A novel diffuse interface approach to brittle fracture

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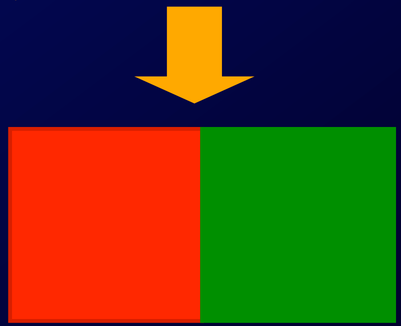
Outline

- Introduction and Motivation.
- Continuum model for brittle fracture.
- Convalidation of the model in well controlled geometries.
- Some application examples.
- Conclusions and future work.

Introduction

Many problems in condensed matter physics deal with
sharp interfaces:



like:

- solidification
- dendritic growth
- grain growth
- solid-solid transformation
- magnetic domains
- fracture

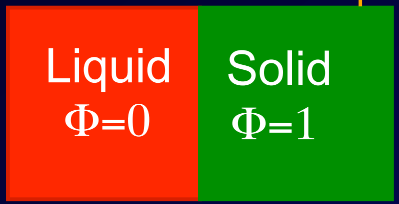
Solutions:

1) Boundary conditions at the interface. Heavy to deal.....each time a new problem !!

2) Atomistic models. Numerically heavy and how to cross to the macroscopic beh.?

3) Diffuse interface technique (including phase field models) :
regularization, additional field ϕ !!.

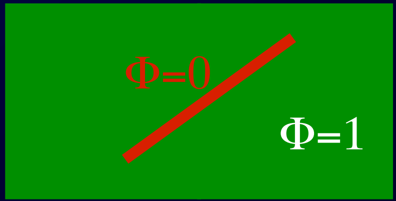
Example:



ϕ is an "external" degree of freedom
How to deal with its dynamics???

Motivation

Phase field models for fracture:



I. S. Aranson, V. A. Kalatsky, and V. M. Vinokur, Phys. Rev.Lett. 85, 118 (2000).

A. Karma, D. A. Kessler, and H. Levine, Phys. Rev. Lett. 87, 045501 (2001).

L. O. Eastgate, J. P. Sethna, M. Rauscher, T. Cretegny, C.S. Chen, and C. R. Myers, Phys. Rev. E 65, 036117 (2002).

All previous have in common an external degree of freedom !

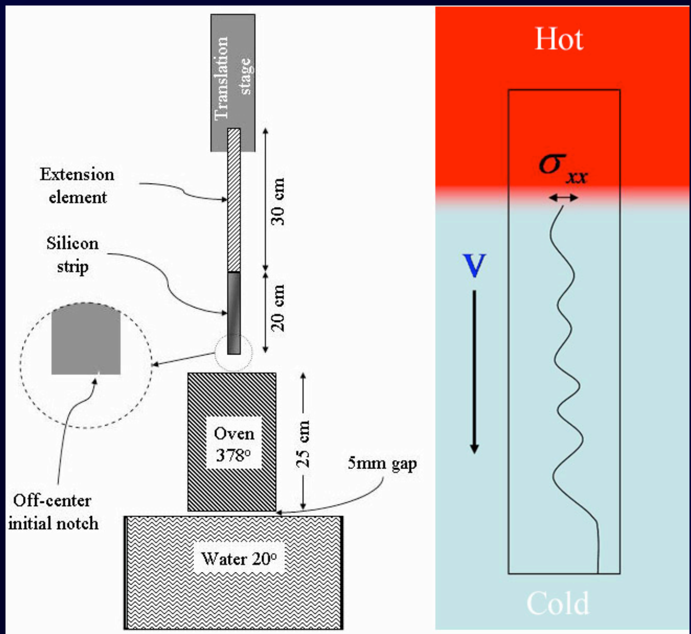
Our aim.......

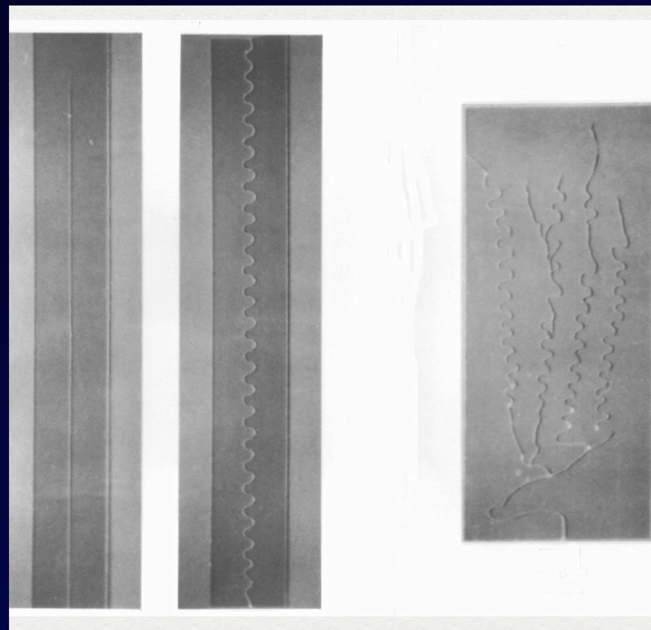
"Obtain a diffuse interface approach for the propagation of cracks able to describe the properties of "isotropic materials" independently of the underlying numerical mesh without adding extra degrees of freedom."

Motivation

Need to supplement macroscopic transport physics with a **regularizing short scale physics** in order to obtain a self-consistent theoretical framework for many problems: dendritic solidification, viscous fingering, and many examples in fracture physics as:

1)Quasi-equilibrium cracks propagation under uniaxial loading or thermal gradient





Yuse, Sano, Nature (1993)

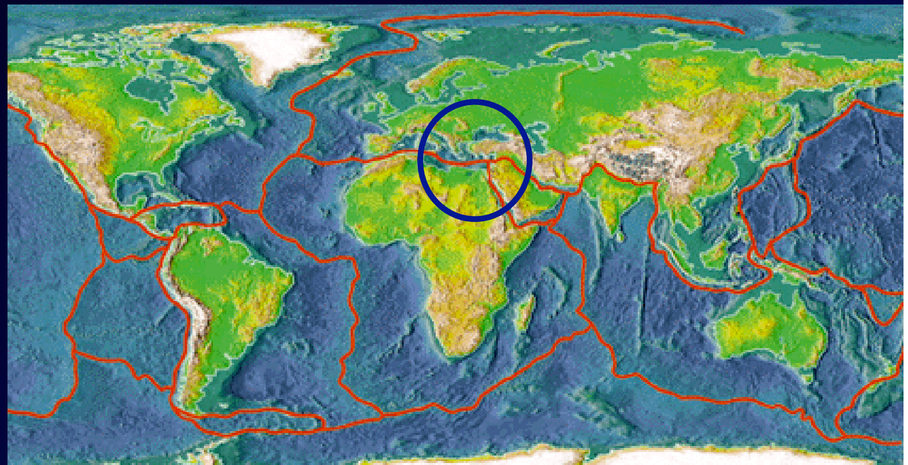
Motivation

2) Cracks due to shrinking:

- changes in humidity concentration
- nonuniform temperature distribution

Picture from Salar (salty surface) Uyuni, Bolivia.

Length scale ~ meters



Tectonic plates

Length scale ~ km

Motivation

3) Columnar fracturing in basaltic lava, sedimentary rocks…

Bariloche
Argentina

Svartifoss,
Skaftafell National Park, Iceland

Model

Fundamental variables: "strain tensor components"

$$\varepsilon_{ij} \equiv \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

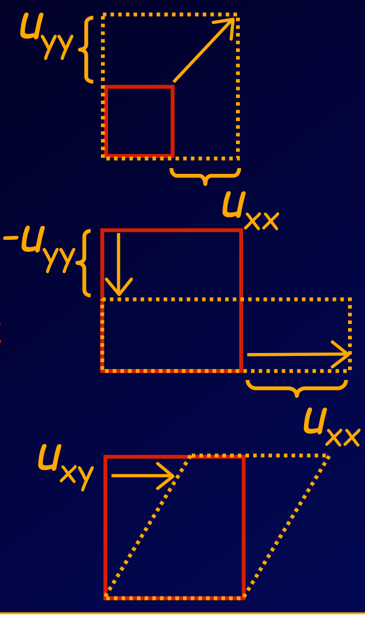
Displacements with respect to the unperturbated position $u_i^0(\mathbf{r})$

For a 2D geometry we choose:

$e_1 = (u_{xx} + u_{yy}) / 2 = (\varepsilon_{11} + \varepsilon_{22}) / 2$

$e_2 = (u_{xx} - u_{yy}) / 2 = (\varepsilon_{11} - \varepsilon_{22}) / 2$

$e_3 = (u_{xy} + u_{yx}) = \varepsilon_{12} = \varepsilon_{21}$



Attention!! Variables e_1 , e_2 and e_3 are not independent !

St Venant Condition

$\nabla \times (\nabla \times \mathbf{e}) = 0$

$(\partial^2_x + \partial^2_y)\, e_1 - (\partial^2_x - \partial^2_y)\, e_2 - 2\partial_x\partial_y\, e_3 = 0$

Textures in ferroelastic materials and martensites:
Lookman, S.R. Shenoy, Rasmussen, Saxena and Bishop, PRB (2003).
S.R.Shenoy etal., PRB (1999).

Model

Local free energy density F_L (e) ?

1) For small $u_i(r)$ and small e should be… :

$$F_L^0(\varepsilon) = C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}/2$$

→ " Elasticity "

Bulk and shear modulus

For isotropic material (our first aim)

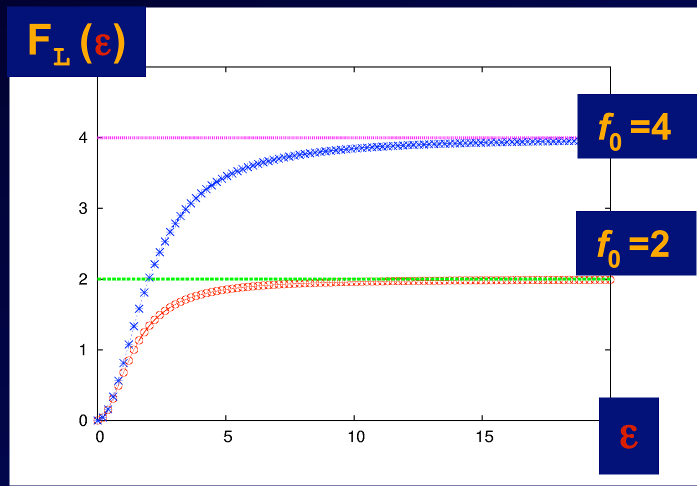
$$F_L^0(\varepsilon) = 2B\, e_1^2 + 2\mu\, (e_2^2 + e_3^2)$$

Rotational Invariance

- Two crucial ingredients:

2) How to account for fracture at large strains ?

$$F_L(\varepsilon) = \frac{g\, F_L^0(\varepsilon)}{[1 + F_L^0(\varepsilon)/f_0]}$$



Lim $F_L(\varepsilon) = f_0$ (related with the crack energy)
$\varepsilon \to \infty$

" A crack is nucleating when $F_L^0(\varepsilon) \sim f_0$ "

