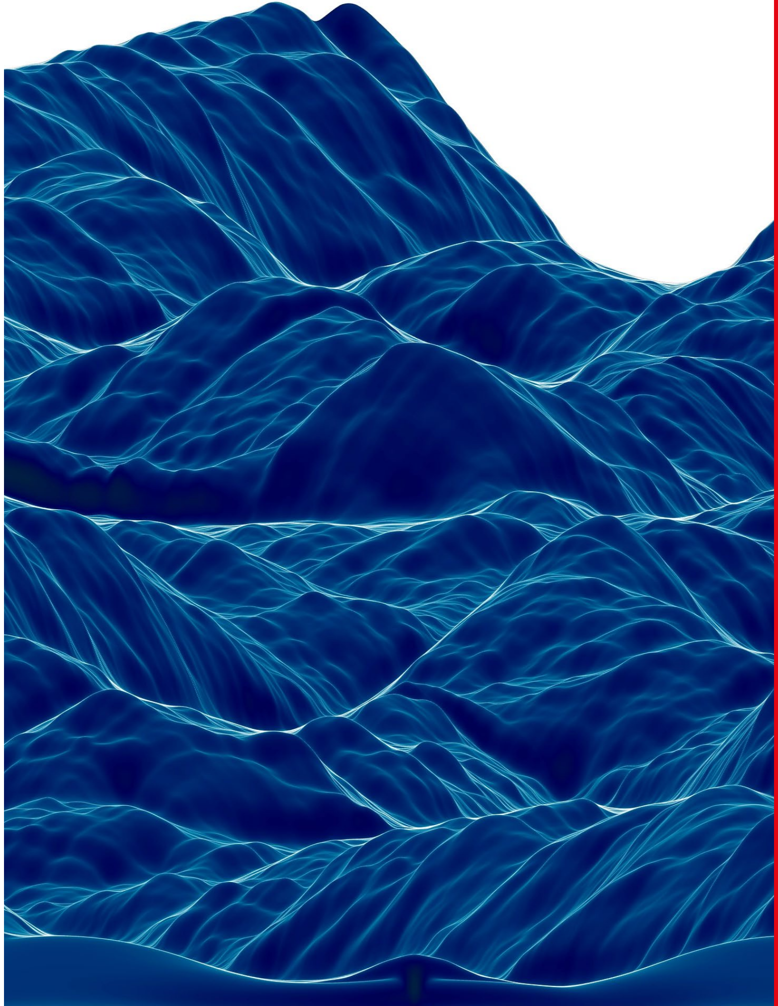


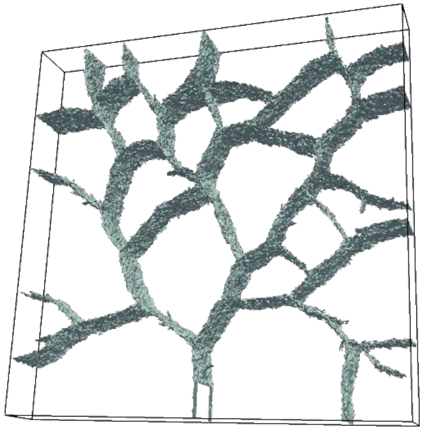
FE modeling of fracture mechanics

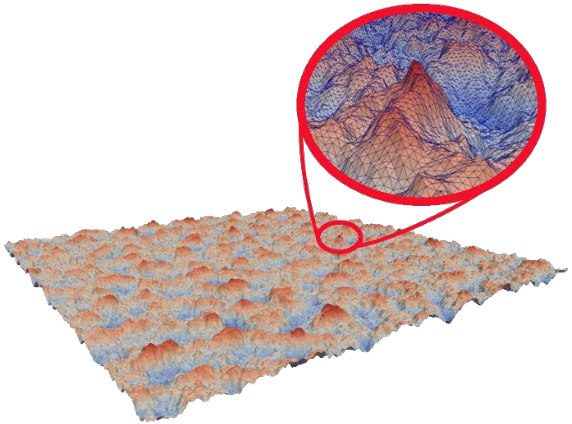
Computational Solid Mechanics Laboratory
lsms.epfl.ch
Director: J.F. Molinari

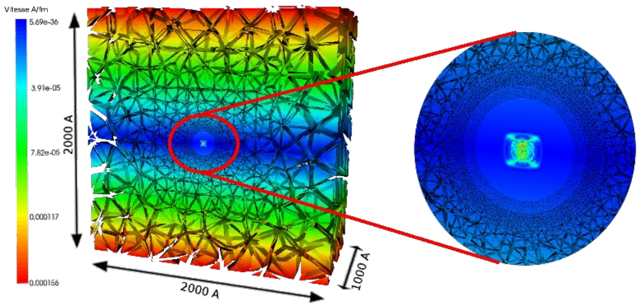
Affiliated with
ENAC (Civil Engineering)
and STI (Materials Science) schools at EPFL

LSMS activities

- Mechanics of materials and structures
- Interdisciplinary research (civil engineering, mechanics, materials science, geoenginering and geophysics, scientific computing, applied mathematics)
- Theory and simulations (and experiments through collaborations)
- Alumni LSMS – LSMS - EPFL
- Two main areas: damage mechanics and tribology across scales







Numerical simulations: software at LSMS

- Track record of development of novel numerical methods and open-source software (extensive V&V; all on GitLab; demonstrated HPC capabilities)
- Akantu Cracklet Tamaas Libmultiscale

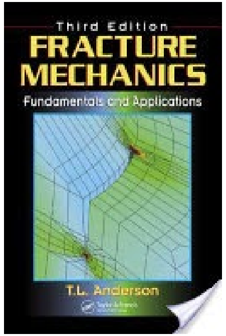
- Open-source software for granular materials, ex LAMMPS
- Two in-house codes examples:
  - Akantu: general purpose FE software (statics and dynamics, contact detection, cohesive elements, non-local continuum damage, phase-field fracture)
  - Cracklet: spectral boundary element code for elastodynamics of cracks and sliding friction (Geubelle and Rice 1995; Breitefeld and Geubelle 1998); very fast (discretization of interface only; semi-infinite elastic bodies in contact)

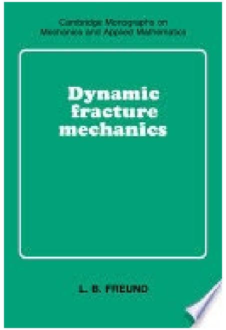

PSSST
WOULD YOU BE INTERESTED IN SOME...
?
FREE
SOFTWARE
OPEN SOURCE

Part 1: Numerical methods for modeling fracture of materials and structures

- Brief recap of LEFM
- FEM approaches for fracture mechanics
- Discrete approach : cohesive zone approach
- Non-local continuum damage and phase-field approach

Linear elastic fracture mechanics





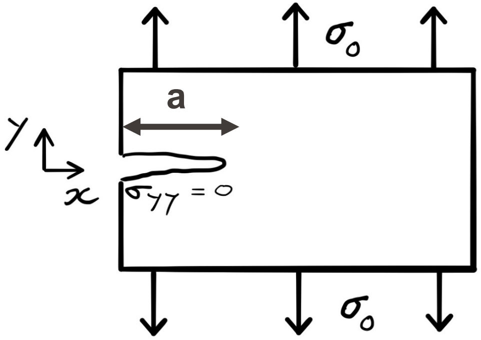
Not a class on fracture mechanics

Further reading: Anderson's or Freund's books

Defects exist in materials and structures (Inglis 1919)

Notion of damage tolerance: defects exist, will they propagate?

