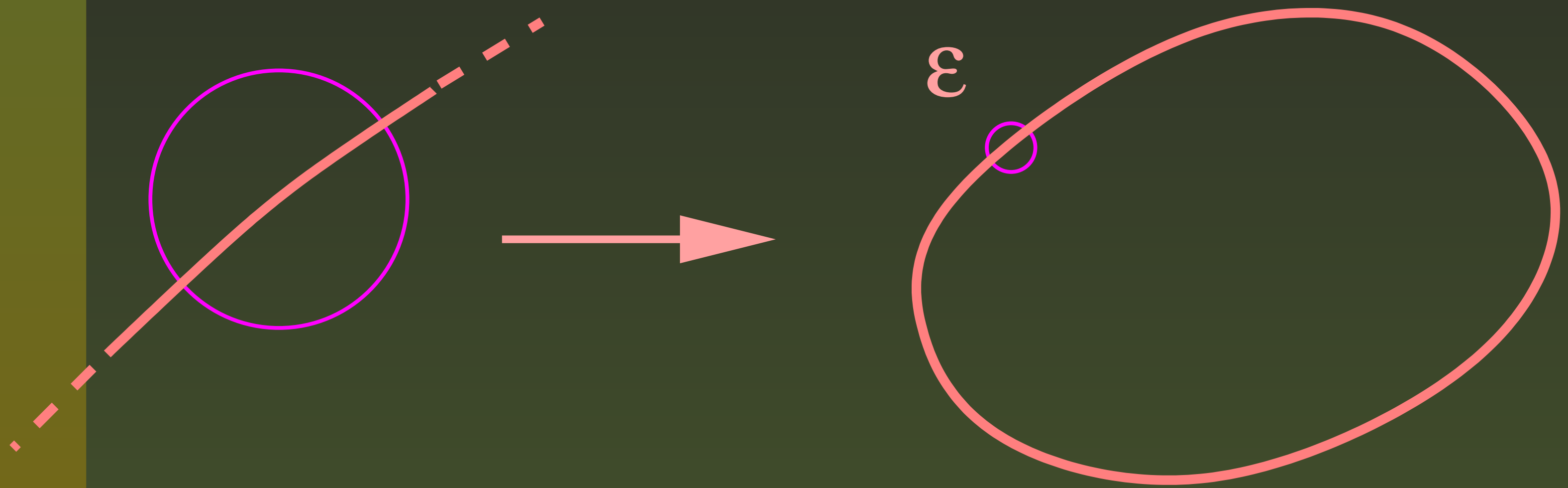
$\Longrightarrow$

$$\frac{\partial \rho^\varepsilon}{\partial t} = (c_0^\varepsilon \star \rho^\varepsilon)\,|\nabla \rho^\varepsilon| \quad \text{on} \quad \mathbb{R}^n$$

with

$$c_0^\varepsilon(x) = \frac{1}{\varepsilon^{n+1}|\ln \varepsilon|} c_0\left(\frac{x}{\varepsilon}\right)$$

At large scale



Slepčev level sets formulation

$$\frac{\partial \rho}{\partial t} = (c_0 \star \rho)\,|\nabla \rho| \quad \text{on} \quad \mathbb{R}^n \quad \text{with} \quad \rho \in \{0,1\}$$

is replaced for ρ continuous by

$$\frac{\partial \rho}{\partial t} = \left\{ \left(c_0 \star 1_{\{\rho(\cdot,t) \geq \rho(x,t)\}} \right)(x) \right\} |\nabla \rho| \quad \text{on} \quad \mathbb{R}^n$$

with

- $\geq$ for subsolutions
- $>$ for supersolutions

Convergence to anisotropic MCM

Theorem 1 [Da Lio, Forcadel, M.]
In the Slepcev formulation, and under certain regularity assumptions, as ε goes to zero, ρ^ε converges to ρ^0 solution of

$$\frac{\partial \rho^0}{\partial t} = F_g(D^2\rho^0, \nabla\rho^0)$$

where

$$F_g(M,p) = \text{trace}\left(M \cdot A_g\left(\frac{p}{|p|}\right)\right)$$

$$A_g\left(\frac{p}{|p|}\right) = \int_{\mathbb{S}^{n-1}\cap p^\perp} \left(\frac{1}{2} g(\theta)\theta \otimes \theta\right)\, d\theta$$

Similar results

- [Garroni, Muller] (Gamma limit, stationnary pb)
- [Merriman, Bence, Osher] algorithm
- [Evans], [Barles, Georgelin], [Ishii], [Ishii, Pires, Souganidis], ...