$g(r_{ij}) \sim 0$ ➔ Preexistent cracks

$g(r_{ij}) \sim 1$ ➔ Random inhomogeneities

Model

3) How to avoid influence from the numerical mesh? " REGULARIZATION "

$$F_{\nabla}(\varepsilon) = \sum_{i=1,2,3} \alpha_i \, (\nabla e_i)^2$$

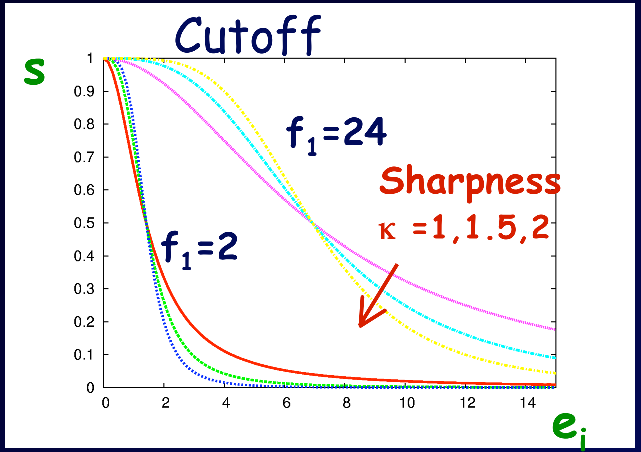
choosing $\alpha_2 = \alpha_3$ (rot. invariance)

$$F_{\nabla}(\varepsilon) = \sum_{i=1,2,3} \alpha_i \, (\nabla e_i)^2 \, s(e_i)$$

→ $s(e_i) = (1 + (F_L^0/f_1)^{\kappa})^{-1}$

↓

Smooth interfaces, 'a way to soften variables'



Finally ...the full free energy density is defined:

$$F = F_L + F_{\nabla}$$

$$= F_L^0(e)/[1+F_L^0(e)/f_0] + \sum_{i=1,2,3} \alpha_i \, (\nabla e_i)^2 \, s(e_i)$$

Elasticity + fracture REGULARIZATION

Like a G.Landau free energy: with order parameter, own elastic deformations

Model: equations of motion

Including a kinetic term, $T \sim \rho(du/dt)^2/2$ the eqs of motion in Fourier space, where E_i are Fourier transforms of e_i:

Inertial term

Potential Force

Dissipation

Constraint: St. Venant

$$\frac{4\rho}{k_x^2 k_y^2}(k^2 \ddot{E}_1 + (k_x^2 - k_y^2)\ddot{E}_2) = -\frac{\delta F}{\delta E_1^*} - A_1 \dot{E}_1 + k^2 \Lambda$$

$$\frac{4\rho}{k_x^2 k_y^2}((k_x^2 - k_y^2)\ddot{E}_1 + k^2 \ddot{E}_2) = -\frac{\delta F}{\delta E_2^*} - A_2 \dot{E}_2 + (k_y^2 - k_x^2)\Lambda$$

$$0 = -\frac{\delta F}{\delta E_3^*} - A_3 \dot{E}_3 - 2k_x k_y \Lambda$$

A_i = phen. damping cte

Lagrange mult.

Molecular Dynamics simulations:

-Overdamped regime

-Periodic boundary conditions

-Square and rectangular mesh

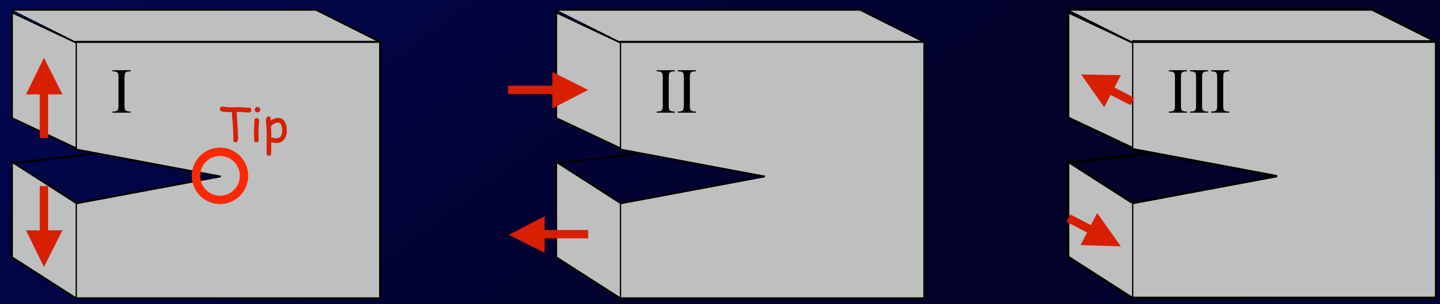
-System sizes: 128x128, 512x512, 768x768, 768x256…

St. Venant condition in FS:

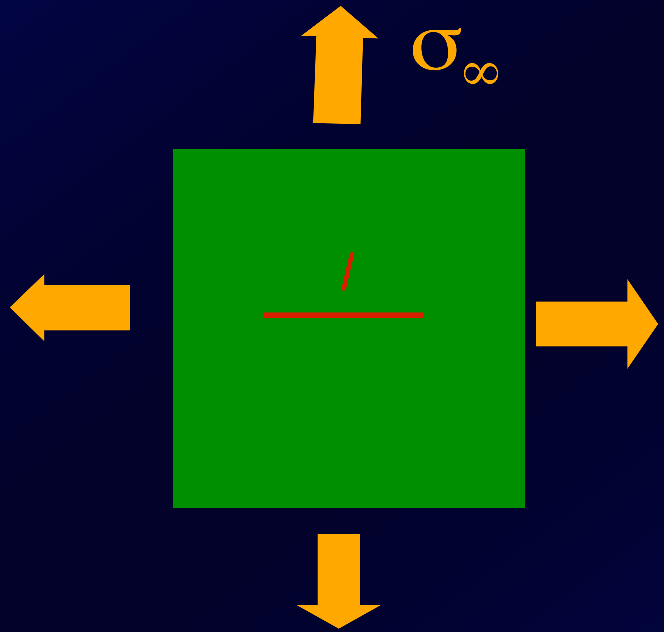
$$(k_x^2+k_y^2)E_1 - (k_x^2-k_y^2)E_2 - 2k_x k_y E_3 = 0$$

Convalidation of the model: "Griffith law"

Loadings modes: I, II, III



Griffith law (GL) ? Under uniform loading (Mode I).......



GL ➡ For $\sigma > \sigma_c$ breaks and

$$\sigma_c \sim l^{-\beta} = l^{-0.5}$$

Deduced just considering :

elastic energy + crack energy

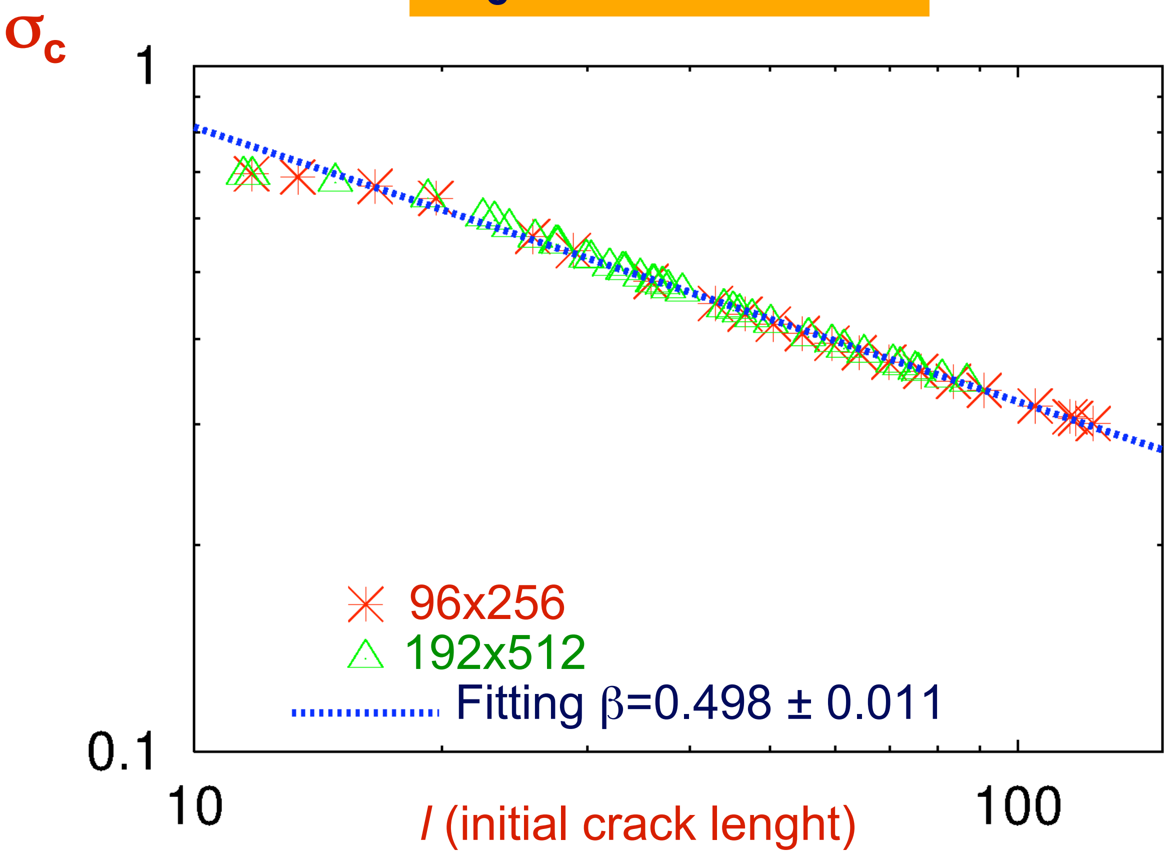
"all models for fracture should fullfill it"

Griffith criterion: results

Model without regularization, $\alpha_i=0$

↪ $F = F_L + F_V = F_L^0(e)/[1+F_L^0(e)/f_0]$

$\sigma_c \sim l^{-\beta}$, β = ??

