Damage gradient/phase-field models for brittle fracture

Jérémy Bleyer

Master M2 Mécanique des Solides : matériaux et structures
Endommagement

Outline

Variational approach to fracture [Francfort & Marigo, 1998]

Two-fields minimum principle: displacement $u(t)$, crack location $\Gamma(t)$
The solution $(u(t), \Gamma(t))$ realizes the minimum of the sum of potential and fracture energy:

$$\boxed{\mathcal{E}(u,\Gamma) = \mathcal{E}_{pot}(u,\Gamma) + E_f(\Gamma) = \int_{\Omega\setminus\Gamma} \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon}\,\mathrm{dx} - W_{ext}(u) + G_c|\Gamma|}$$

for all Γ such that $\Gamma(s) \subset \Gamma\ \forall s < t$ and all kinematically admissible displacement u at time t

extends Griffith theory by letting the crack choose its own **future path** based on a minimum energy principle

impossible to solve in practice $\Rightarrow$ need **approximate numerical strategies**

Regularization à la Ambrosio-Tortorelli

Francfort & Marigo variational approach similar to image segmentation using the Mumford-Shah functional [Ambrosio & Tortorelli, 1990]
$\Rightarrow$ mathematical works in this domain lead to the **Ambrosio-Tortorelli** approximation

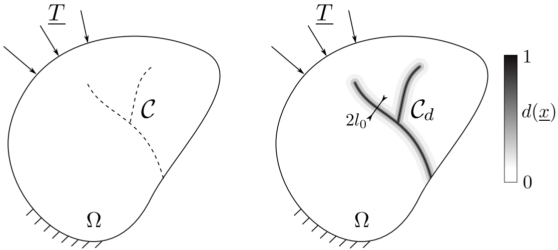
adaptation to the variational approach of fracture by [Bourdin et al., 2000]

$$\boxed{\mathcal{E}_{pot}(u,d) = \int_\Omega (1-d)^2 \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} \,\mathrm{dx} - W_{ext}(u)}$$

$$\boxed{\mathcal{E}_f(d) = \frac{G_c}{c_w}\int_\Omega \left(\frac{w(d)}{\ell_0} + \ell_0\|\nabla d\|^2\right)\mathrm{dx}}$$

$d \in [0;1]$ is a continuous field representing the fracture location ($d = 1$) in a **smeared** fashion
ℓ_0 is a regularization parameter which must be small
$w(d)$ a continuous strictly-monotonic function with $w(0) = 0$ and $w(1) = 1$
c_w a numerical constant associated with w

Regularization properties



Two-fields minimum principle: $u(t)$, $d(t)$ minimizes the total energy:

$$u(t), d(t) = \arg\min_{u,d} \mathcal{E}_{pot}(u, d) + \mathcal{E}_f(d)$$

with the irreversibility condition $\dot{d} \geq 0$
ℓ_0 will drive the size of the localization zone of the smeared crack representation

Convergence result

the solution (u, d) **converges** to (u, Γ) solution of the FM problem in the sense of Γ-convergence when $\ell_0 \to 0$, in part. $E_f(d) \to G_c|\Gamma|$

Reinterpretation as a damage gradient model

If $\ell_0 = 0$ we formally have a **local** damage model (with all its known issues)
when $\ell_0 \neq 0$, we can see it as a **damage** gradient model (dissipation potential depending both on $\dot{d}$ and $\nabla\dot{d}$) following the framework of standard generalized materials
in this interpretation, ℓ_0 may not be seen as a pure mathematical regularization parameter but an **additional material** parameter

Popular choices for $w(d)$

- AT1 model:

$$\boxed{a(d) = (1-d)^2, \quad w(d) = d, \quad c_w = \frac{8}{3}}$$

- AT2 model:

$$\boxed{a(d) = (1-d)^2, \quad w(d) = d^2, \quad c_w = 2}$$

$a(d)$ is the stiffness degradation function (continuous, monotonically decreasing, $a(0) = 1$, $a(1) = 0$)

Why phase-field models ?

Models for phase-separation of mixtures (binary alloys for instance) show similar equations the main difference is that they employ a double-well potential $w(d) \propto d^2(1-d)^2$ to penalize intermediate phase densities

First-order optimality conditions

Directional derivative for u: **linear variational elasticity problem** at **fixed** d

$$\left.\frac{\partial \mathcal{E}_{tot}}{\partial u}\right|_{(u,d)}(v,0) = 0 \Rightarrow \int_\Omega a(d)\boldsymbol{\varepsilon}_u : \mathbb{C} : \boldsymbol{\varepsilon}_v \,\mathrm{dx} = W_{ext}(v) \quad \forall v$$

Directional derivative for d:

$$\left.\frac{\partial \mathcal{E}_{tot}}{\partial d}\right|_{(u,d)}(0,\beta) \geq 0 \Rightarrow \begin{array}{c} \displaystyle\int_\Omega \left(a'(d)\frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon}\right)\beta \,\mathrm{dx} + \\ \displaystyle\frac{G_c}{c_w}\int_\Omega \left(\frac{w'(d)}{\ell_0}\beta + \ell_0 \nabla d \cdot \nabla \beta\right)\mathrm{dx} \end{array} \geq 0$$

$\forall \beta \geq 0$ which accounts for the **irreversibility** condition, we have a **variational inequality** it yields the following evolution laws:

$$\boxed{f(\boldsymbol{\varepsilon}, d) = -a'(d)\frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} - \frac{G_c w'(d)}{c_w \ell_0} + 2\frac{G_c \ell_0}{c_w}\Delta d \leq 0} \quad \text{(non-local damage criterion)}$$

and $\dot{d} \geq 0$, $\dot{d} f(\boldsymbol{\varepsilon}, d) = 0$.

