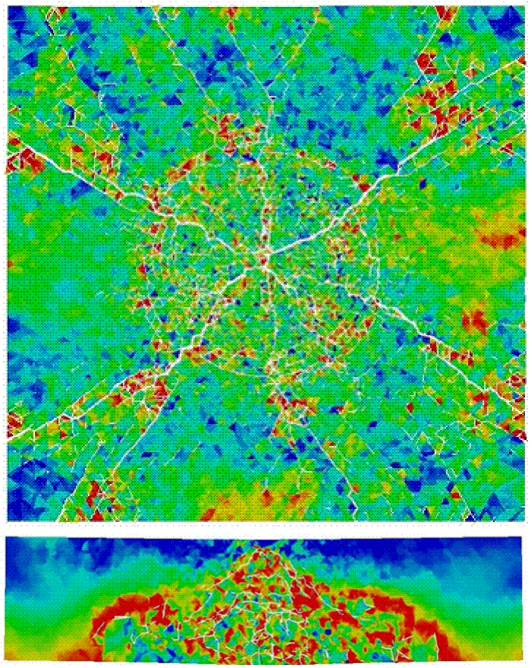
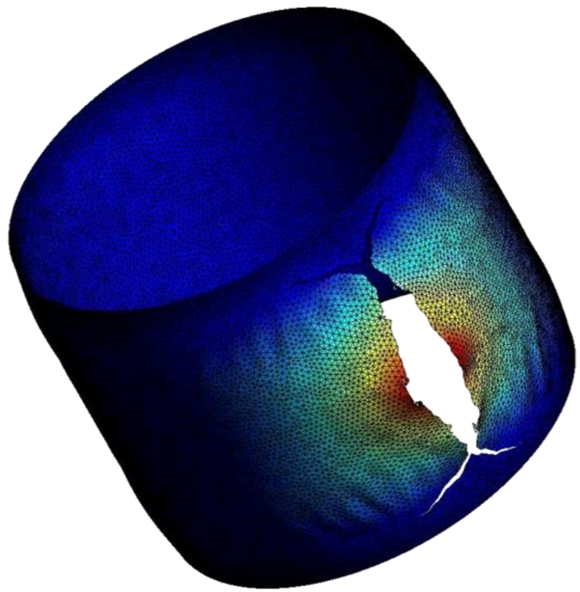
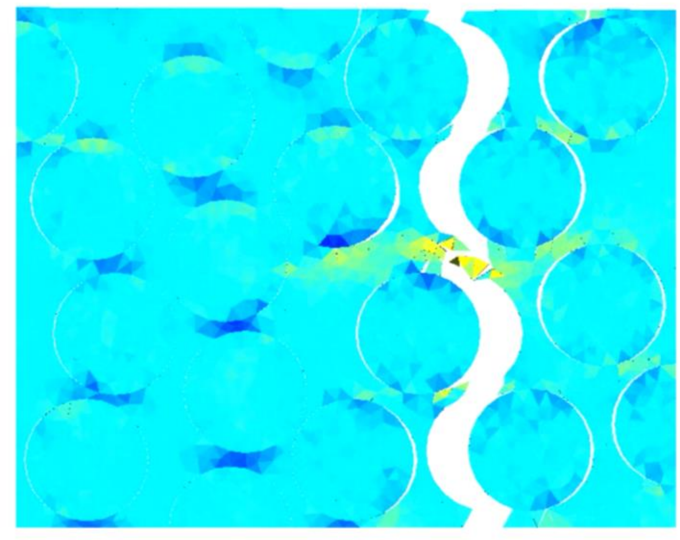
University of Liège
Aerospace & Mechanical Engineering

Computational Fracture Mechanics

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- Some fracture mechanics principles
  - Brittle/ductile materials & Fatigue
  - Linear elastic fracture mechanics
- Computational fracture mechanics for brittle materials
  - Crack propagation
  - Cohesive models
  - XFEM
- Computational fracture mechanics for ductile materials
  - Damage models
- Multiscale methods
  - Composite materials
  - Atomistic models

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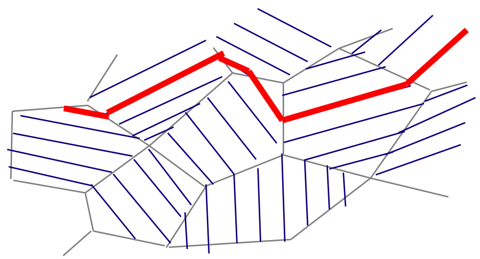
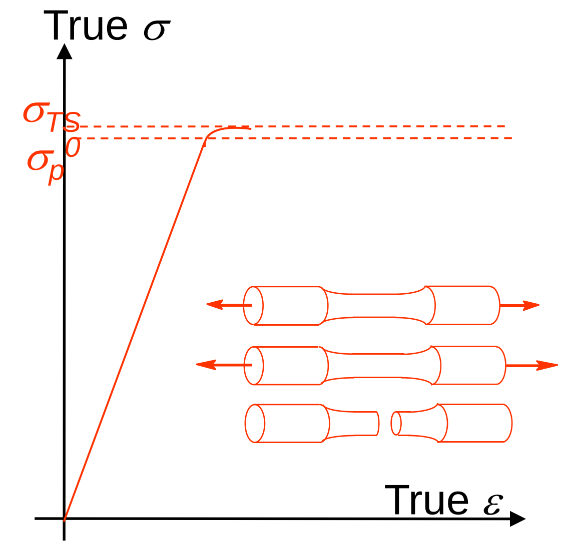
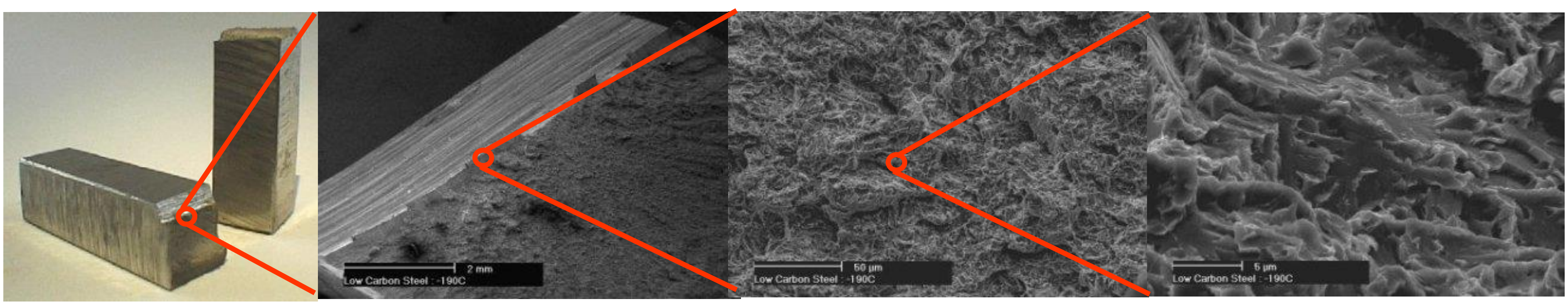
Brittle / ductile fracture