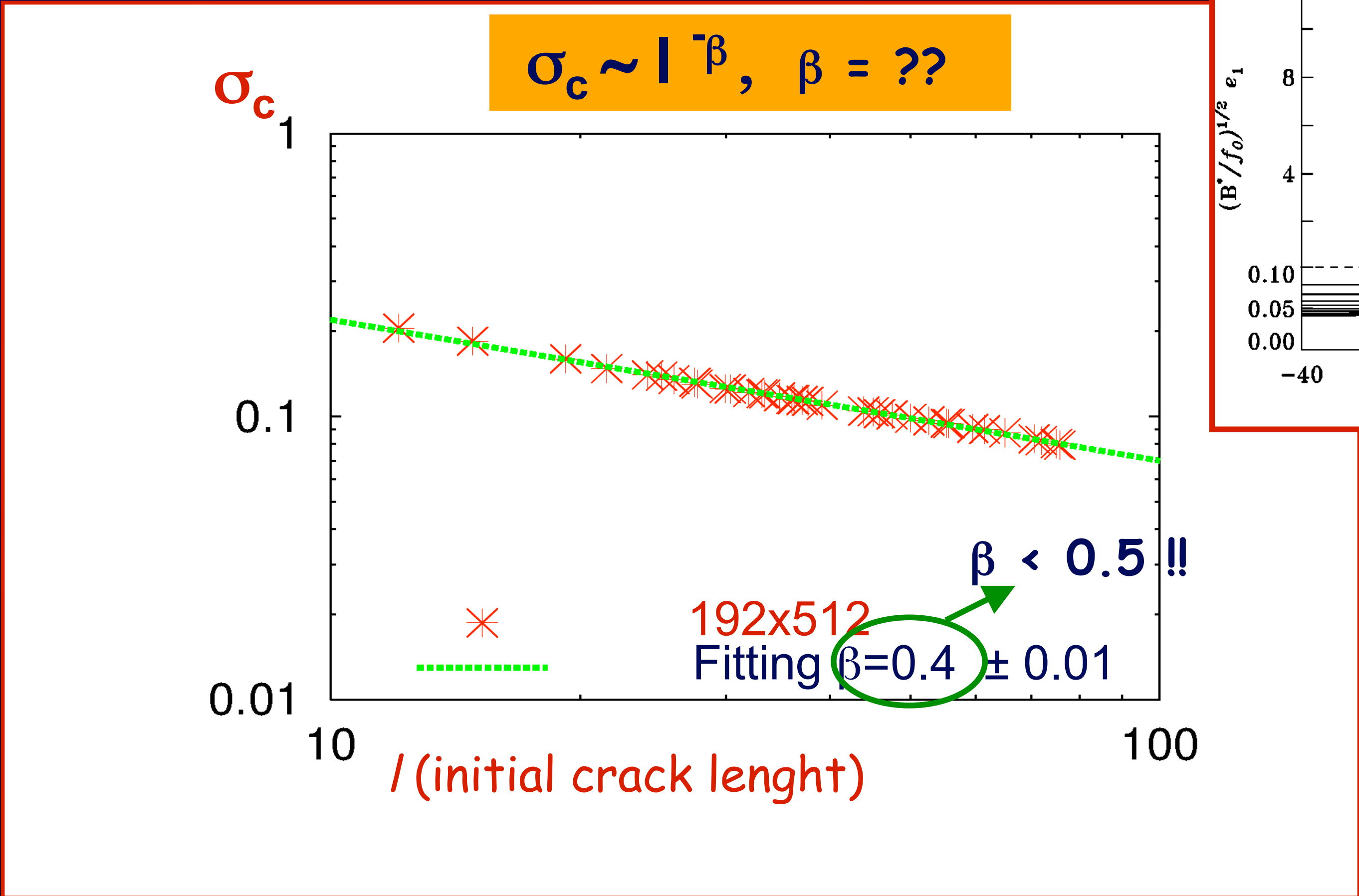


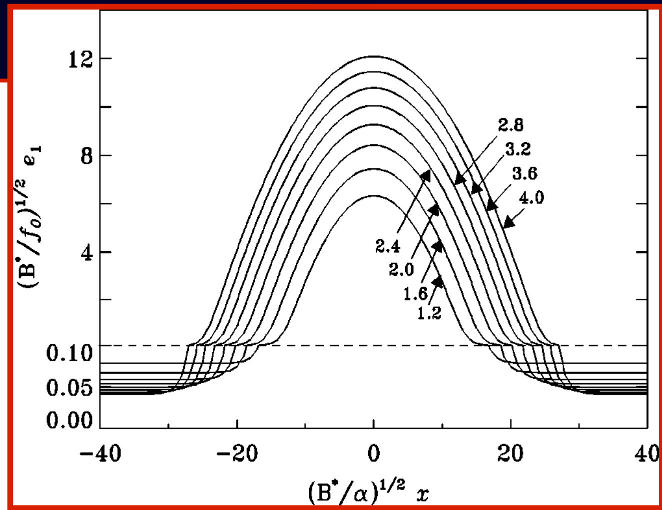
Very nice GL....but it is not an isotropic model !!

Griffith criterion: results

Model with regularization, α_i=0.25, and $f_1 \rightarrow \infty$ (without cutoff)

↪ $F = F_L + F_\nabla = F_L^0(e)/[1+F_L^0(e)/f_0] + \sum_{i=1,2,3} \alpha_i (\nabla e_i)^2$ ~~$s(e_i)$~~

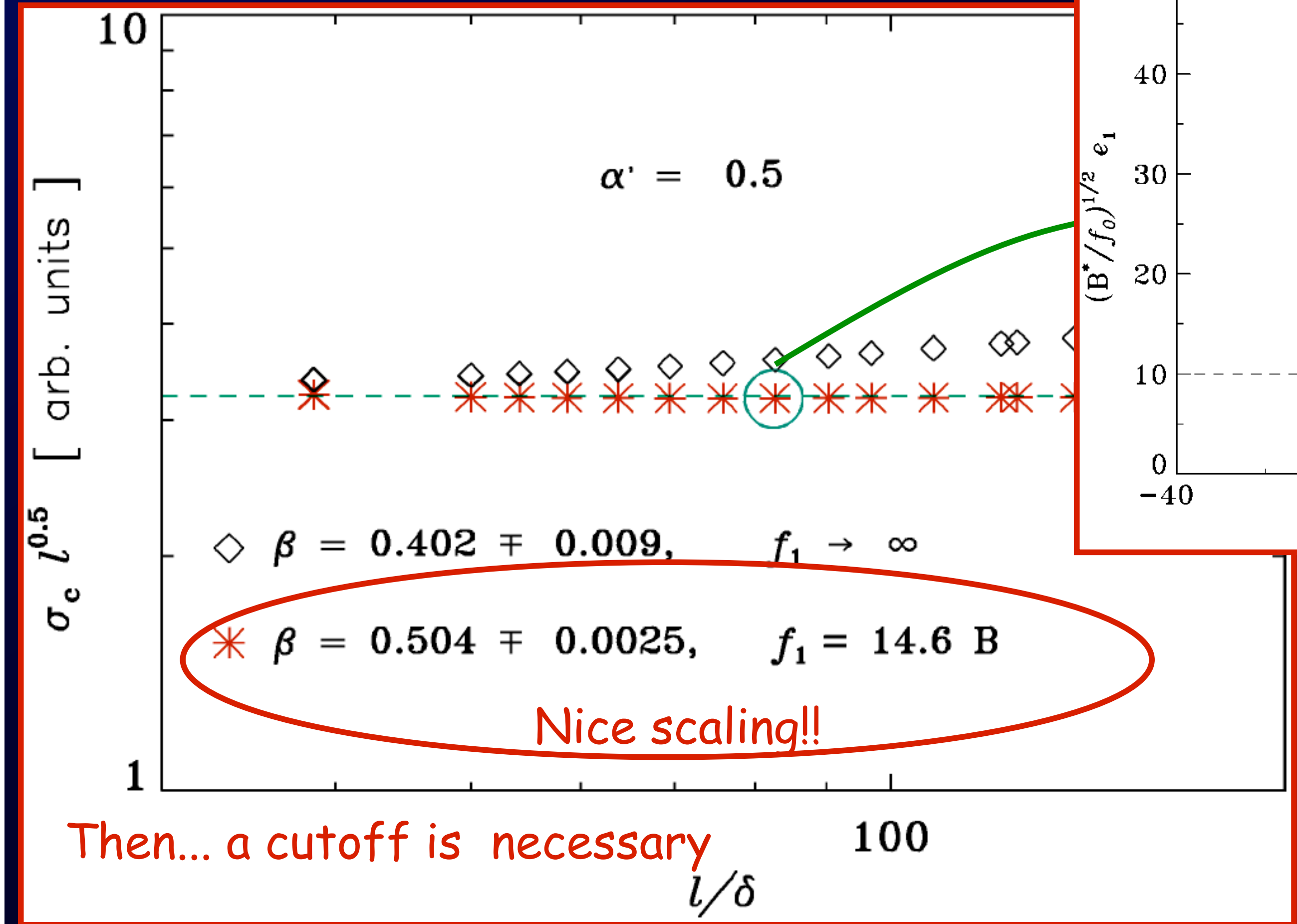


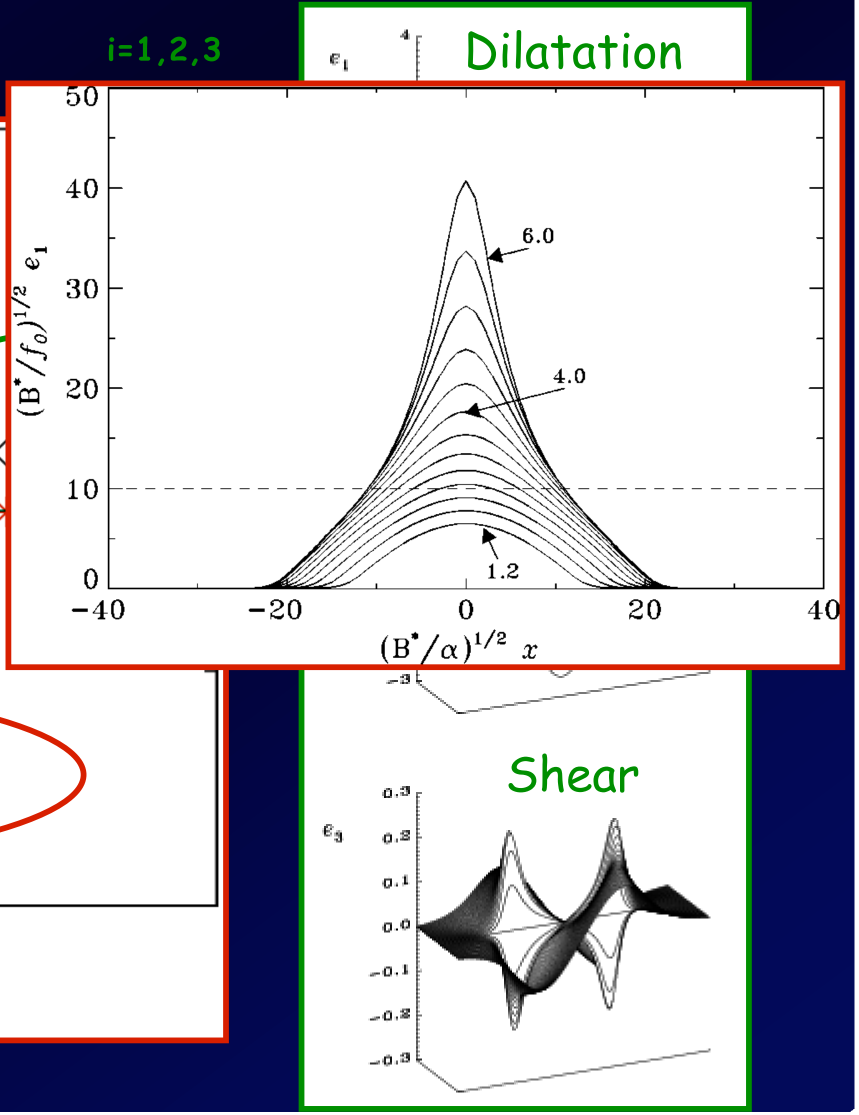


Griffith criterion: results

Model with regularization, α_i=0.25 + finite f_1 (cutoff)