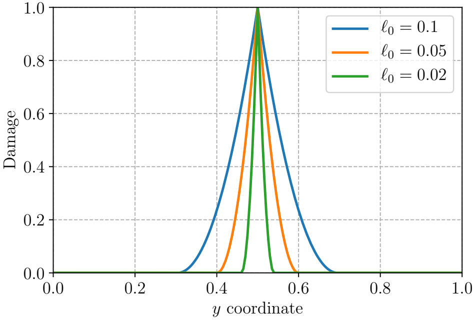
Localized solutions for AT1

Localized solution with $d = 1$ at $x = x_0$:

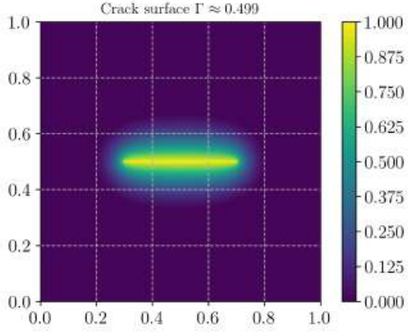
$$d(x) = \left(\frac{|x - x_0|}{2\ell_0} - 1\right)^2 \text{ on } [x_0 - 2\ell_0, x_0 + 2\ell_0],\ d = 0 \text{ otherwise}$$

localized zone of **finite support** (width $4\ell_0$)

c_w computed such that $\dfrac{1}{c_w}\displaystyle\int_{x_0-2\ell_0}^{x_0+2\ell_0} \left(\frac{w(d(x))}{\ell_0} + \ell_0 (d'(x))^2\right) \mathrm{dx} = 1$



(a) 1D solution



(b) $\ell_0 = 0.1$ for $|\Gamma| = 0.4$

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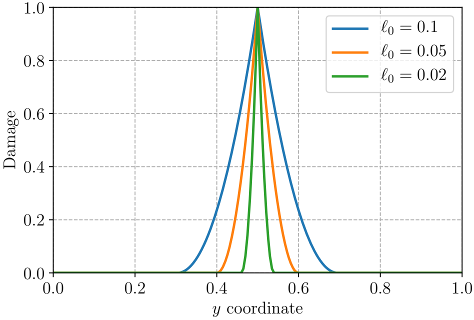

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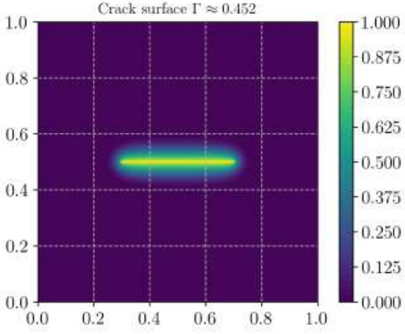

(b) $\ell_0 = 0.05$ for $|\Gamma| = 0.4$

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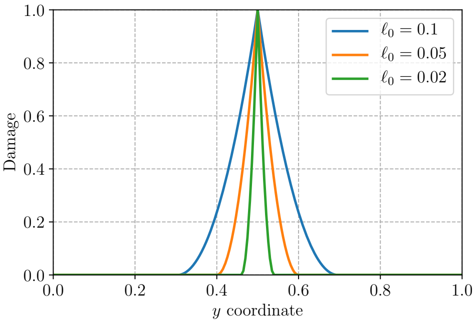

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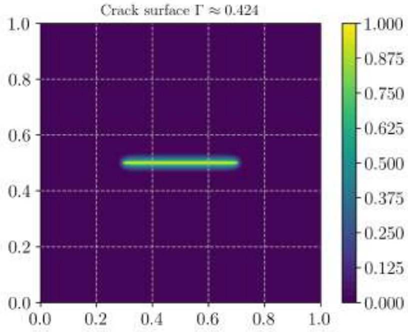

(b) $\ell_0 = 0.02$ for $|\Gamma| = 0.4$

Localized solutions for AT2

Localized solution with $d = 1$ at $x = x_0$: $\quad d(x) = \exp\left(-\dfrac{|x - x_0|}{\ell_0}\right)$

localized solution of **infinite support** but characteristic width is ℓ_0

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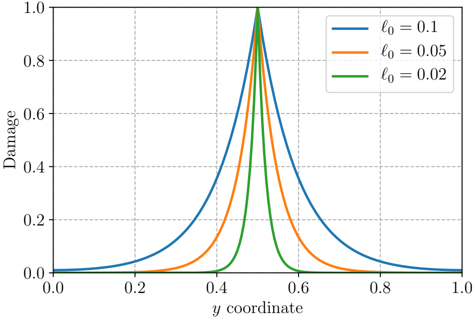

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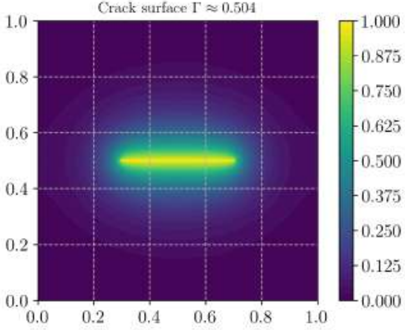

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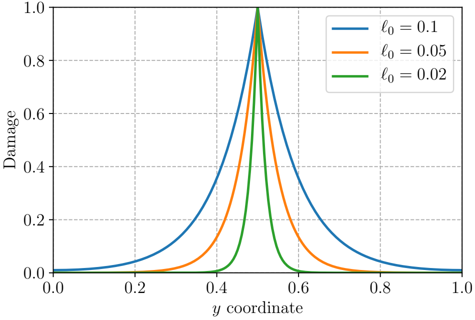

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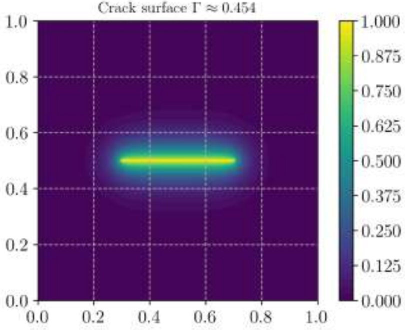

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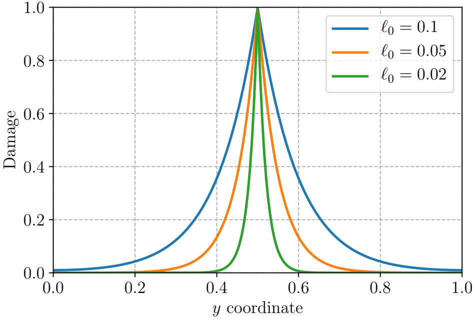

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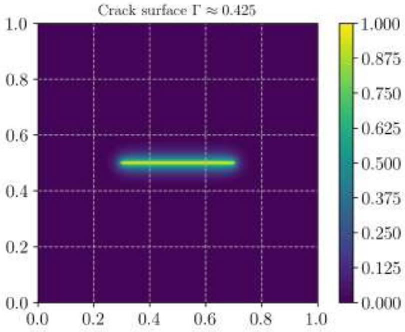