Mode I crack (within LEFM)



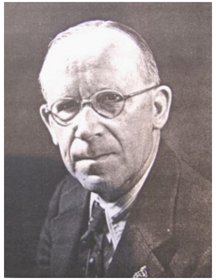
Stress drop on crack faces (zero stress)

$\Rightarrow$ Stress singularity ($1/r^{1/2}$) at crack tip

Stress intensity factor: $K_I \propto \sigma_0 \sqrt{a}$

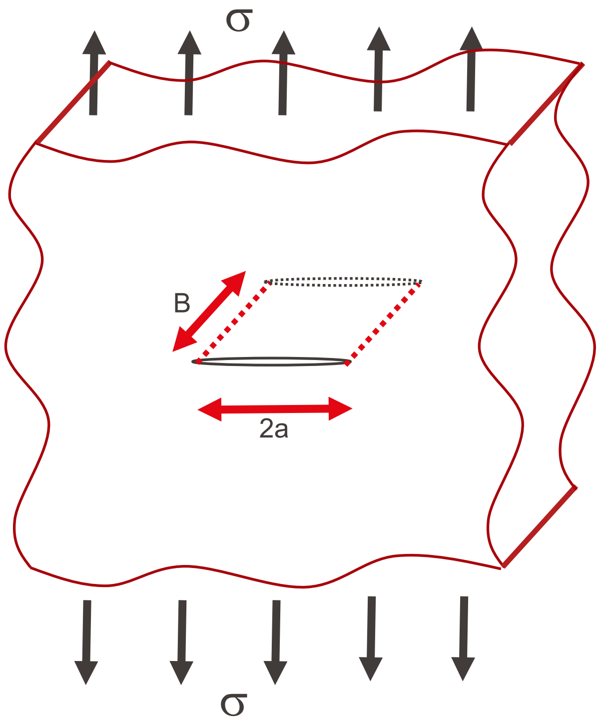
Energy balance: $G = G_c$ $\qquad G = \dfrac{{K_I}^2}{E}$

Griffith's energy criterion; global approach



Alan Arnold Griffith

Plate under far field load, through crack (1920)



Critical point for propagation of a crack

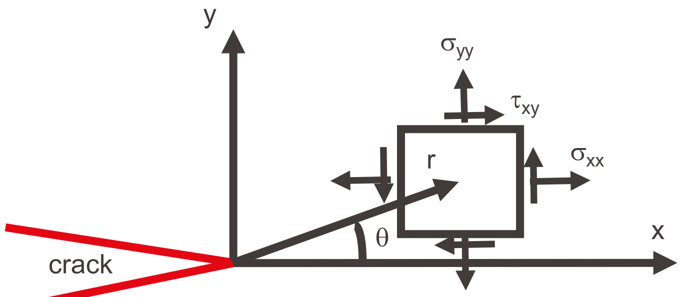
$$\frac{dE}{dA} = \frac{dE_{pot}}{dA} + \frac{dW_S}{dA} \leq 0$$

$$E_{pot} = E_{pot0} - \pi\frac{\sigma^2 a^2 B}{E}$$

$$W_S = 4aB\gamma_S = 2A\gamma_S$$

$$\boxed{\sigma_f = \sqrt{\frac{2E\gamma_s}{\pi a}}}$$

Local approach



∃ analytical solutions:
Westgaard 1939, Irwin 1957,
Sneddon 1946, Williams 1957

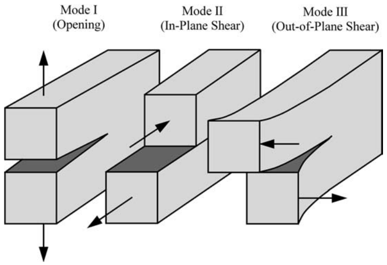
Stress intensity factor (depends on geometry and load)

$$\sigma_{ij} = \left(\frac{K}{\sqrt{2\pi r}}\right) fij(\theta) + \sum_{m=0}^{\infty} A_m \, r^{\frac{m}{2}} \, g_{ij}{}^{(m)}(\theta)$$

Limit $r \rightarrow 0,$ leading term is in $\frac{1}{\sqrt{r}}$

Stress singularity at crack tip !

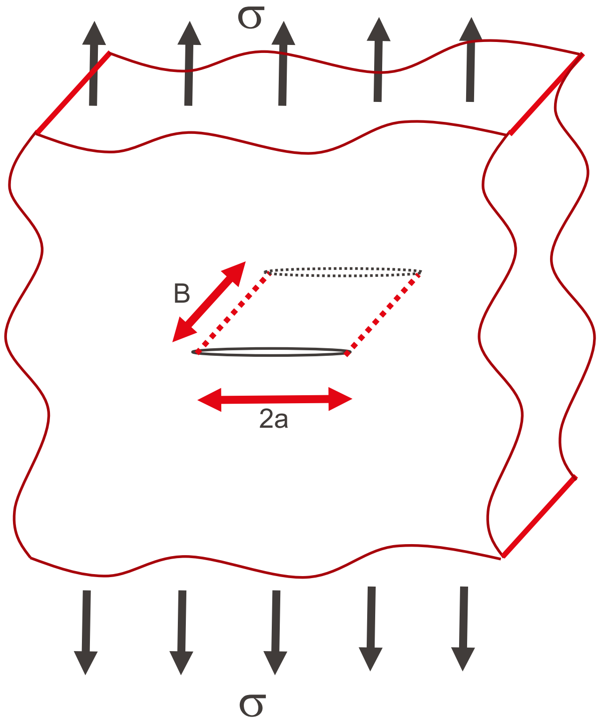
3 modes of rupture
Mode I (opening)
Mode II (in-plane shear)
Mode III (out-of-plane shear)
(image from Anderson)



$f_{ij}{}^{I}(\theta), f_{ij}{}^{II}(\theta),$ and $f_{ij}{}^{III}(\theta)$ are known adimentional functions of θ, and are independent of geometry

- Known analytical solution for through crack: $K_I = \sigma\sqrt{\pi a}$

Equivalence between local and global approach



Energy release rate:

$$G = -\frac{dE_{pot}}{dA} = \frac{\square^{2} a}{E}$$

Stress intensity factor:

$$K_I = \sigma\sqrt{\pi a}$$

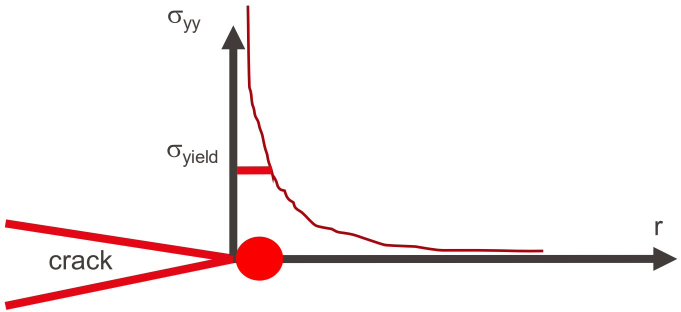
$$G = \frac{{K_I}^2}{E}$$

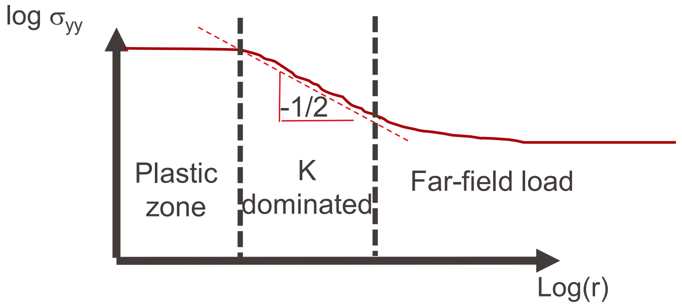
Mixed-mode:

$$G = \frac{{K_I}^2}{E'} + \frac{{K_{II}}^2}{E'} + \frac{{K_{III}}^2}{2\mu}$$

Fracture: $G = G_c$

Crack tip plasticity





If no K dominated zone (and no separation of scale), then no LEFM, and we enter the realm of finite fracture mechanics

Stress singularity at crack tip, but stresses cannot be infinite

→ Plastic zone must exist

Its size can be estimated in some cases

Example, Rice and Palmer:

$$l_z = \frac{9\pi E G_c}{32(1-\nu^2)\sigma_c^2}$$

Numerically, non-linear zone added at crack tip (cohesive zone removes singlularity)