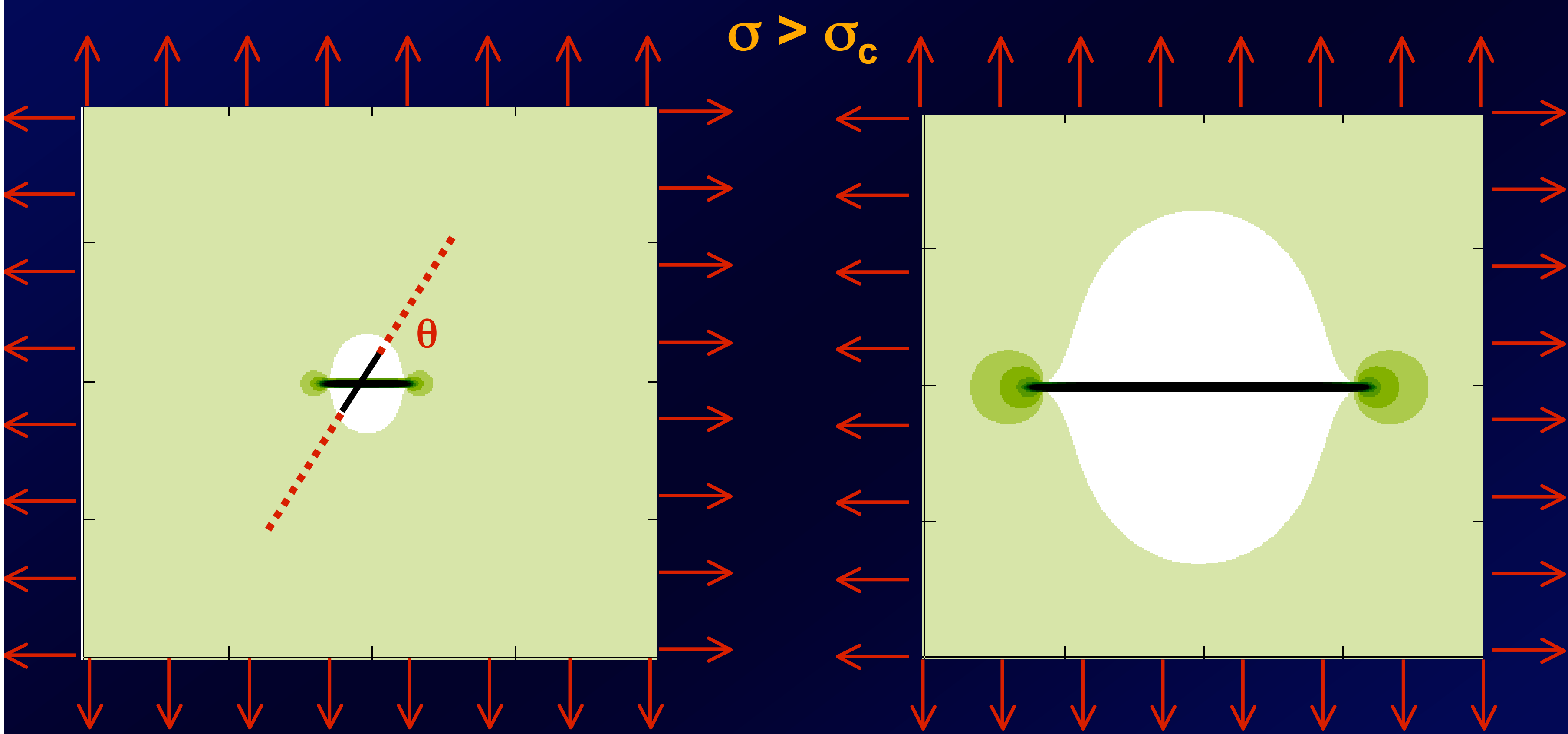
$$\hookrightarrow F = F_L + F_\nabla = F_L^0(e)/[1+F_L^0(e)/f_0] + \sum_{i=1,2,3} \alpha_i (\nabla e_i)^2 \; s(e_i)$$





Results in well controlled geometries

Uniform loading (Mode I): σ remote stress



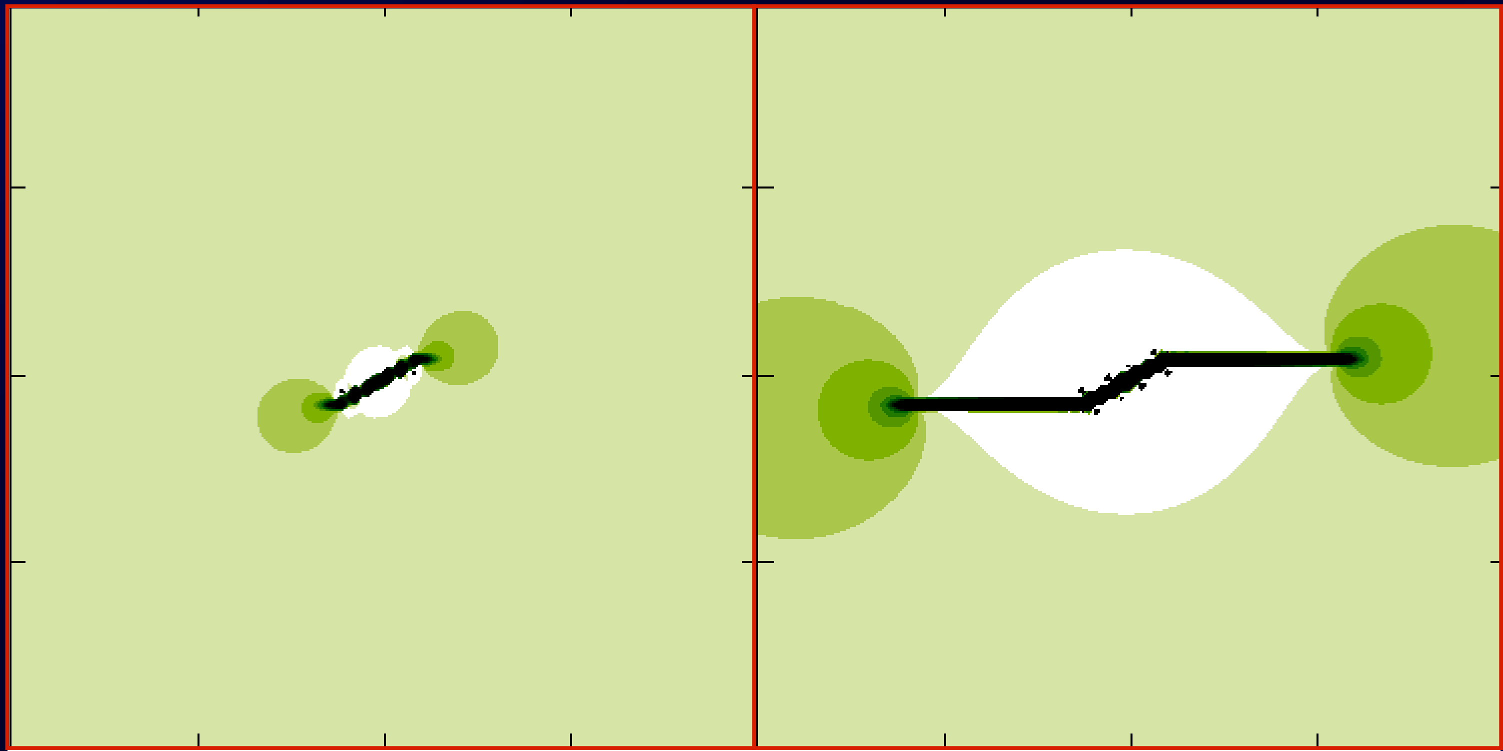
Crack propagation

Results in well controlled geometries

Uniform loading: σ remote stress

$$\sigma > \sigma_c$$

Without regularization terms !!



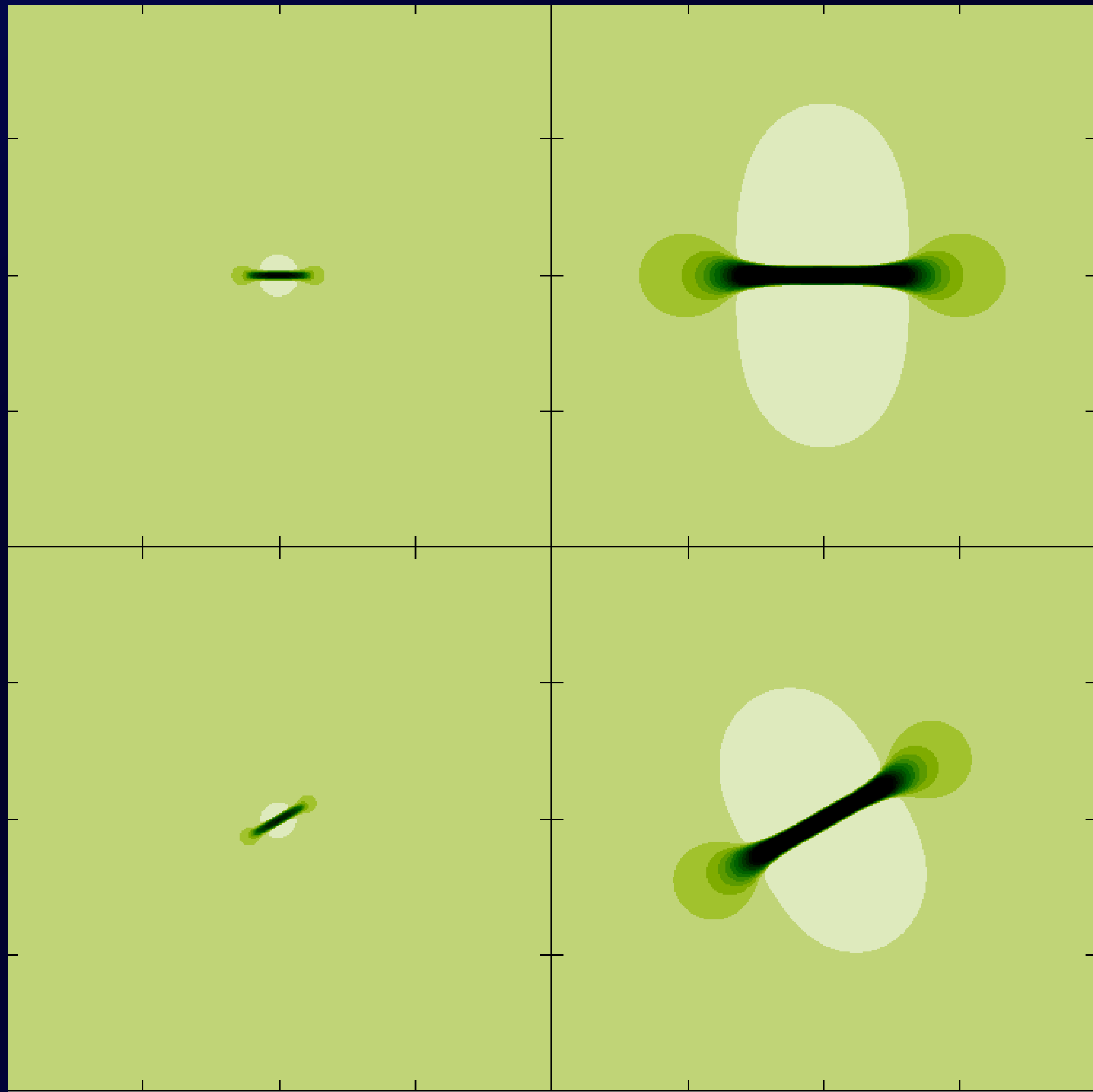
Typical drawback in many discrete models for fracture !!
Clear effects of underlying numerical mesh.......