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Outline

Numerical implementation

Classical strategy[1]: **alternate minimization**

[1] other possibilities exist

Numerical implementation

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at time t_{n+1}, we know the past solution (u_n, d_n), we iterate:

$$
\begin{array}{l}
u_{n+1}^0 = u_n \text{ and } d_{n+1}^0 = d_n \\
\text{for } i = 1, \ldots, N_{\text{iter max}} : \\
\quad u_{n+1}^i = \arg\min\limits_{v} \mathcal{E}_{tot}(v, d_{n+1}^i) \qquad (1) \\
\quad d_{n+1}^i = \arg\min\limits_{d_n \leq d \leq 1} \mathcal{E}_{tot}(u_{n+1}^i, d) \qquad (2) \\
\quad \text{stop if } \|(u_{n+1}^i, d_{n+1}^i) - (u_{n+1}^{i-1}, d_{n+1}^{i-1})\| \leq \texttt{tol}
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Problem (1) = **standard elasticity problem** with fixed value of $d = d^i_{n+1}$
Problem (2) for AT1/AT2 = **minimizing a quadratic energy** in terms of d with bound constraints $d_n \leq d \leq 1$

$\Rightarrow$ there exist **dedicated solvers** (e.g. TAO distributed with PETSc)

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$\Rightarrow$ there exist **dedicated solvers** (e.g. TAO distributed with PETSc)

Warning

we must find a global minimum of $\mathcal{E}_{tot}$ $\Rightarrow$ extremely difficult as $\mathcal{E}_{tot}$ is **non-convex**
alternate minimization will only converge to **critical points** (not necessarily a minimum)

[1] other possibilities exist

Open-source implementation

Next week: extension of previous local damage script to damage gradient very close to

Corrado Maurini and Tianyi Li implementation using FEniCS
`https://bitbucket.org/cmaurini/gradient-damage`

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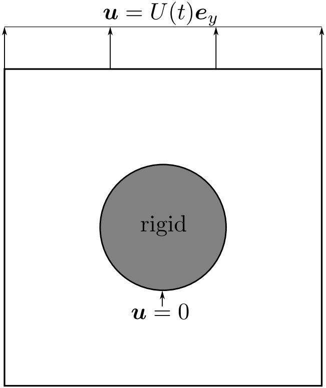
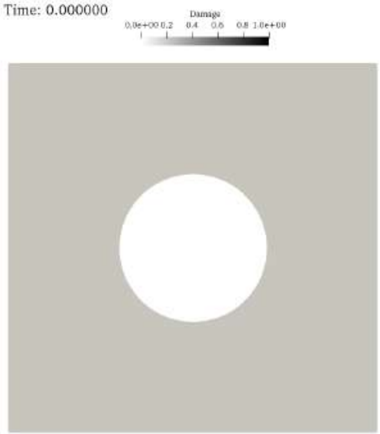
Example: Traction of a plate with a stiff inclusion [Bourdin et al., 2000]

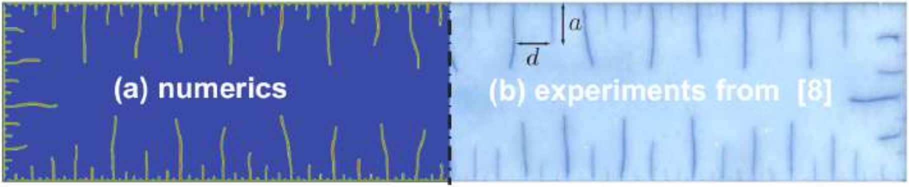




Application to a thermal shock problem

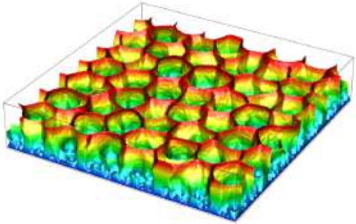
Thermal strains: strain energy is now $(1-d)^2\dfrac{1}{2}(\varepsilon - \varepsilon^{th}) : \mathbb{C} : (\varepsilon - \varepsilon^{th})$ with $\varepsilon^{th} = \alpha \Delta T 1$

Ceramic plate in a cold bath:



Numerics from [Bourdin et al., 2014]

Experiments from [Shao et al., 2011]



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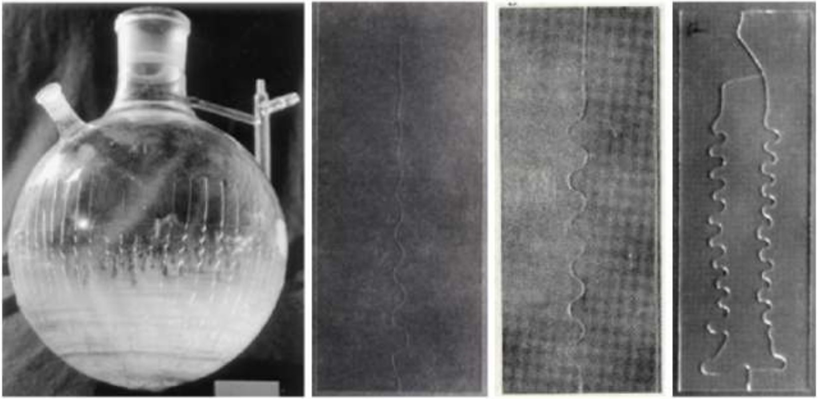
Rapid cooling of a strip of glass: **osciallatory cracks**

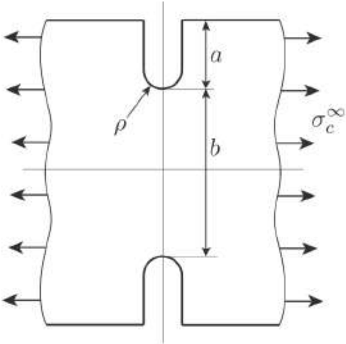


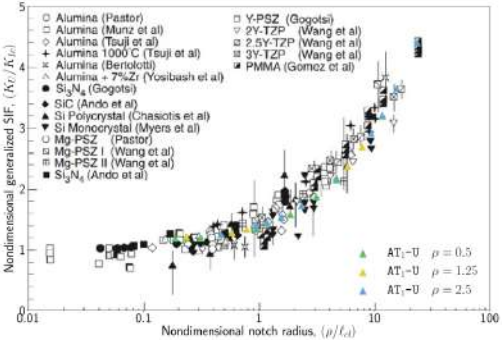
Simulation 1 Simulation 2

[B. Bourdin website]