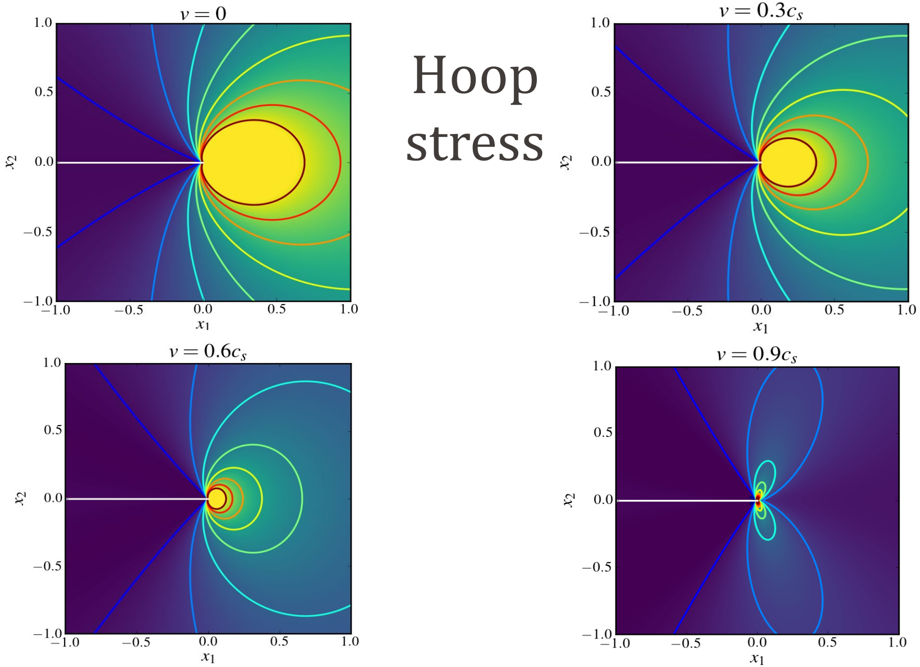
Mesh size must be smaller than this lengthscale

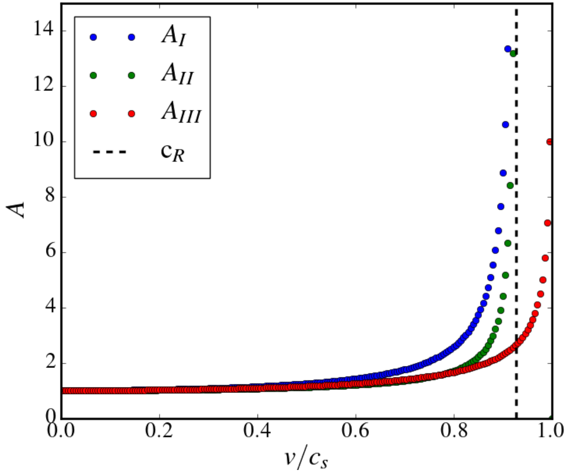
Dynamic crack propagation

Molinari

Freund 1990, Kostrov and Das 1988, process zone size shrinks with crack speed

$$G(a,v) = \frac{1-\nu^2}{E}\left[A_I(v)K_I^2 + A_{II}(v)K_{II}^2\right] + \frac{1}{2\mu}A_{III}(v)K_{III}^2$$





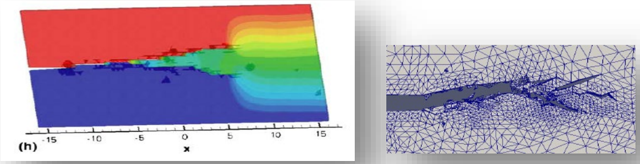
Part 1: Numerical methods for modeling fracture of materials

- Brief recap of LEFM
- **FEM approaches for fracture**
- Discrete approach : cohesive zone approach
- Non-local continuum damage and phase-field approach

A wide choice of numerical methods for fracture mechanics (beyond mesh erosion…)

Cohesive element approach (*Camacho, Ortiz, Pandolfi, Needleman …*)

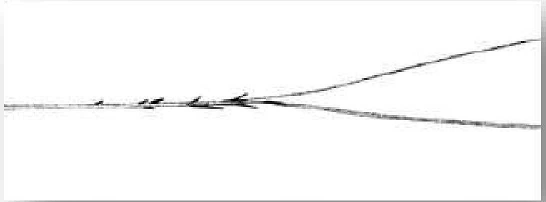
+ Crack description closest to frac. mech.
+ Ability to handle contact
- Mesh dependency (if no remeshing)



Zhou, Molinari and Shioya, Eng. Fract. Mech. (2005)

X-FEM (*Belytschko, Moës, …*)

+ No mesh dependency
- Need ad hoc criterion for crack branching

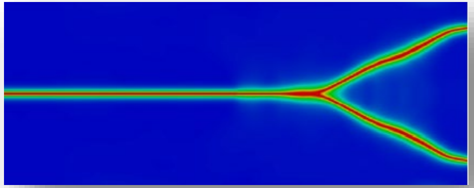


Song, Wang and Belytschko, Comput. Mech. (2008)

A wide choice of numerical methods for fracture mechanics

Phase field (*Karma, Bourdin, Marigo, Miehe, de Lorenzis…*)

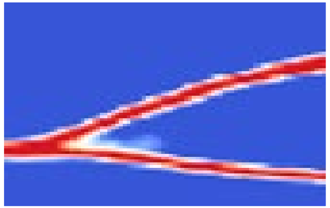
+ Crack path convergence
- Computational cost



Borden, et al., CMAME. (2012)

Classical Non-local continuum damage (*Bazant, Pijaudier-Cabot, Jirasek …*)

+ Crack path convergence
- Computational cost



+ Eigenerosion (*Ortiz Pandolfi*), **TLS** *(Moës),* **Peridynamics, MPM, CLIP...**

Discrete approach: cohesive zone model

- Cohesive zone model, Dugdale Barrenblat 1960's
- Cohesive element: Camacho Ortiz (2D) 1996, Pandolfi Ortiz (3D) 1999, Xu Needleman 1993, Rose et.al., etc…

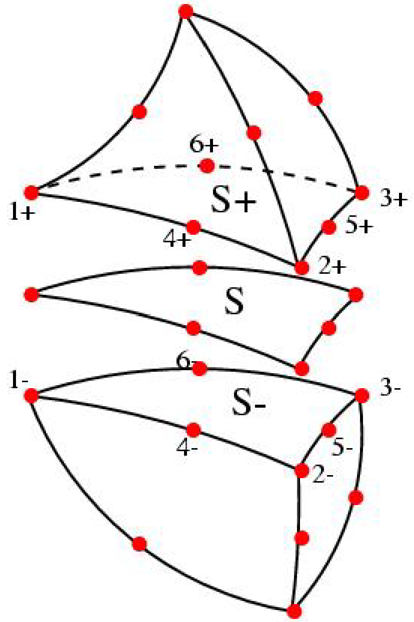
- Cohesive elements glue two neighboring elements

  Cracks created within ordinary elements boundaries (Mesh dependency)

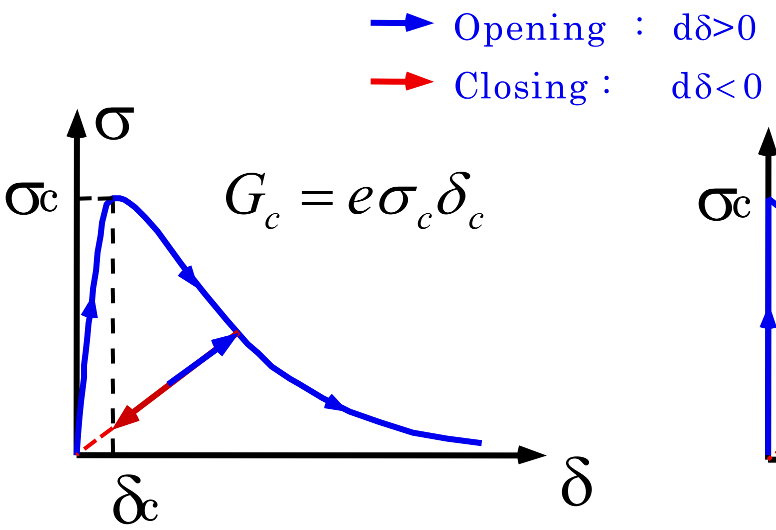
  Computationally expensive ($h_{FE} < l_Z < W$)
- Cracks explicitly described by cohesive elements