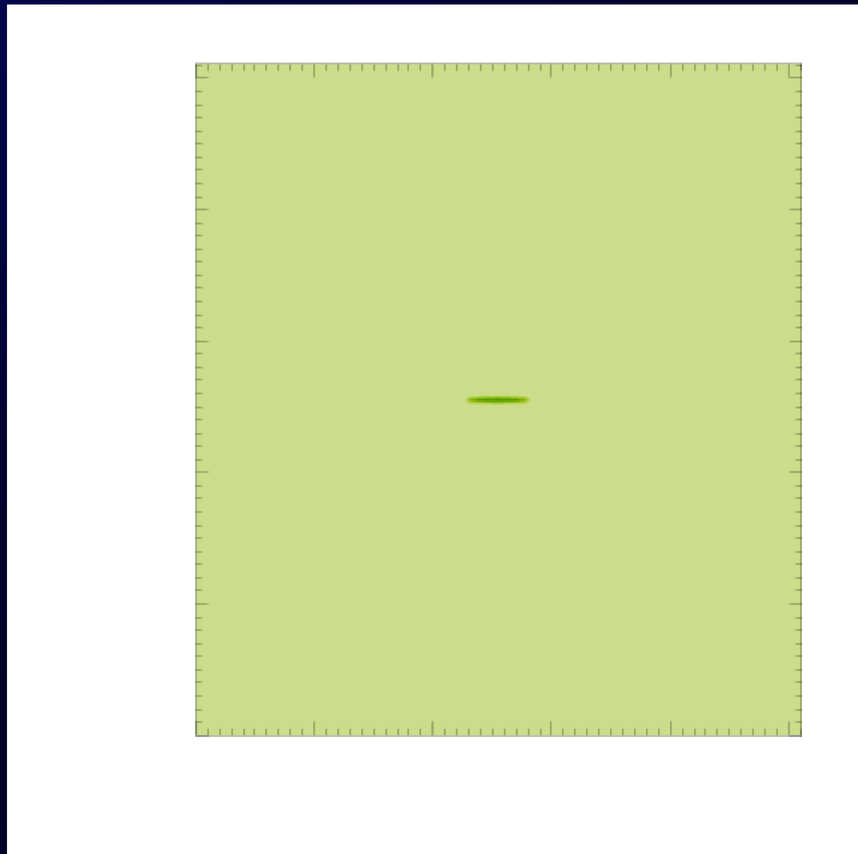
Results including REGULARIZATION

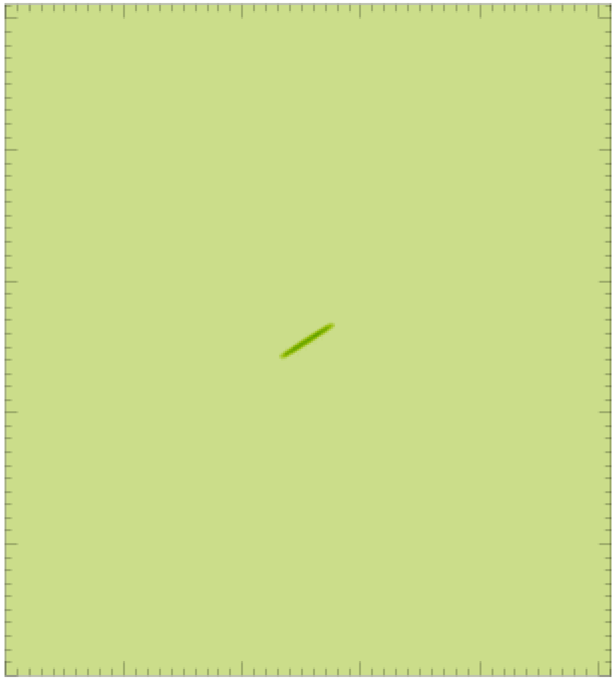
Uniform loading:

σ remote stress:

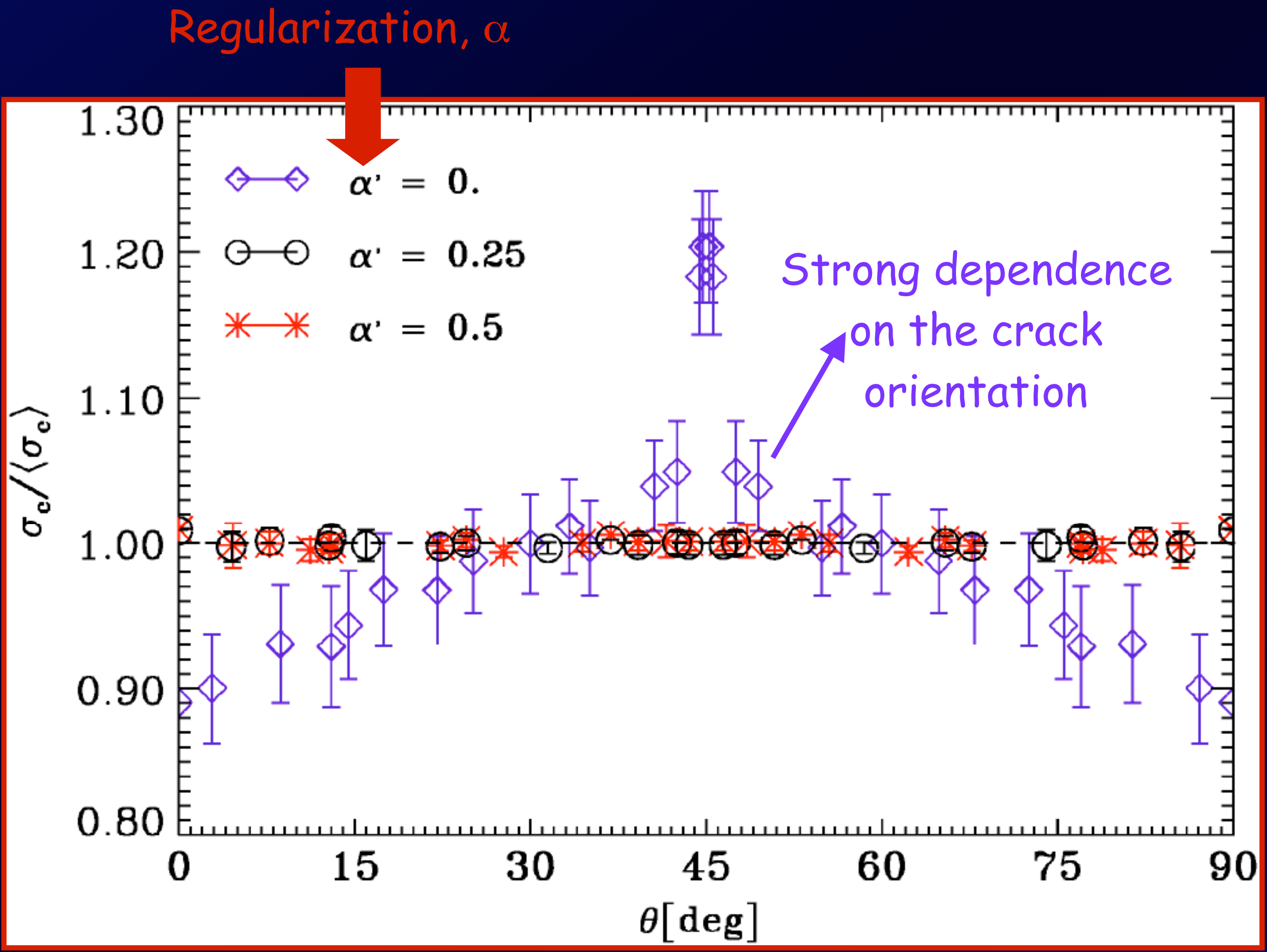
$\sigma > \sigma_c$







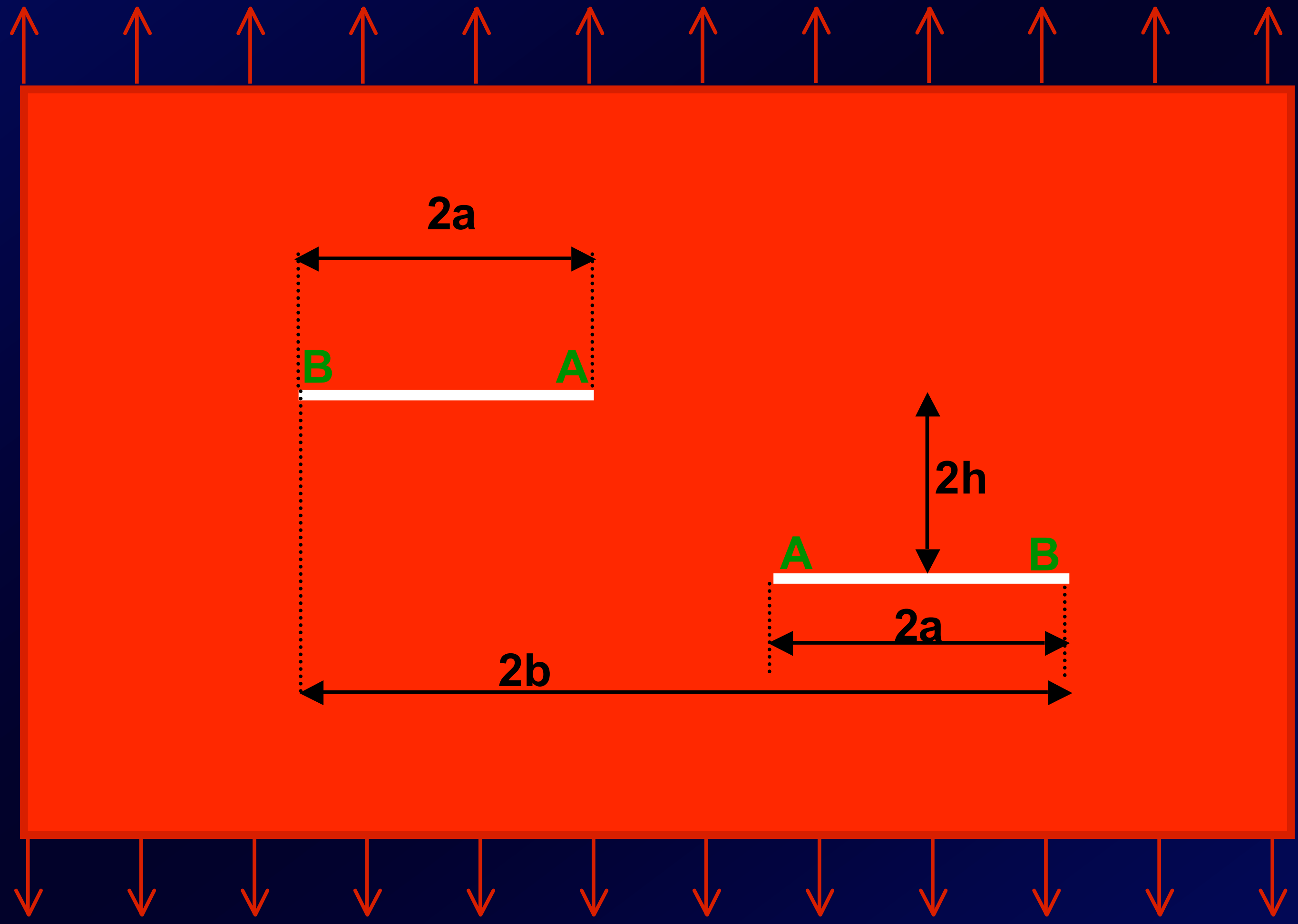
Critical remote stress dependence on angle