Crack nucleation [Tanné et al., 2018]

Role of ℓ_0 ? Critical stress for crack nucleation at notches

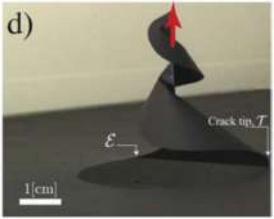




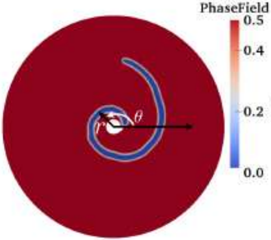
Extension to fracture of thin shells [Li et al., 2018]

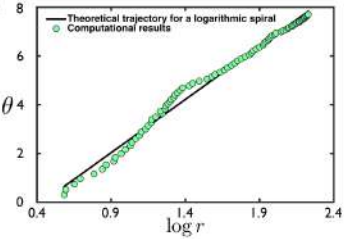
Strain energy of a thin shell:
membrane strain $\boldsymbol{e}$ and curvature strain $\boldsymbol{\chi}$ (Koiter thin shell)

$$\mathcal{E}_{el}(u) = \int_\omega (1-d)^2 \psi(\boldsymbol{e}, \boldsymbol{\chi})\, \mathrm{dx}$$



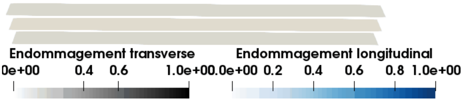
Romero, et.al, *Soft Matter*, 2013



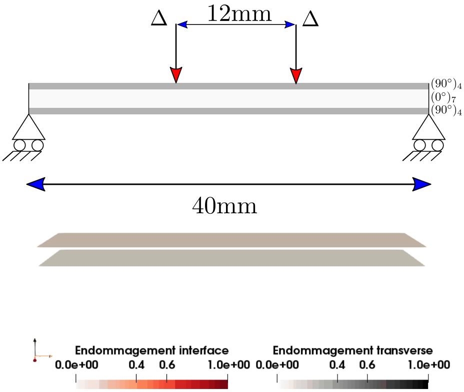


Multicracking and delamination [Th. Paul Bouteiller, 2022]

Traction

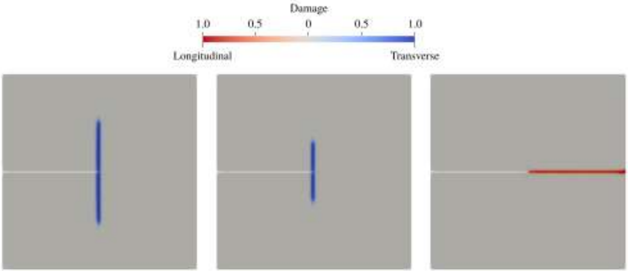


Bending



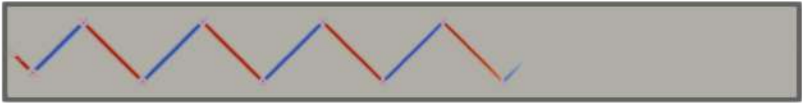
Crack propagation in anisotropic media

Crack kinking in anisotropic material [Bleyer et Alessi, 2018]



$G_{cy} = 0.05\,G_{cx}$ $\quad$ $G_{cy} = 0.09\,G_{cx}$ $\quad$ $G_{cy} = 0.1\,G_{cx}$

Zig-zag cracks in polycrystals [Scherer et al., 2022]



Outline

Dynamic brittle fracture: open questions

Open questions: crack path, velocity, crack branching/fragmentation, dissipated energy ?

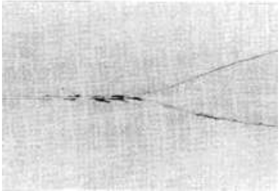
Fundamental aspects of LEFM (nominally brittle materials)

- mode-I crack limiting speed: c_R
- dynamic energy release rate G: Griffith criterion $G = G_c(v)$

Experimental results

- experimental limiting velocity: $0.4 - 0.7c_R$
- branching: single crack description is not OK anymore
- large increase of apparent G_c at high speed

explained by **crack-tip instabilities** developping microbranches [Sharon et Fineberg, 1996], increase of fracture surface roughness



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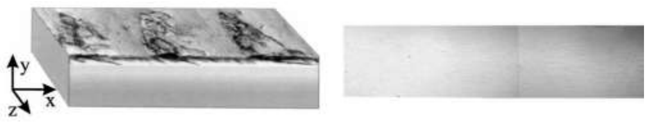

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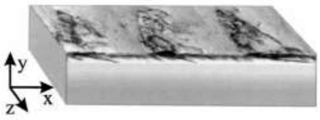

Dynamic brittle fracture: open questions

Open questions: crack path, velocity, crack branching/fragmentation, dissipated energy ?

Fundamental aspects of LEFM (nominally brittle materials)

- mode-I crack limiting speed: c_R
- dynamic energy release rate G: Griffith criterion $G = G_c(v)$

Experimental results

- experimental limiting velocity: $0.4 - 0.7c_R$
- branching: single crack description is not OK anymore
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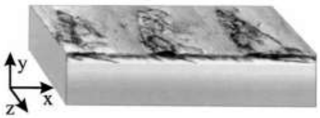

Extension of phase-field approach to dynamics

We simply add a kinetic energy term **not affected by the damage variable**:

$$\mathcal{E}_{kin}(u, d) = \int_\Omega \frac{\rho}{2} \|\dot{\boldsymbol{u}}\|^2 \,\mathrm{dx}$$

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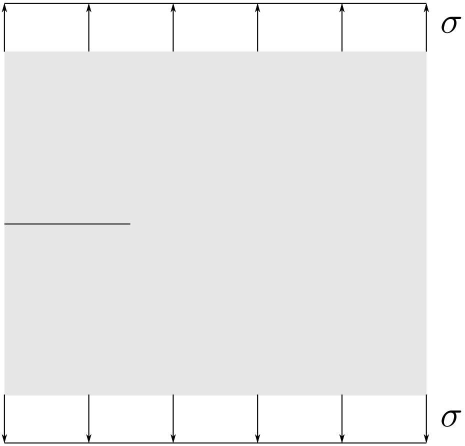
Note: **no mathematical results** of $\Gamma-$convergence in this dynamic setting
$\Rightarrow$ open question