  Easy to handle branching, fragmentation

  Can incorporate contact
- The opening/closing properties of cohesive elements are governed by a cohesive law

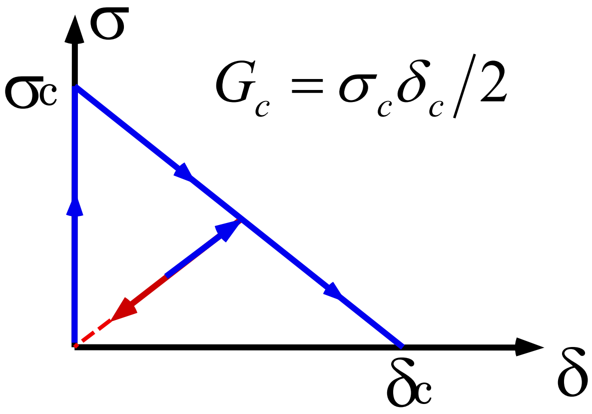


Two classical cohesive laws



Intrinsic exponential irreversible model (Smith-Ferrante Law)

Physically reasonable but modifies structural response



Extrinsic linear irreversible model (Camacho Ortiz)

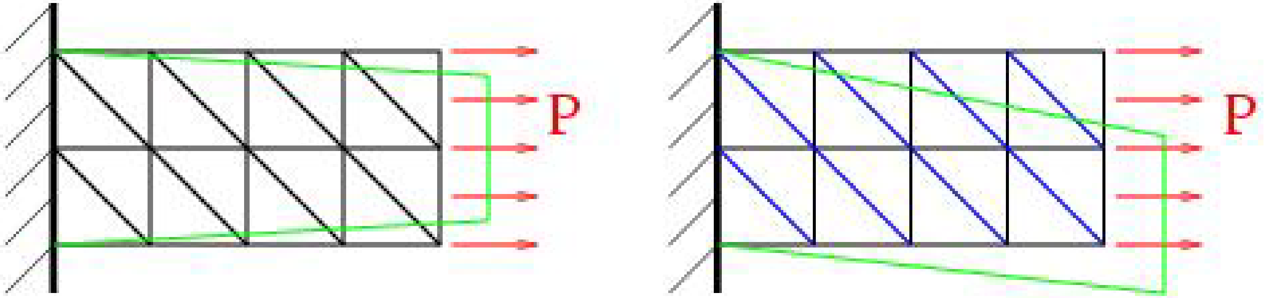
Does not modify elastic properties

Needs to be introduced dynamically

Why extrinsic is often a better choice

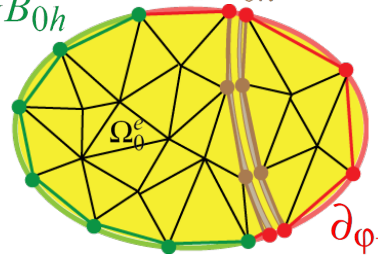
- Introduce a cohesive element if at a given time the opening forces applied on a facet (adjacent to two elements) is larger than a critical traction
- This is computationally challenging (particularly if mesh partition on parallel computers):

  3D dynamic insertion ➡ keep track of facets, edges, duplicated nodes…
- Can create stress perturbations
- But results in computational savings
- And removes “cohesive elements induced” mesh anisotropy

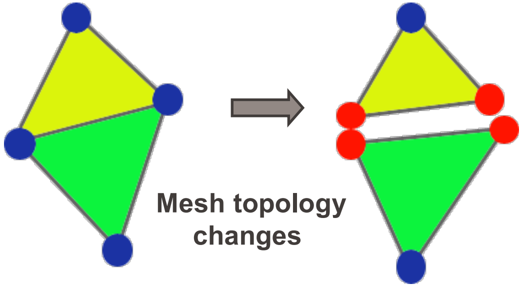


EPFL

FEM implementation (PVW)



Dynamic insertion of cohesive elements



Space discretization: $$B_{0h} = \bigcup_{e=0}^{N} \Omega_0^e$$

Continuum term

$$\int_{B_{0h}} \left(\rho_0\, \ddot{\varphi}_h\, \delta\varphi_h + P_h : \nabla_0 \varphi_h\, \delta\varphi_h \right) dV - \int_{\partial_N B_{0h}} \bar{T}\, \delta\varphi_h dS - \int_{B_{0h}} \rho_0\, B\, \delta\varphi_h dV$$

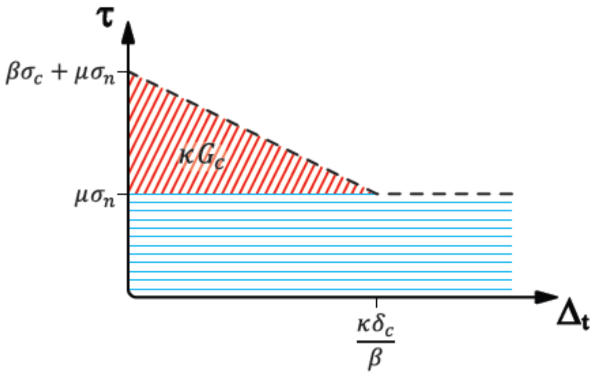
Cohesive term

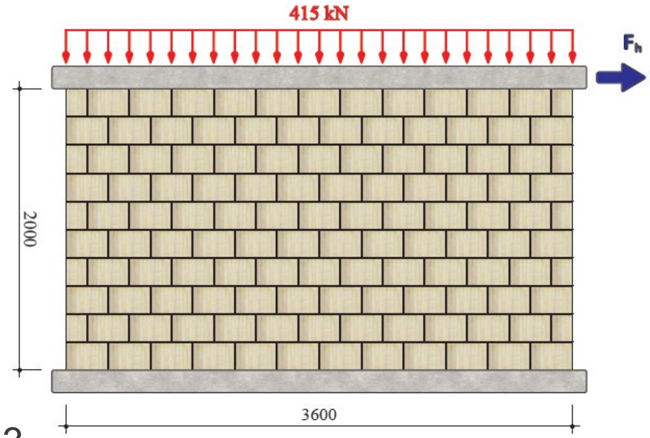
$$+ \int_{\partial_I B_{0h}} T([\![\varphi_h]\!])\, [\![\delta\varphi_h]\!] dS = 0$$

Jump operator:

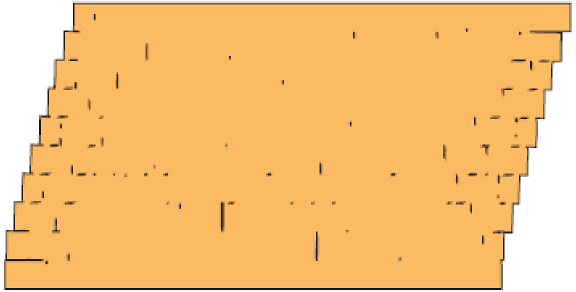
$$[\![\bullet]\!] = \bullet^+ - \bullet^-$$

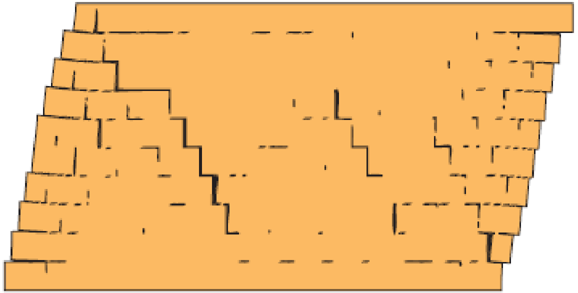
Ex: masonry wall subject to seismic load