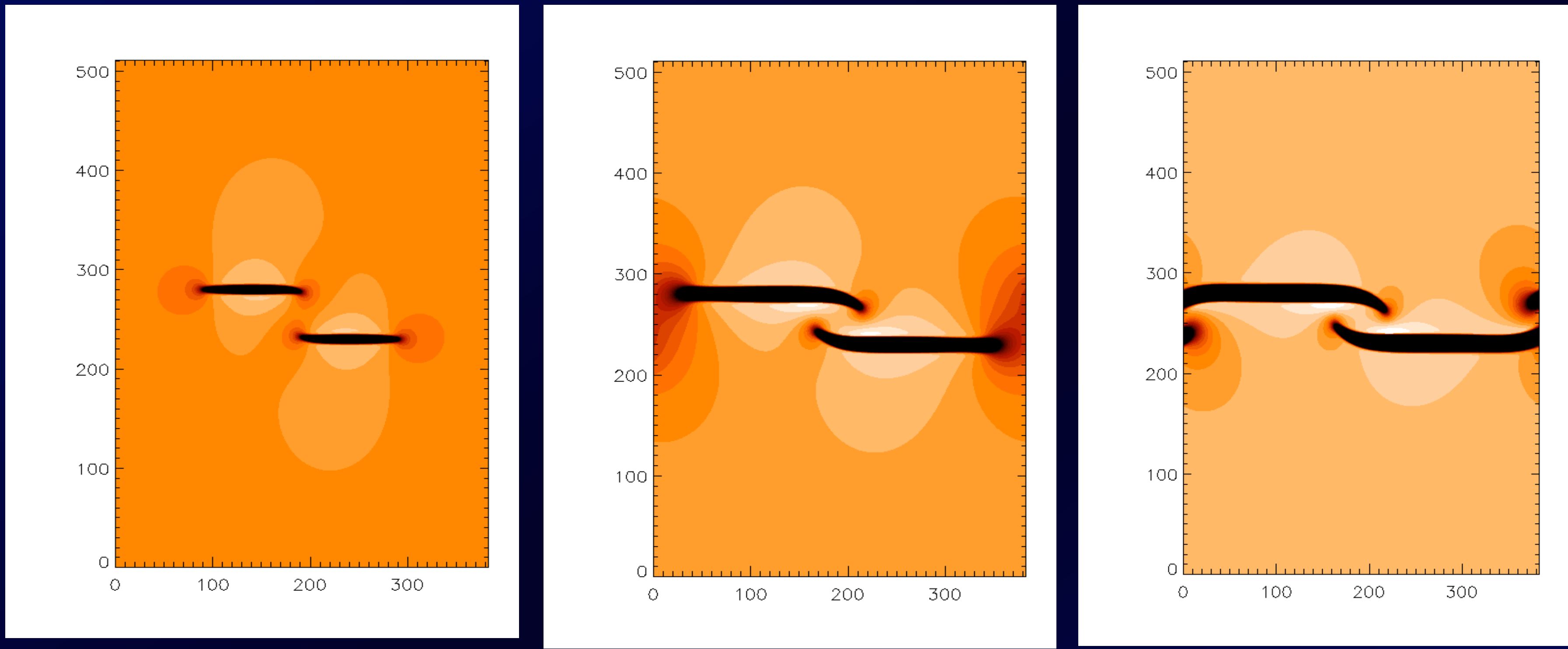
REGULARIZATION ➔ critical stress independent of the angle!

We succeed obtaining an isotropic model !!