In-plane tearing problem

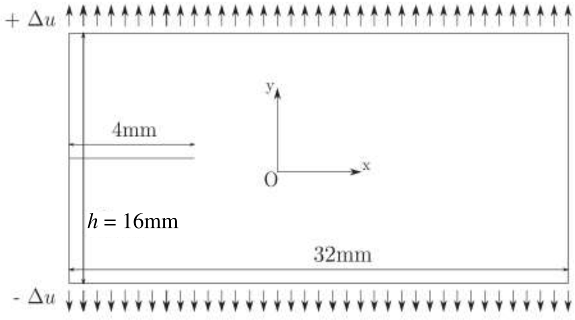
Mode I loading with prescribed stress échelon on top and bottom



Small stress   Medium stress   Large stress

Prestrained plate

Prestrained state, fixed boundaries during propagation [Zhou, 1996]
$E = 3.09$ GPa, $\nu = 0.35$, $\rho = 1180$ kg/m^3, $G_c = 300$ J/m^2, $c_R = 906$ m/s



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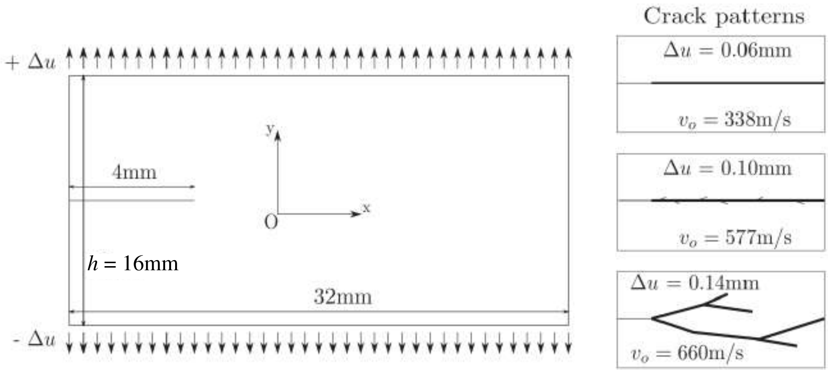
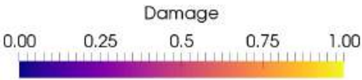


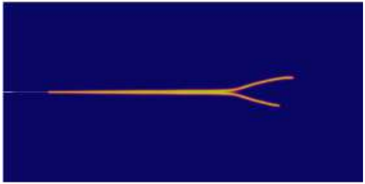
- experimental results: simple propagation for small loading, microbranching then macrobranching at higher loads
- band geometry ⇒ LEFM solution: crack should accelerate up to c_R

Damage fields [Bleyer et al., 2016]

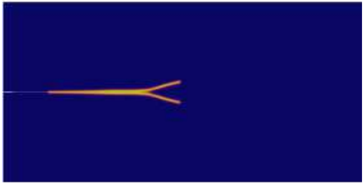


(a) $\Delta U = 0.035$ mm at $t = 40$ μs

(b) $\Delta U = 0.038$ mm at $t = 40$ μs

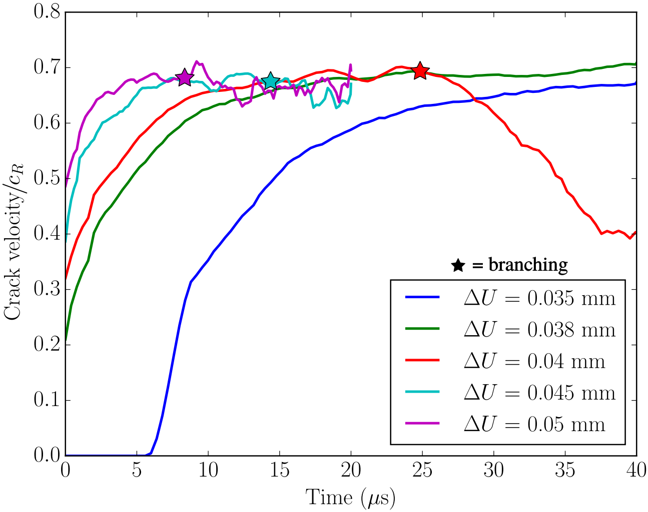


(c) $\Delta U = 0.040$ mm at $t = 40$ μs



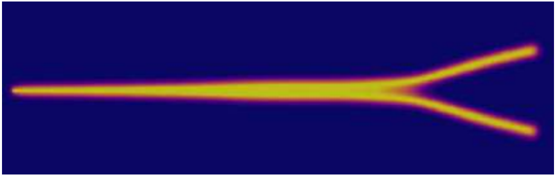
(d) $\Delta U = 0.045$ mm at $t = 20$ μs

Crack velocity [Bleyer et al., 2016]



existence of a **limiting speed** $v_{lim} \approx 0.68 c_R$

Damage broadening before branching [Bleyer et al., 2016]



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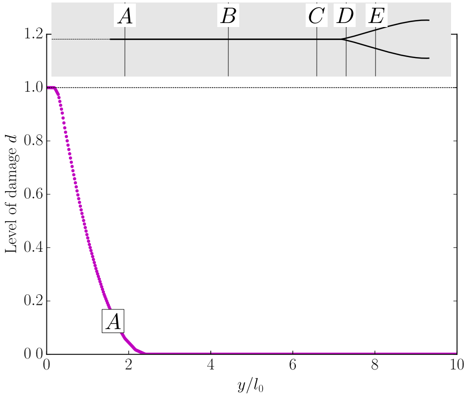

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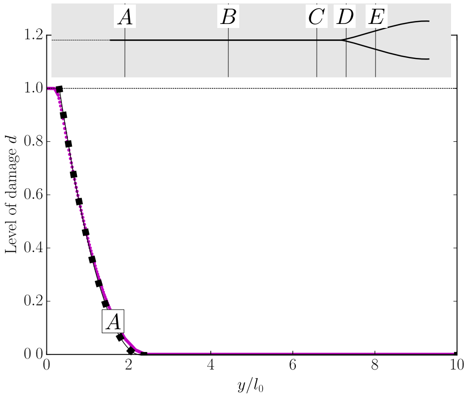