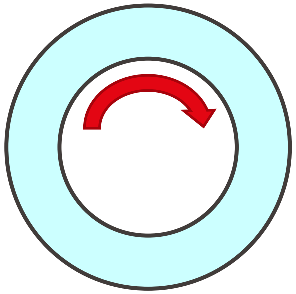
Snozzi, Molinari, IJNME, 2013
Masonry wall loaded in shear at two loading rates





But beware: mesh dependency of crack path

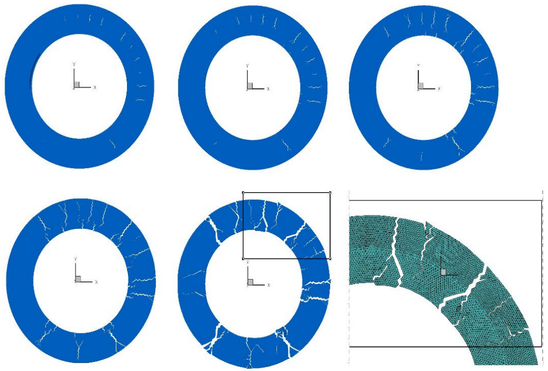
Fragmentation of a rotating brittle ceramic (SiN) ring under centrifugal force



Symmetry: Mesh dependency of fracture paths if no adaptive meshing

Hoop stress maximum at inner radius: cracks initiate there and propagate outward

Strange:



Pathological mesh dependency!

Not only crack paths depend on mesh

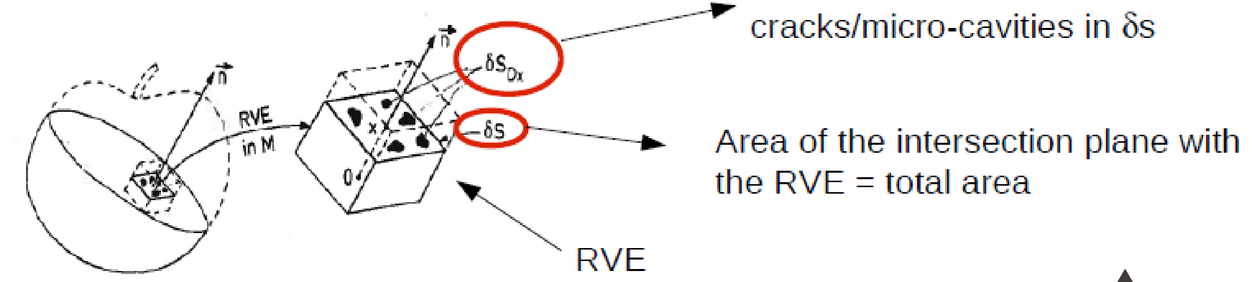
But they initiate in middle of ring
(where small elements are perpendicular to load)
(can be fixed: “Weibull” cohesive elements, Zhou Molinari, IJNME, 2004)

Part 1: Numerical methods for modeling dynamic fracture of materials

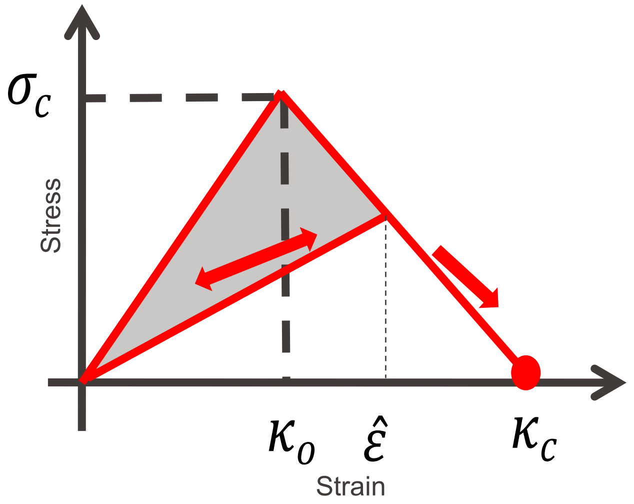
- Brief recap of LEFM
- Many FEM approaches for dynamic fracture
- Discrete approach : cohesive zone approach
- **Non-local continuum damage and phase-field approach**

Continuum damage mechanics

1D surface damage variable



From a course on damage mechanics, J. Lemaitre



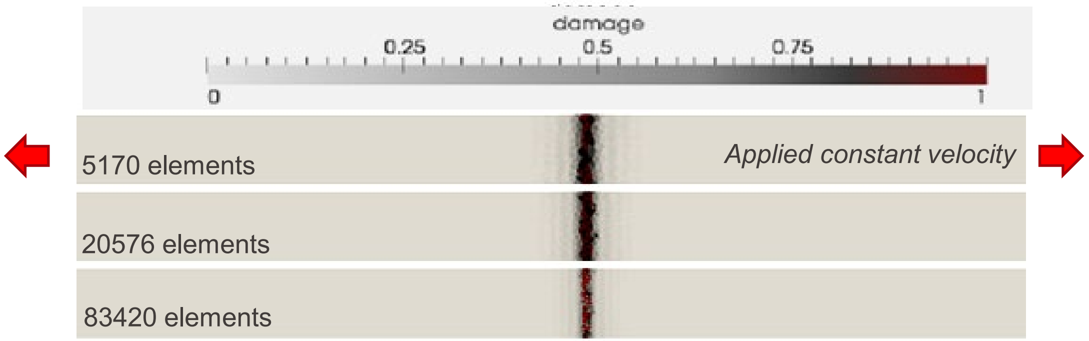
Definition of continuous damage variable (Kachanov 58):

D between 0 and 1

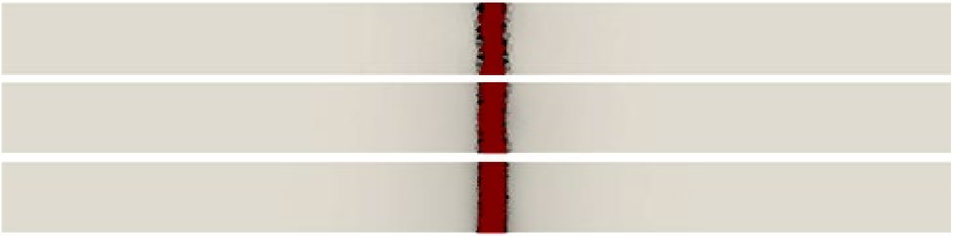
$$\bar{\sigma} = (1 - D)\bar{\bar{\bar{E}}} : \bar{\varepsilon}$$

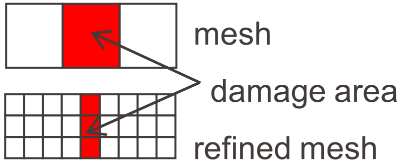
Many variations beyond this scalar definition of D

Local versus non-local continuum damage

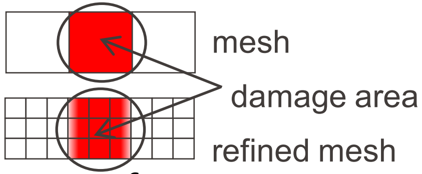


Several methods to avoid localization
Gradient, Delay, **Integral type** (for illustration)…
Requires choice of interaction length scale