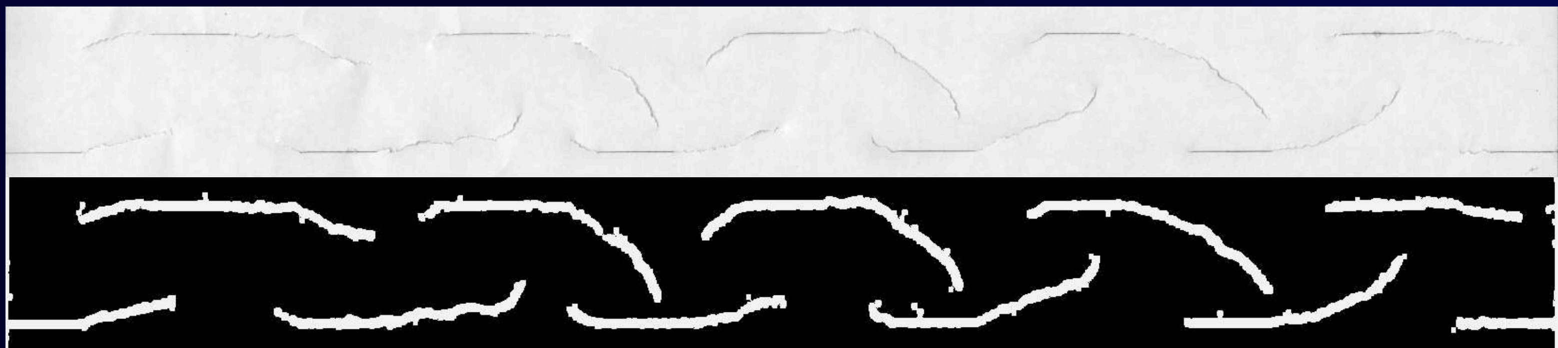
Equal skew-parallel cracks problem



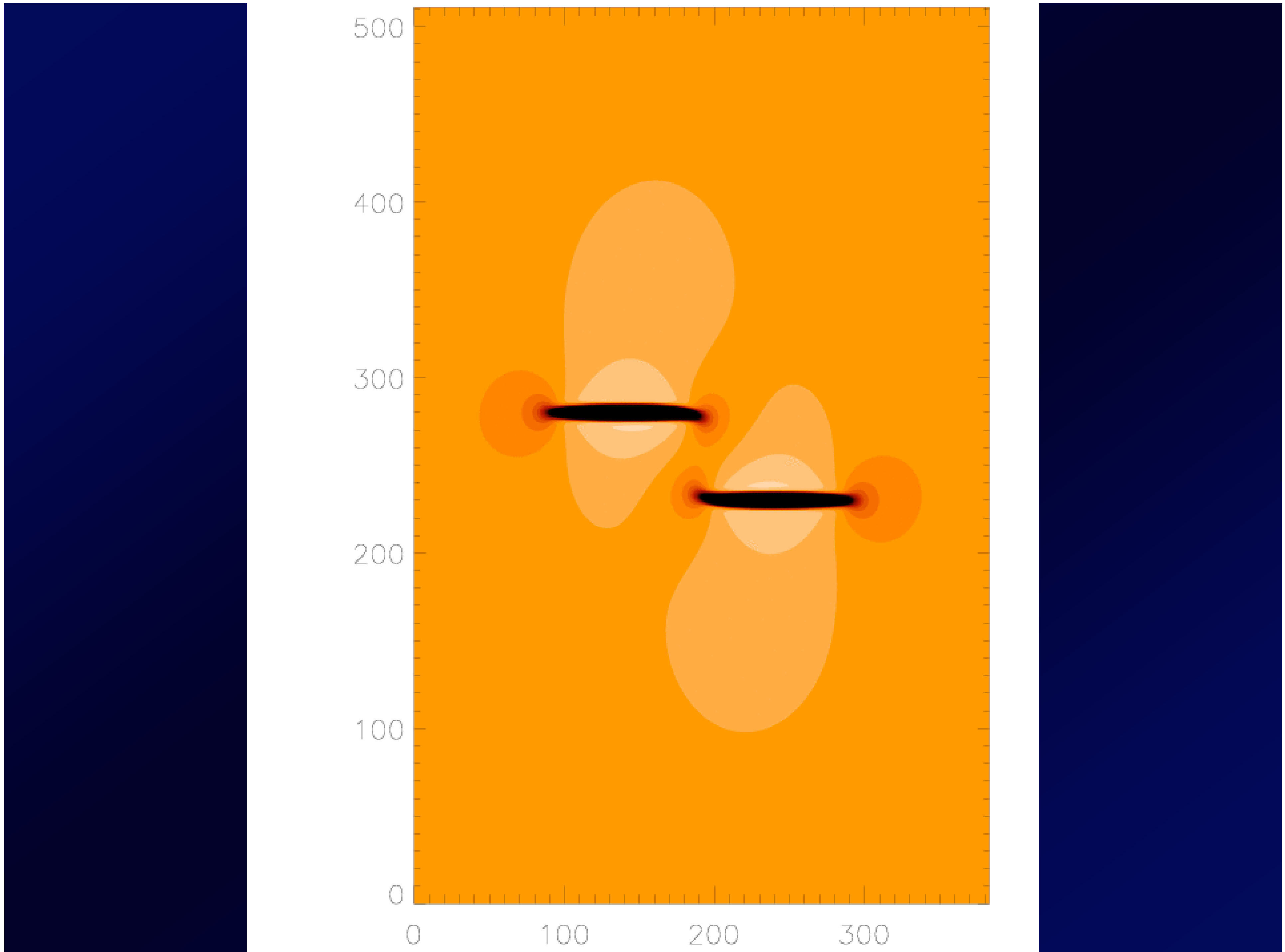
Equal skew-parallel cracks problem



S. Ciliberto's Group experiment, Universite de Lyon, France. Cond-Mat July 2008.

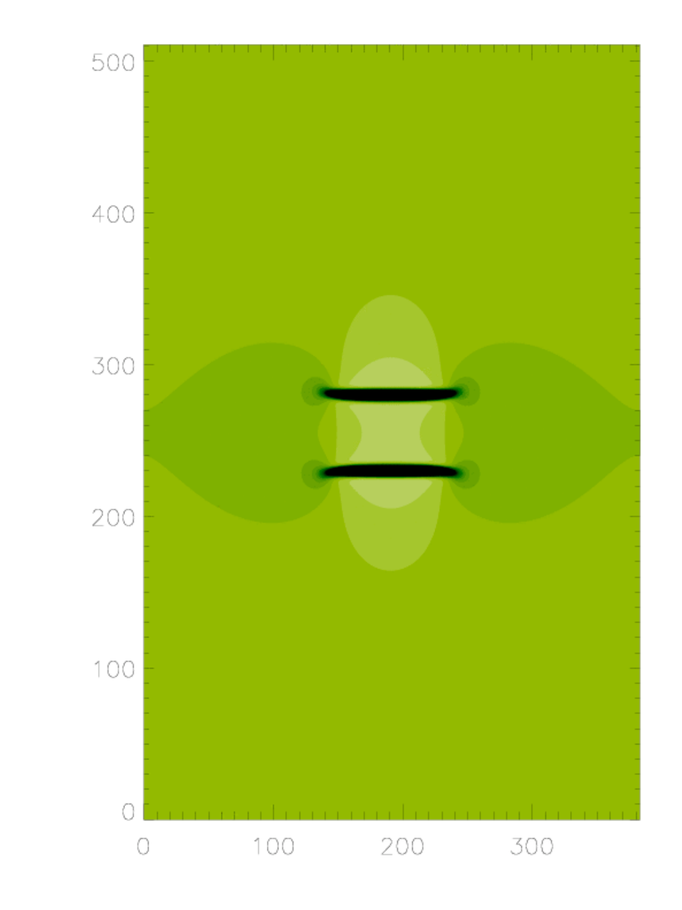


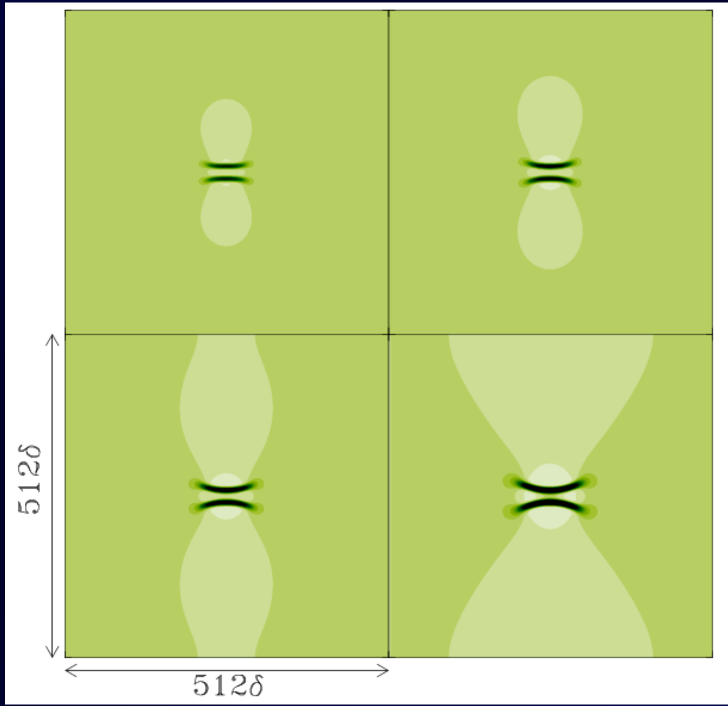
Loaded 2d brittle sample of fax paper sheet (Alrey) with a tensile Machine.



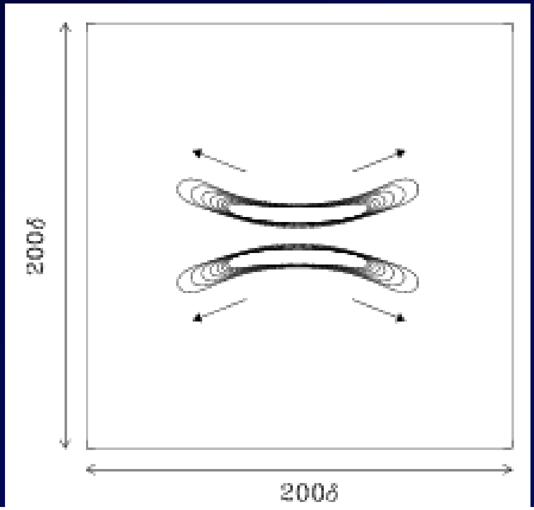
500
400
300
200
100
0
0
100
200
300

Parallel cracks problem





Crack propagation:
snapshots vs time.



Conclusions

Advantages of this model for brittle fracture:

§ Does not include additional degrees of freedom: the full set of variables are the components of the strain tensor.

§ Well defined Newtonian dynamics (plus damping).

§ Largely reduced number of uncontrolled parameters.

§ Information of 'existence and direction' of fracture in a single cell of a computational mesh.

§ Rotational invariant theory.

Summarizing.....

The diffuse interface approach for brittle fracture
is able to reproduce well stablished facts in
fracture physics
and REGULARIZATION makes
results insensitive to the numerical
mesh used "fact not at all trivial in crack modeling".
PRE 71, 036110 (2005).

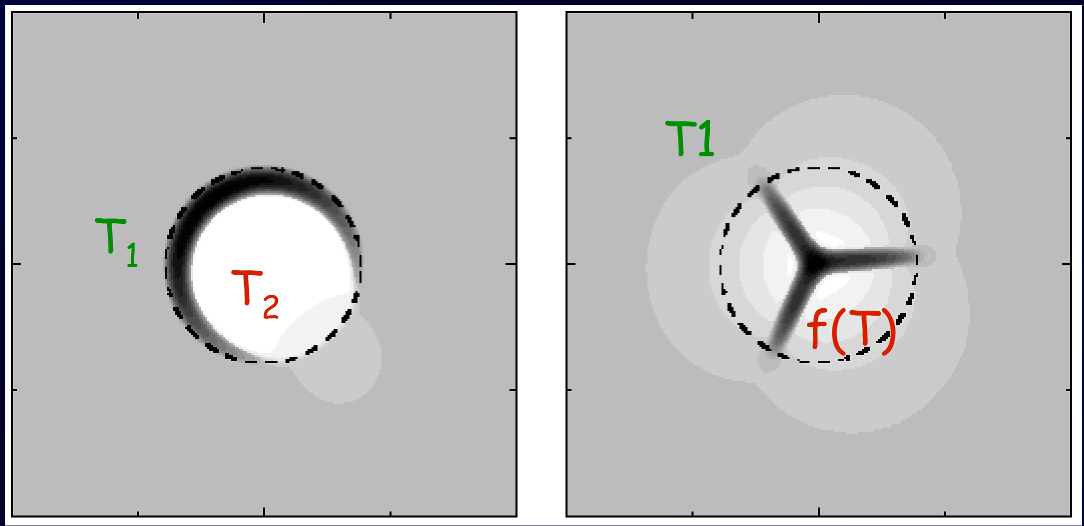
Applications and future work

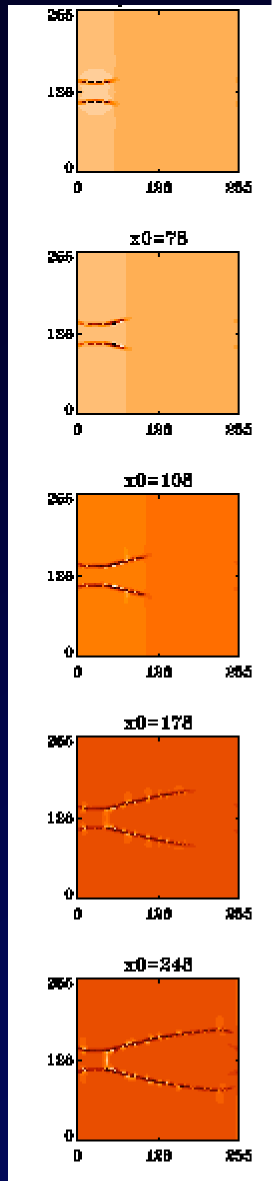
⇨Quasi-static crack propagation problems:

1) Systems under pression.

2) Systems under thermal gradient.

3) Minimum cracks energy configuration (non uniform temperature distribution).



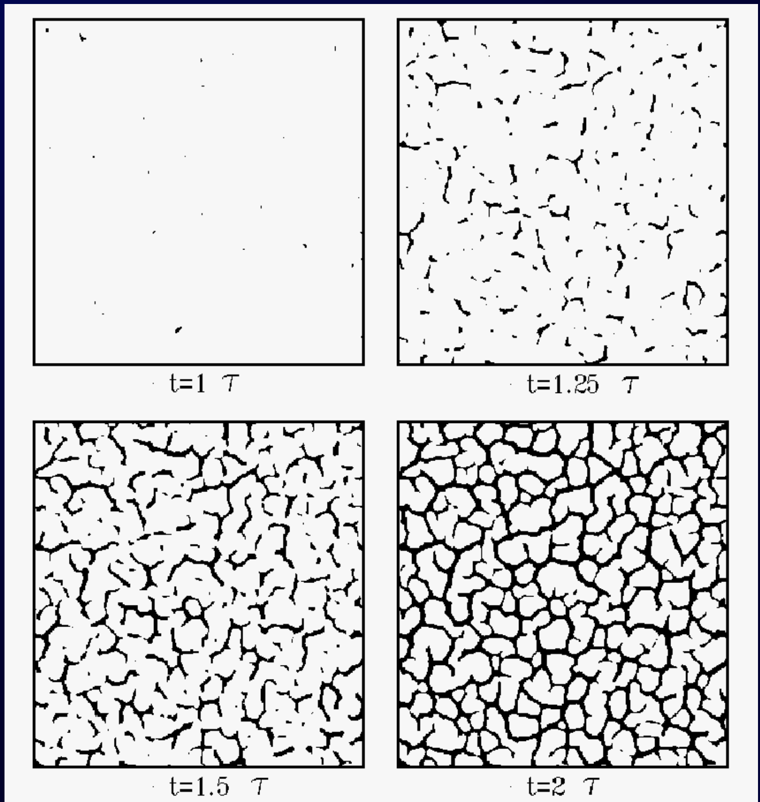




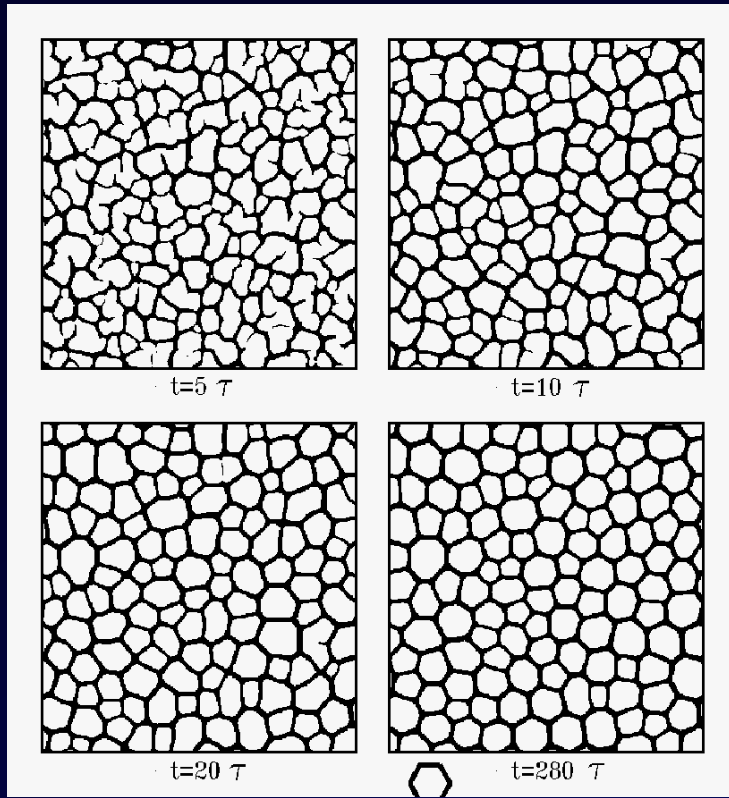
Applications

⇨Crack maturation : Model applied to a thin layer elastically attached to a substrate + disorder