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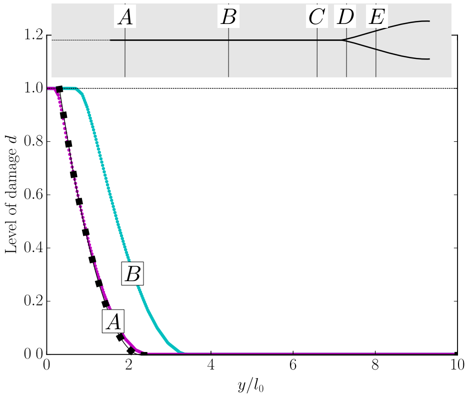

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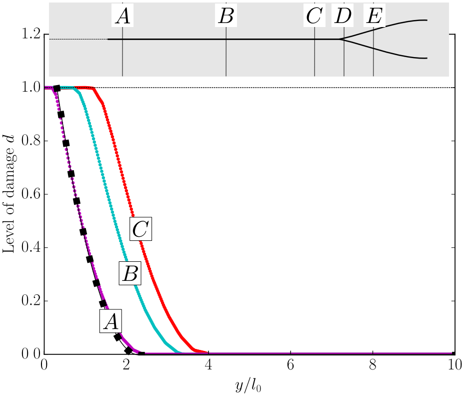

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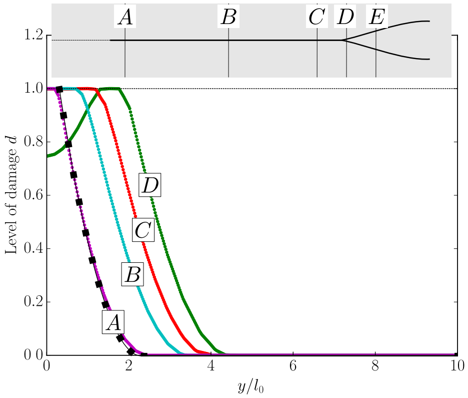

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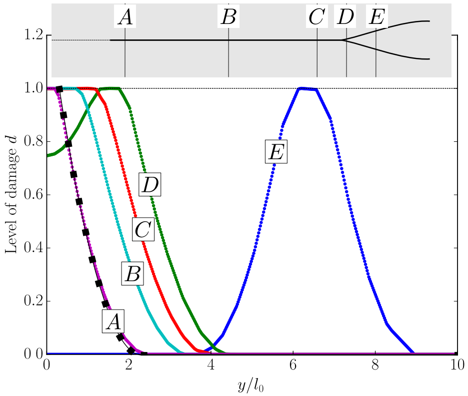
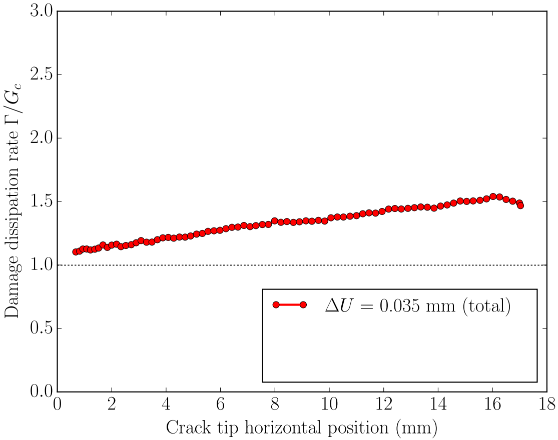


Apparent fracture energy [Bleyer et al., 2016]

$\Gamma = dE_{frac}/da$ seen as the apparent fracture energy



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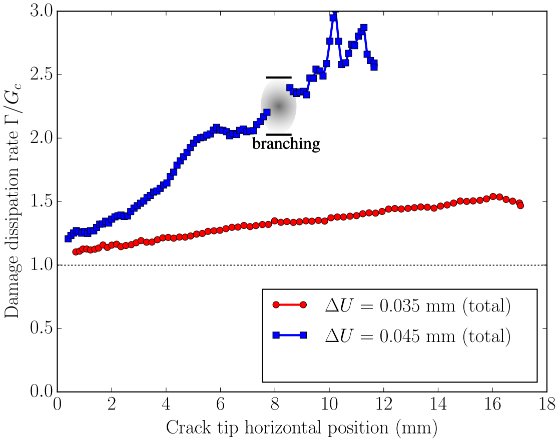

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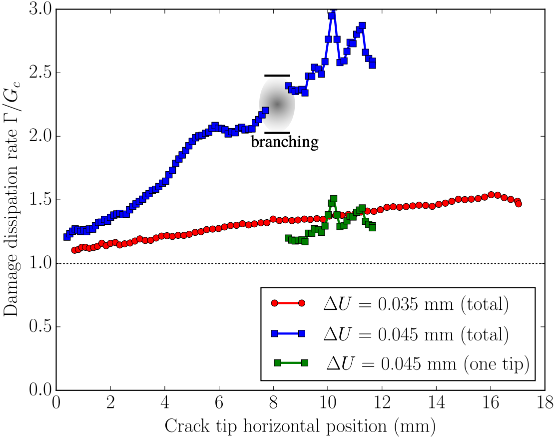

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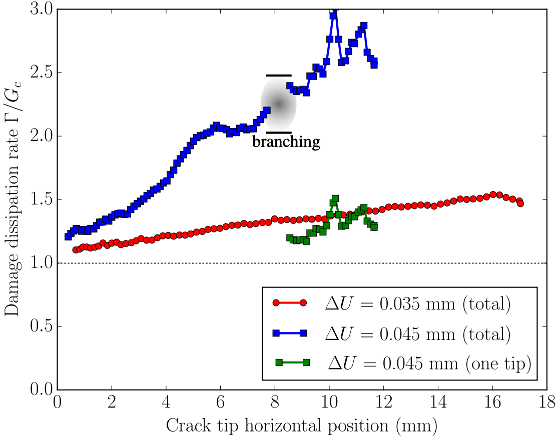
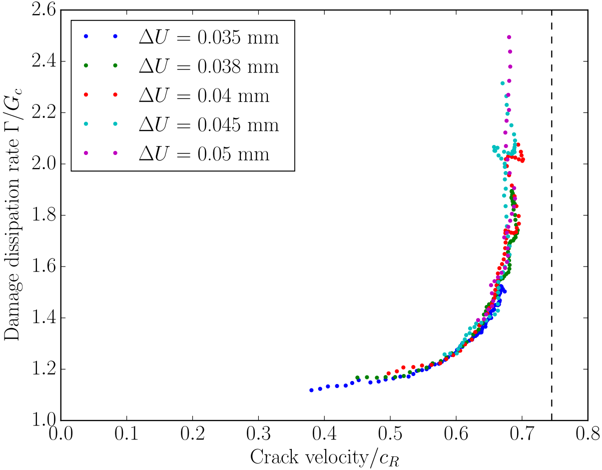


suggest a **critical value** of $\Gamma \approx 2G_c$ associated with branching

Velocity-toughening mechanism [Bleyer et al., 2016]