Ill-posed problem:
equilibrium balance
becomes elliptic in dynamics



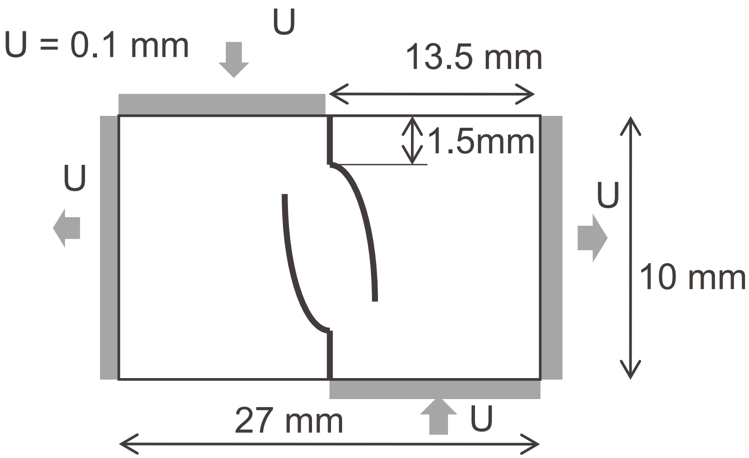
$$\varepsilon_{eq}^{nl}(\vec{x}) = \int_{\Omega} \alpha(\vec{x},\vec{s})\varepsilon_{eq}(\vec{s})d\vec{s}$$

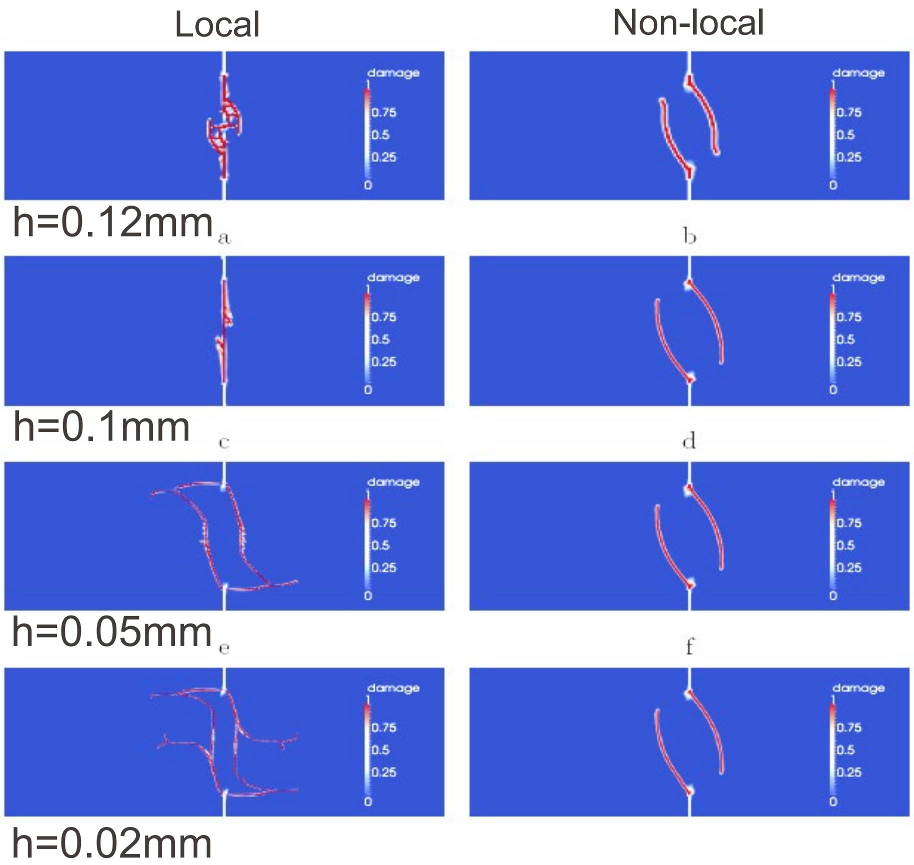
Pijaudier-Cabot and Bazant, J. Eng. Mech. (1987)

NL damage; mesh convergence

Nooru Mohamed test

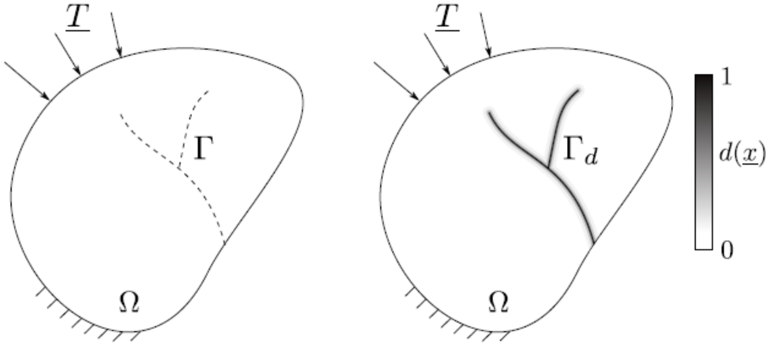
Wolff Richart Molinari, IJNME, 2015

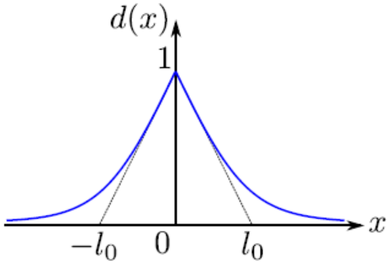




Phase-field: variational approach to fracture

The crack discontinuous topology is regularized by a **continuous** phase-field function $d(\underline{x}) \in [0;1]$ and a length scale l_0





$$l_0^2 \Delta d - d = 0 \quad \Longrightarrow \quad \min \Gamma_{l_0}(d) = \int_\Omega \left(\frac{d^2}{2l_0} + \frac{l_0}{2} \|\nabla d\|^2 \right) d\Omega$$

Better suited for :

- complex crack paths : dynamic crack branching, instabilities
- crack propagation in heterogeneous media
- multiphysics coupling

Phase-field: variational approach to fracture

Francfort and Marigo; Bourdin, Francfort and Marigo, J of Elasticity, 2008

$$E(\underline{u}, \Gamma) = \int_{\Omega \backslash \Gamma} \psi(\underline{\epsilon}) d\Omega + g_c |\Gamma|$$

The state at t_{n+1} is obtained as :

$$\min E(\underline{u}, \Gamma) \quad \forall \underline{u} \in KA(\Gamma, t_n) \text{ and } \Gamma \supseteq \Gamma_n$$

alleviates some limitations of Griffith theory but is ill-posed
$\Rightarrow$ regularization of the crack surface with a phase-field

$$\min E(\underline{u}, \Gamma_d) \quad \forall \underline{u} \in KA(\Gamma_d, t_n) \text{ and } \Gamma_d \supseteq \Gamma_{dn}$$

where

$$E(\underline{u}, \Gamma_d) = \int_{\Omega} \psi(\underline{\epsilon}, d) d\Omega + g_c \int_{\Omega} \left(\frac{d^2}{2 l_0} + \frac{l_0}{2} \|\nabla d\|^2 \right) d\Omega$$

irreversibility : $\dot{d} \geq 0$
strong link with **damage gradient models**

Phase-field: variational approach to fracture

$d(\underline{x})$ is viewed as a scalar **damage variable**

- elastic energy density $\psi(\underline{\underline{\varepsilon}}, d)$
- dissipated energy density $w(d) + w_1 l_0^2 \|\underline{\nabla} d\|^2$ with $w_1 = w(1)$
- irreversible damage $\dot{d} \geq 0$

variational principle which yields :

$$\begin{aligned} \underline{\underline{\sigma}}(d) &= \partial_\varepsilon \psi(\underline{\underline{\varepsilon}}, d) \\ \rho \underline{\ddot{u}} &= \mathrm{div}(\underline{\underline{\sigma}}(d)) + \underline{f} \\ d &= \arg\min_{\dot{d} \geq 0} \int_\Omega \psi(\underline{\underline{\varepsilon}}, d) d\Omega + \int_\Omega (w(d) + w_1 l_0^2 \|\underline{\nabla} d\|^2) d\Omega \end{aligned}$$

Proven convergence in statics to Griffith when $l_0/L \to 0$

Resolution algorithm : alternate minimization

At fixed u_n, solve for d_{n+1} (constrained optimization for irreversibility)
At fixed d_{n+1}, solve for u_{n+1} : elastodynamics problem with degraded stiffness