Fragmentation: first stage of evolution



Maturation: at longer times



PRE 69, 056212 (2004)

Applications and future work

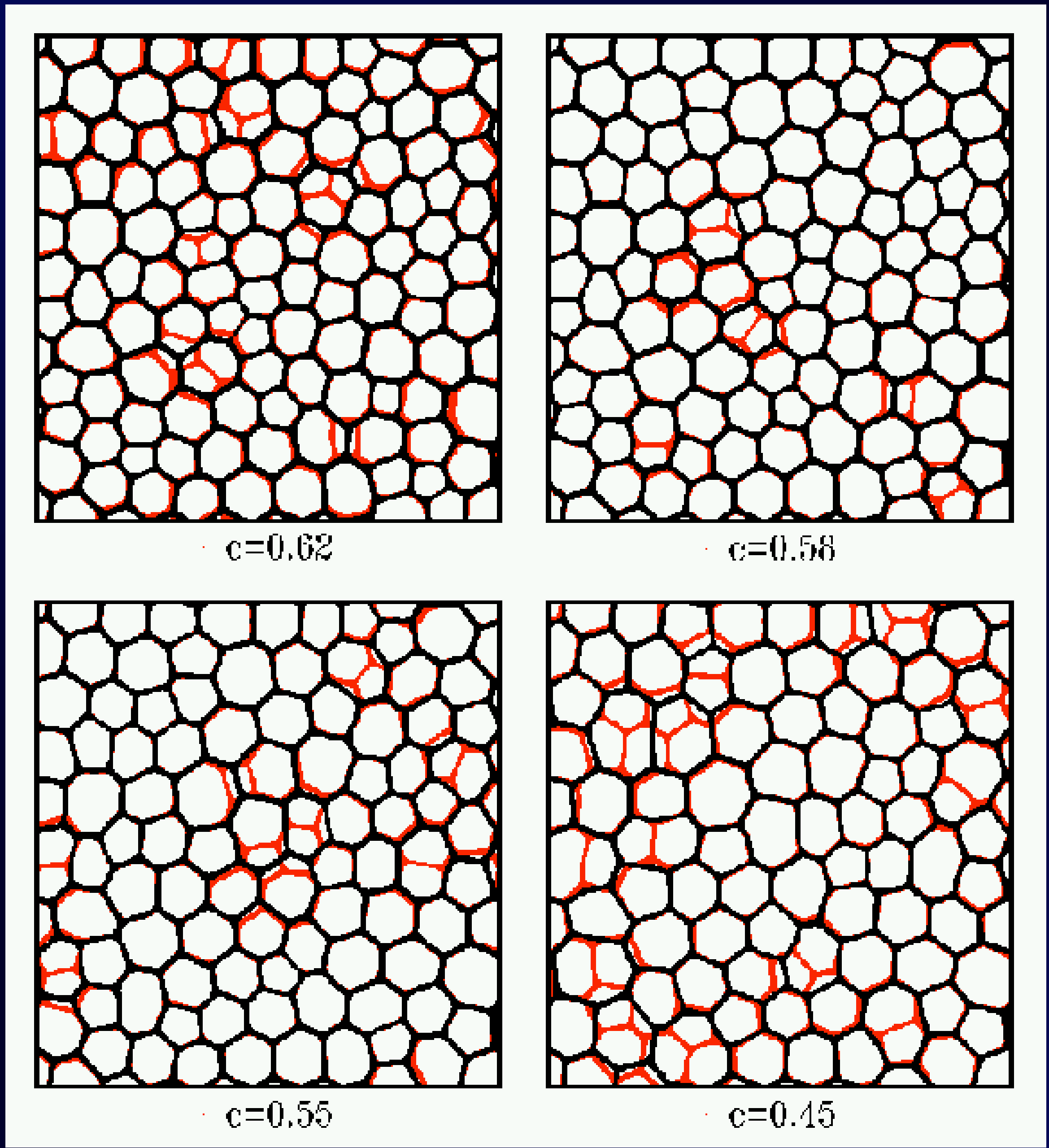
⇨Dynamics of fracture : sound emission, bifurcation, cracks instabilities, …..

Preliminary simulations of the complete dynamics (underdamped or inertial) show indeed well known effects as crack bifurcation and crack oscillations.

⇨ Straightforward extension to 3D problems.

Acknowledgments:
-E. A. Jagla and S. R. Shenoy (ICTP, Italy) and Alain Karma (Northeastern University, Boston) for comments and useful discussions.

$$ Fundings from ICTP & UNESCO.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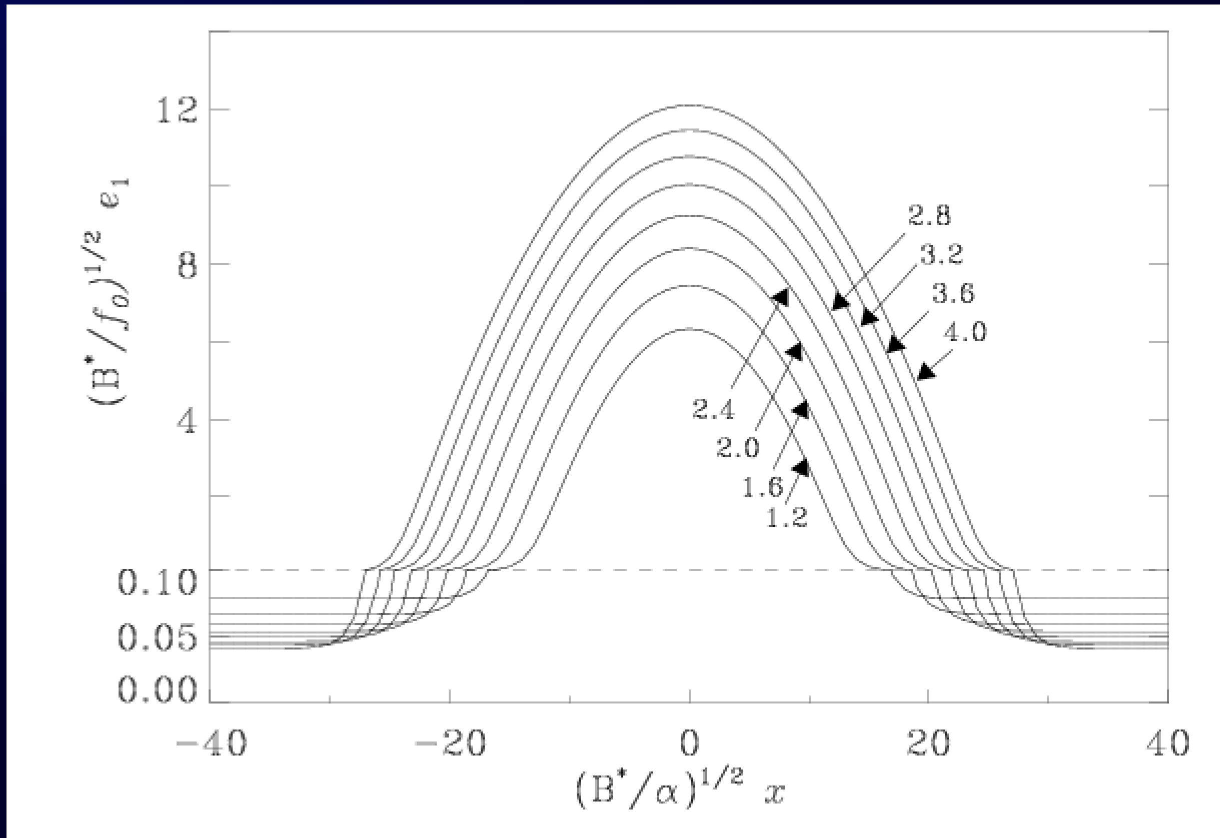

12
8
4
0.10
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$(B^*/f_o)^{1/2}\ e_1$
$(B^*/\alpha)^{1/2}\ x$
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4.0
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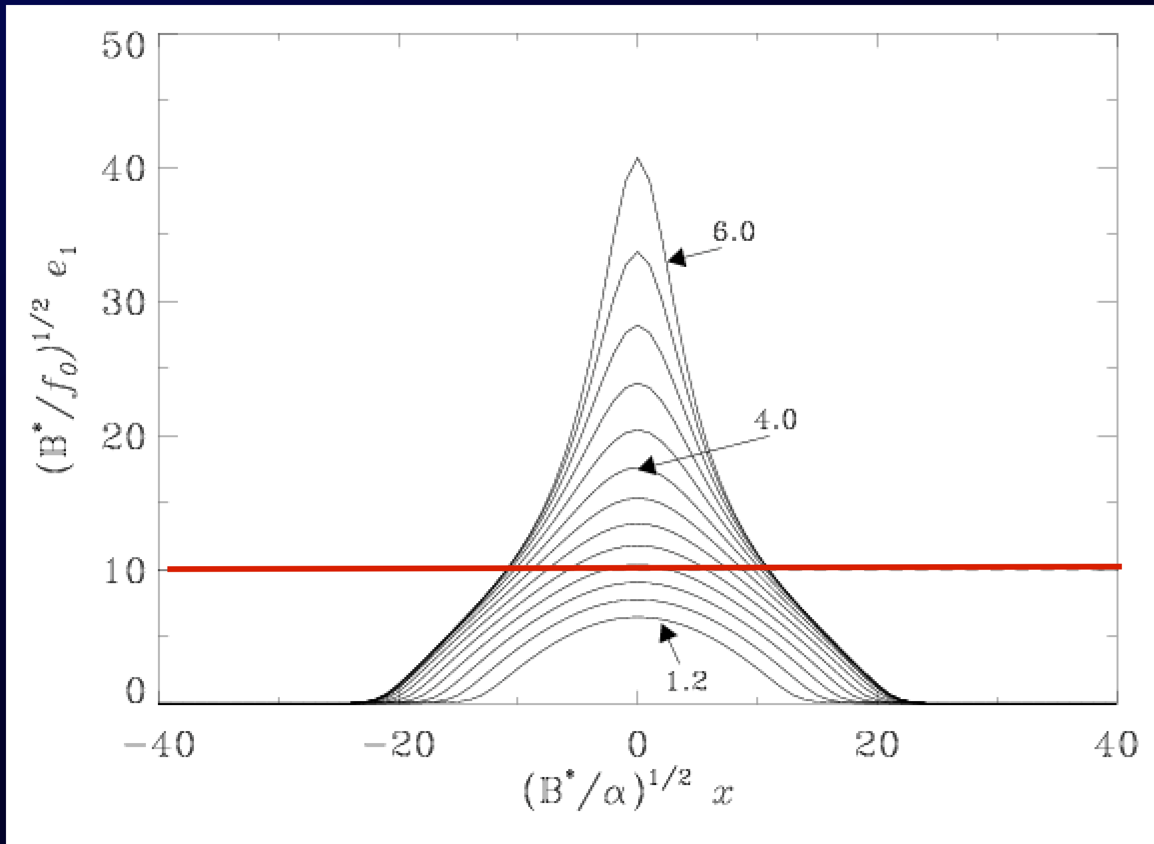
2.0
1.6
1.2



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$(B^*/f_0)^{1/2}\ e_1$
$(B^*/\alpha)^{1/2}\ x$