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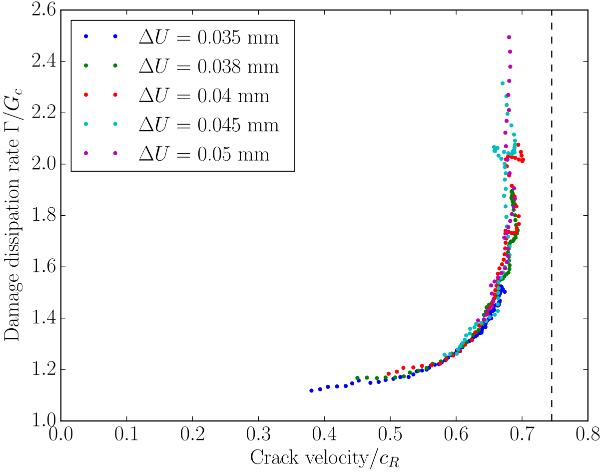

well-defined $\Gamma(v)$ relation, similar to experimentally observed velocity-toughening fracture energies

3D computations : influence of loading [Bleyer & Molinari, 2016]

$\Delta U = 0.04$ mm

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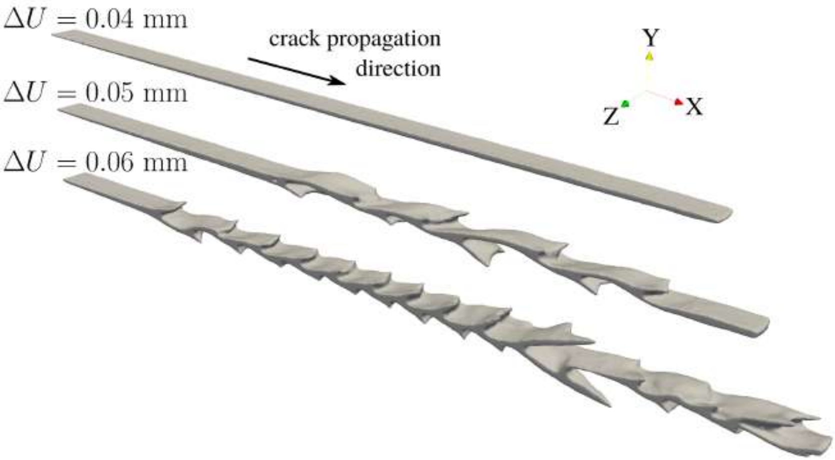

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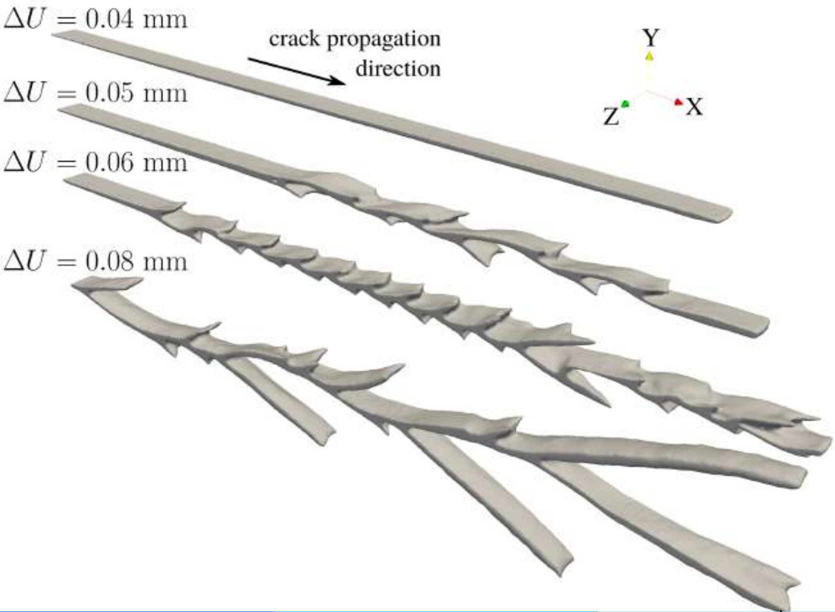

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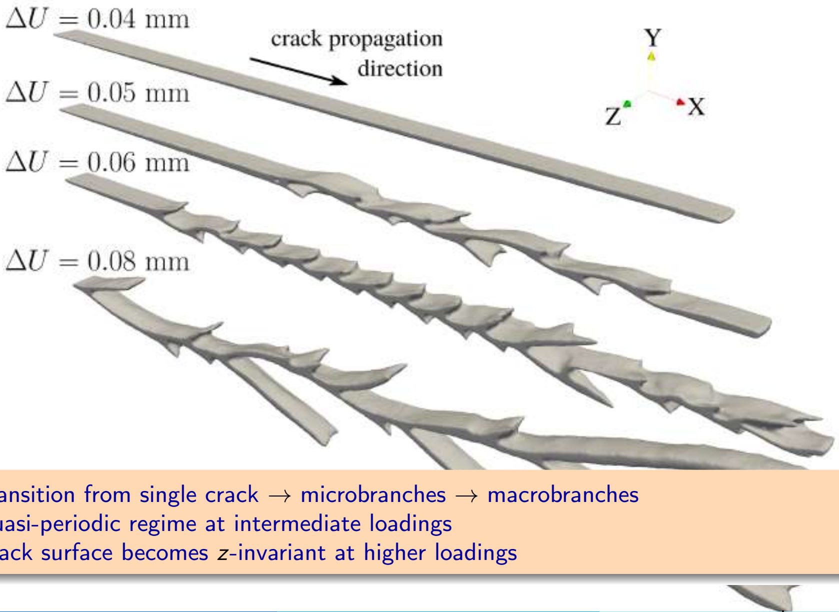

transition from single crack → microbranches → macrobranches
quasi-periodic regime at intermediate loadings
crack surface becomes z-invariant at higher loadings