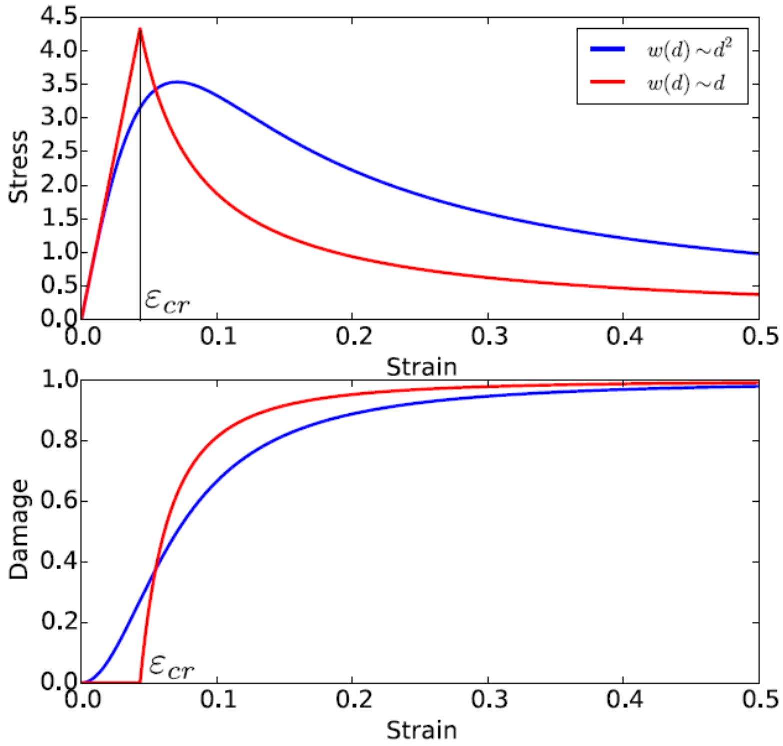
Phase-field: variational approach to fracture

- Stiffness degradation function (isotropic)
  - symmetric $\psi(\underline{\underline{\varepsilon}}, d) = a(d)\psi(\underline{\underline{\varepsilon}})$ with $a(d) = (1-d)^2$
  - unsymmetric [Lancioni and Carfagni, 2009]
    $\psi(\underline{\underline{\varepsilon}}, d) = a(d)\psi^+(\underline{\underline{\varepsilon}}) + \psi^-(\underline{\underline{\varepsilon}})$ with $\psi^+(\underline{\underline{\varepsilon}}) = \frac{\kappa}{2}\langle \mathrm{tr}\,\underline{\underline{\varepsilon}}\rangle_+^2 + \mu\underline{\underline{\varepsilon}}^d : \underline{\underline{\varepsilon}}^d$ and
    $\psi^-(\underline{\underline{\varepsilon}}) = \frac{\kappa}{2}\langle \mathrm{tr}\,\underline{\underline{\varepsilon}}\rangle_-^2$
  - unsymmetric with positive/negative parts of eigenstrains [Miehe and Lambrecht., 2001]

- Dissipation function
  - $w(d) = \dfrac{g_c}{2l_0}d^2$: most widely used model in phase-field literature [Miehe, Borden,...]
  - $w(d) = \dfrac{3g_c}{8l_0}d$: [Pham et al., 2010]

Phase-field: variational approach to fracture

Response to a 1D homogeneous test (same g_c/l_0)



- presence/absence of a purely elastic phase

Implementation choices

Bleyer Roux-Langlois Molinari, IJF, 2017 and Bleyer Molinari, APL, 2017

Many constitutive modeling choices are possible, we follow [Li et al., 2016]

- elastic strain energy density :

$$\psi(\underline{\underline{\varepsilon}}, d) = (1-d)^2 \left(\frac{\kappa}{2} \langle \mathrm{tr}\, \underline{\underline{\varepsilon}} \rangle_+ + \mu \underline{\underline{\varepsilon}}^d : \underline{\underline{\varepsilon}}^d \right) + \frac{\kappa}{2} \langle \mathrm{tr}\, \underline{\underline{\varepsilon}} \rangle_-$$

- non-local fracture energy :

$$w_{frac}(d, \underline{\nabla d}) = \frac{3G_c}{8l_0} \left(d + l_0^2 \|\underline{\nabla d}\|^2 \right)$$

Remark : existence of an elastic phase for this model

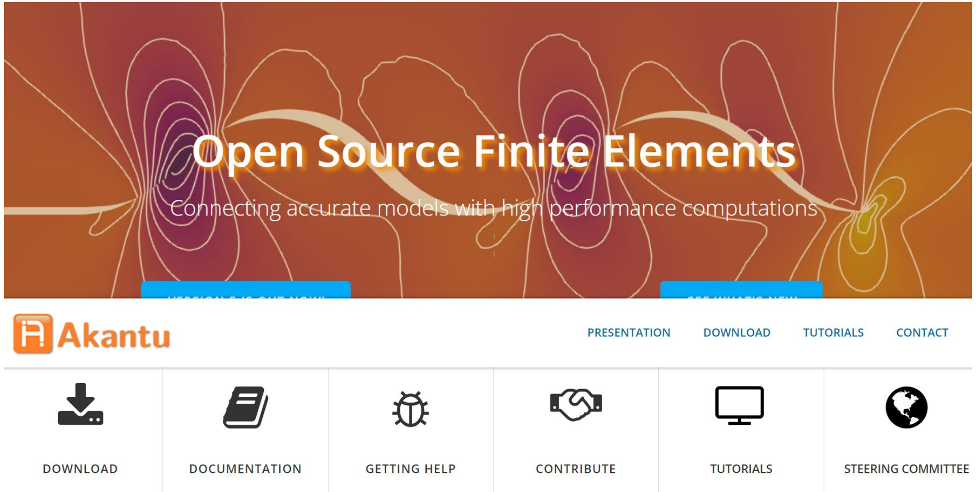
Numerical resolution using a staggered approach :

- minimization of total energy with respect to u : explicit dynamics
- minimization with respect to d : quadratic function with bound constraints ($d_n \leq d_{n+1} \leq 1$) to enforce damage irreversibility

Part 2: Introduction to FE software Akantu

Molinari

- Why Akantu ? Why open source ?
- History and structure
- Example of ongoing project exploiting specific features of Akantu (akantu.ch)
- Tutorials



General considerations on FE software

- Big business: ex. Dassault Systèmes (3,5 billions €)
- **Commercial software :** Ansys, Abaqus, Comsol, …

😇 Stable, robust, certified : great for industry

☹ Cost, “black box”, slow evolution

- **Academic software :** agile but confidential, tailored for specific pbs (Ex: Akantu has unique features for contact and damage mechanics)
- **Our philosophy:**

Knowledge creation and transmission for the greater good (tax payer money)

Open-Source Software development

Timeline of Akantu

2007
Start of LSMS at EPFL
Anciaux (CS backround) is hired

2009
ERC Grant: Open Finite Element
Software as a deliverable

2010
Richart is hired (CS)
First commit of Akantu

2012
V1.0

2016
V2.3
- Python Interface

2020
GitLab

2021
Steering Committee

2022
V4.0
Tutorials

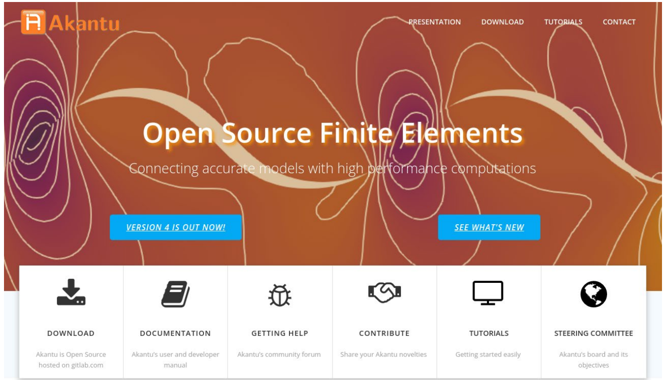
2023
V5.0
C++ 17, Eigen

Akantu today

- 13 years of development
- C++ code with a python interface
- High performance parallel computing
- Hosted on GitLab