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- [Evans], [Barles, Georgelin], [Ishii], [Ishii, Pires, Souganidis], ...
- [Forcadel] : error estimate for a scheme for MCM

Identification of the limit MCM

Theorem 2 [Da Lio, Forcadel, M.]
If u is smooth, then

$$A_g(p) = D^2G(p), \quad F_g(D^2u, \nabla u) = |\nabla u| \,\mathrm{div}\, ((\nabla G)(\nabla u))$$

derives from the energy $\int G(\nabla u)$ with

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derives from the energy $\int G(\nabla u)$ with

$$G = -\frac{1}{2\pi} \hat{L}_g$$

$$L_g = pv \left(\frac{g\left(\frac{x}{|x|}\right)}{|x|^{n+1}} \right)$$

More properties

Theorem 3 [Da Lio, Forcadel, M.]

- $n = 2 :\quad g \geq 0 \iff G$ convex
- $n \geq 3 :\quad \exists G$ convex and $g \not\geq 0$

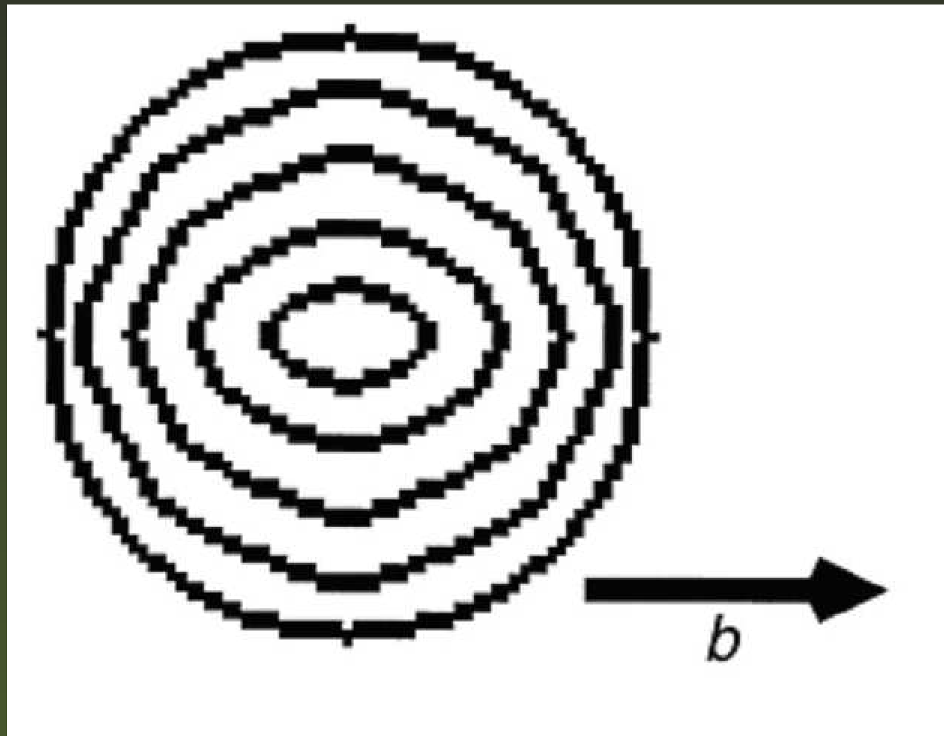
An example in 2D

$$G(x_1, x_2) = \gamma x_1^2 + x_2^2 \quad \text{with} \quad \begin{cases} \gamma = \frac{1}{1-\nu} \in \left(\frac{1}{2}, 2\right) \\ \nu = \text{Poisson ratio} \end{cases}$$

$$g(x_1, x_2) = (2\gamma - 1)x_1^2 + (2 - \gamma)x_2^2$$

(for $x_1^2 + x_2^2 = 1$).

Anisotropic evolution of a circle



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