Influence of plate width [Bleyer & Molinari, 2016]

same loading $\Delta U = 0.06$ mm

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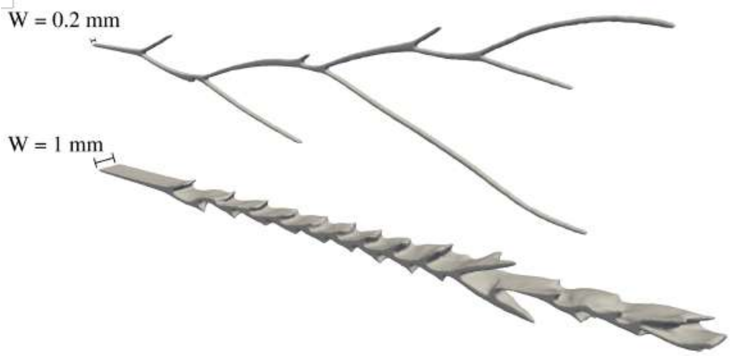

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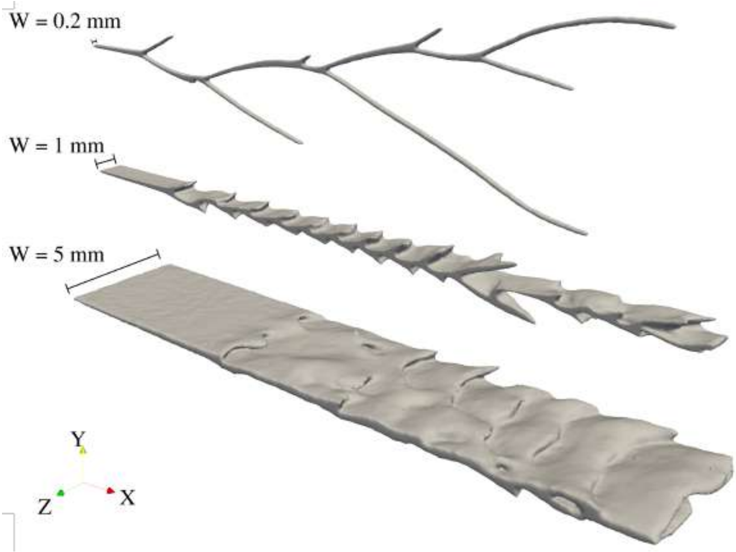

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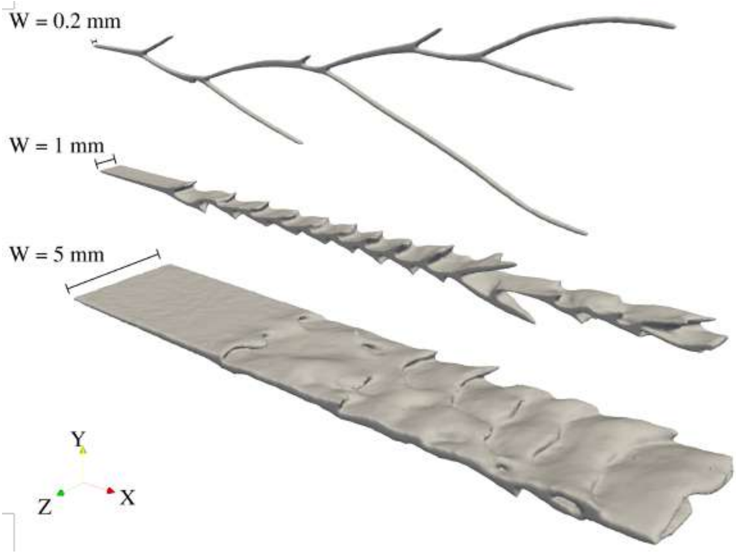
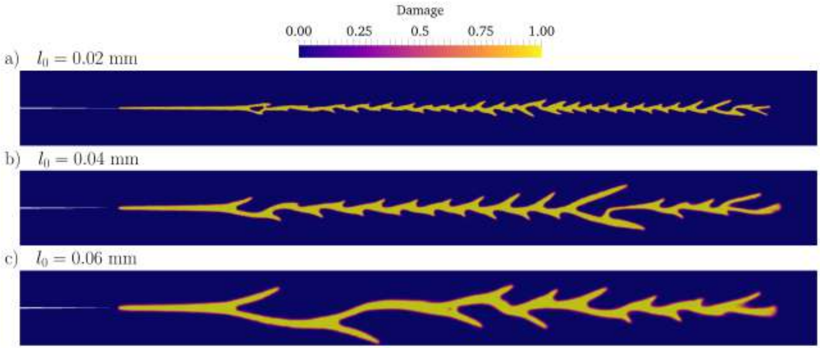


Influence of ℓ_0 [Bleyer & Molinari, 2016]

$\Delta U = 0.06$ mm, $W = 1$ mm



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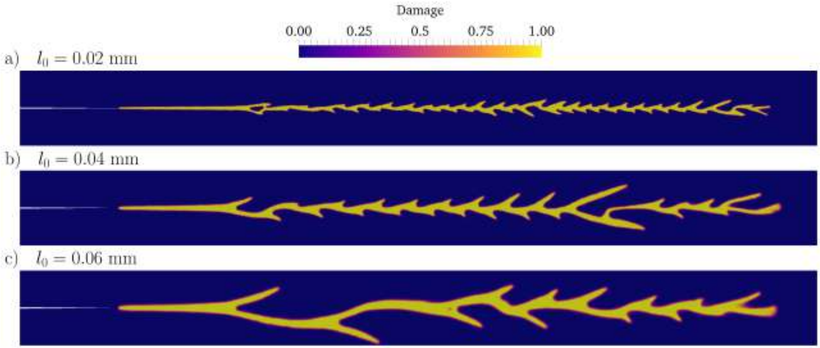

- Δx and $L_{branch} \propto \ell_0$ on average
- dissipated energy almost identical ($\pm 2\%$)!
- no microbranches when ℓ_0 is too large ($\approx W/10$)

Outline

Conclusions

An extremely efficient and popular method

- today's method of choice for simulating fracture
- many extensions: ductile, fatigue, anisotropic, hydraulic fracture...
- simple finite element implementation
- reproduces complex physical phenomena of fracture, some that no other models seem able to do so

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- today's method of choice for simulating fracture
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Open questions and challenges

- we do not compute global minima: physical relevance of critical points ?
- mathematical proofs for extensions by mechanicians (dynamics, cohesive fracture, anisotropy)
- crack interpenetration
- numerical cost (mesh size $h < \ell_0$)

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