(continuous integration and delivery with GitLab tools)

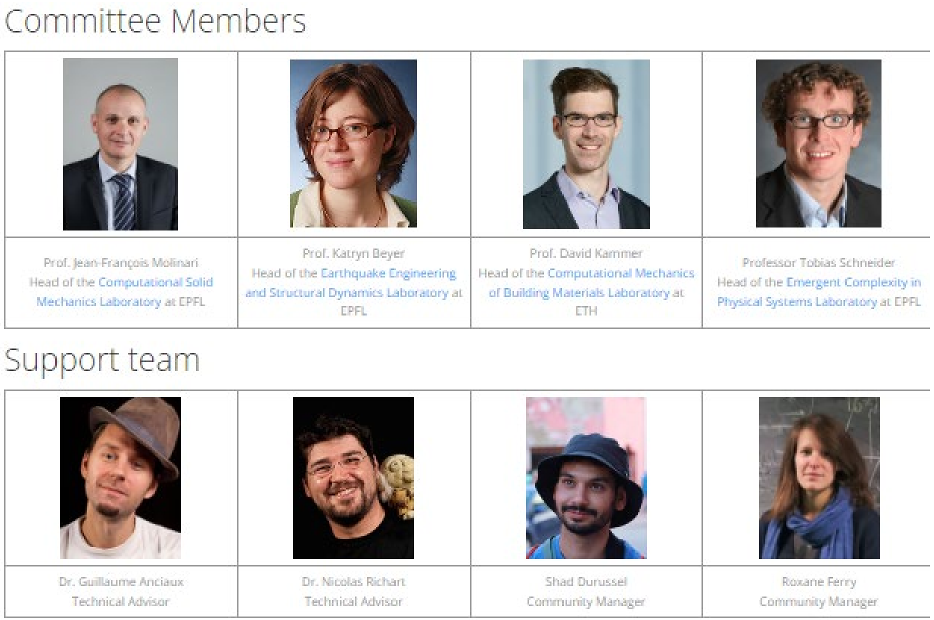
- Full documentation online
- Issues Review and Merge Requests
- Online tutorials on notebooks



- Currently on version 5.0.7
- ~ 110,000 lines of code
- ~ 7,900 commits
- 50+ contributors
- JOSS publication
- https://akantu.ch

Organization

- Steering committee (since 2021)
  - Organize and prioritize the development of new features
  - Guide strategic code changes for performance and multi-physics
- Nurture the broader Akantu’s community by organizing workshops and discussions
- Give personalized support



Akantu's future

- **Steps for community growth**
  - Better visibility of papers published through Akantu (including paper in JOSS)
  - Code dissemination in the academic community and industry
  - Tutorials and events to connect users
- **Use in a teaching environment**
- **Use in industry**
- **Sustainable funding**
- **Valuation / rewarding of developers and contributors ?   (DORA convention)**

Benefits; worth the effort

Reproducibility in science

Transparency

Efficiency

Transfer of knowledge

Sustainability

Visibility

Tutorials and examples

- **Are you a hard core programmer?**
  - Access to source code on gitlab; C++
- **Are you a proficient user ?**
  - Interact with code with Python interface (see online tutorials)
- **Or are you more interested in direct applications ?**
  - Wait for GUI ? 2024 or 2025
  - Or contact LSMS and we can prepare tailor made application for you
  - Some quick simple examples on streamlit: https://cas-eth-ser-molinari.streamlit.app/

Part 3: Applications of Akantu

ASR damage

Multiscale modeling of damage in hydroelectric dams induced by Alkali-Silica-Reaction

EPFL - LSMS
- Lucas Fourel
- Jean-François Molinari

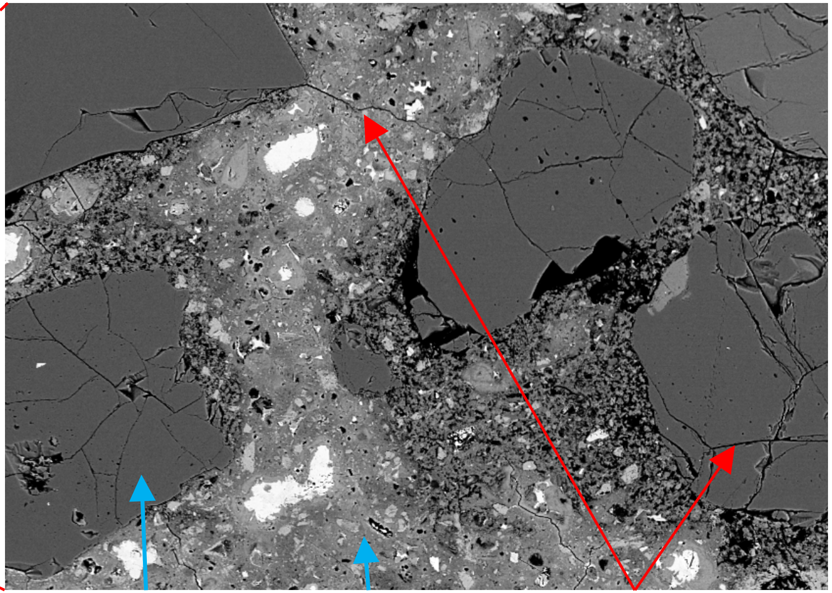
Swiss Federal Office of Energy
- Russell Gunn

Dam operators
- RELL
- Alpiq

Illsee dam, Valais, Switzerland

Concrete mesostructure

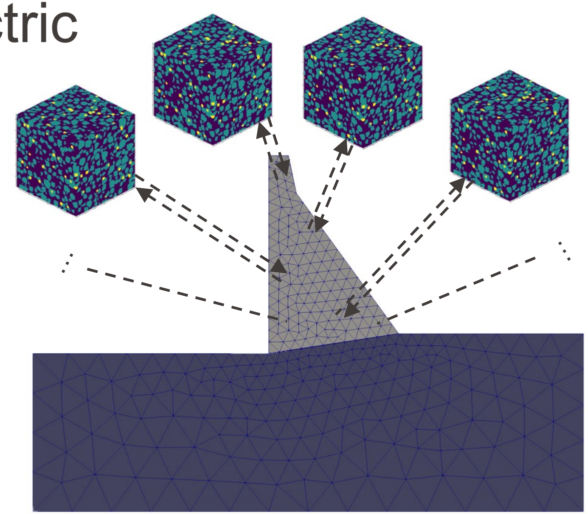
Dunant, 2009



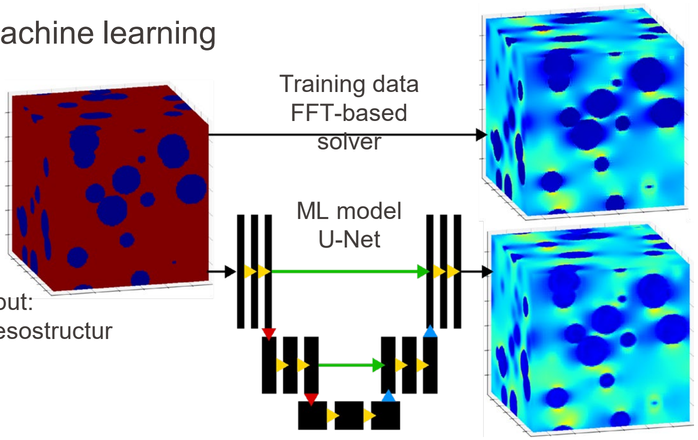
Multiscale modeling of damage in hydroelectric dams induced by Alkali-Silica-Reaction

FFT based solver: chemical swelling + damage

Multiscale approach: FE-FFT



Machine learning



Output:
Stress
distribution

Target

Input:
Mesostructur
e

Prediction