- Mechanism of brittle failure
  - (Almost) no plastic deformations prior to the (macroscopic) failure
  - Cleavage: separation of crystallographic planes
    - In general inside the grains
    - Preferred directions: low bonding
    - Between the grains: corrosion, H_2, …
  - Rupture criterion
    - 1920, Griffith: $\sigma_{\mathrm{TS}}\sqrt{a} \div \sqrt{E\,2\gamma_s}$



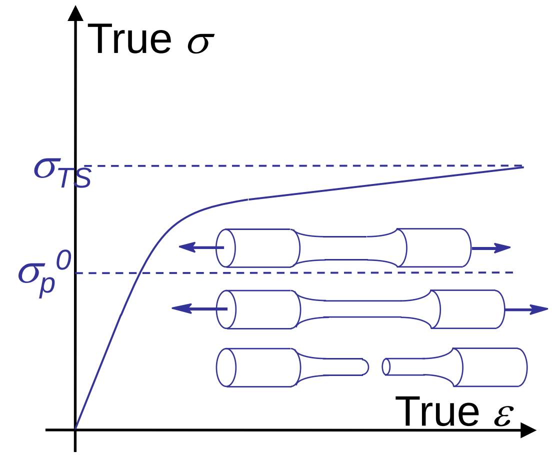


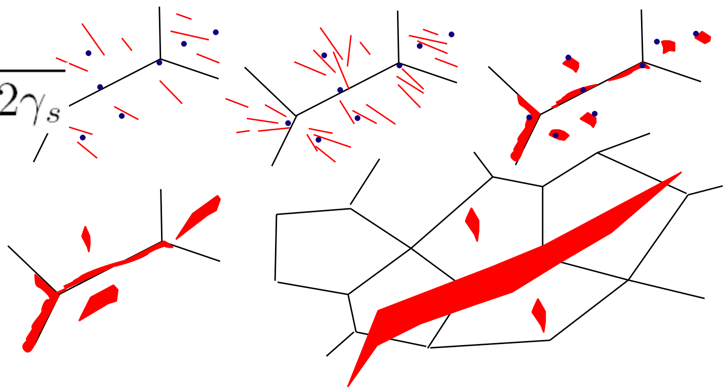


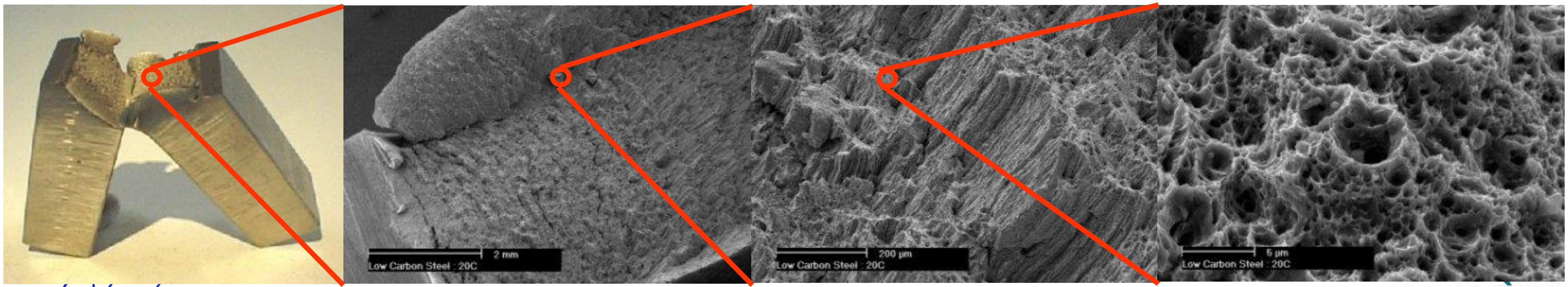
Brittle / ductile fracture

- Mechanism of ductile failure
  - Plastic deformations prior to (macroscopic) failure of the specimen
    - Dislocations motion
      - ⇒ void nucleation around inclusions
      - ⇒ micro cavity coalescence
      - ⇒ crack growth
  - Failure criterion
    - What about Griffith criterion $\sigma_{\mathrm{TS}}\sqrt{a} \div \sqrt{E\,2\gamma_s}$
    - 1950, Irwin, the plastic work at the crack tip should be added to the surface energy:

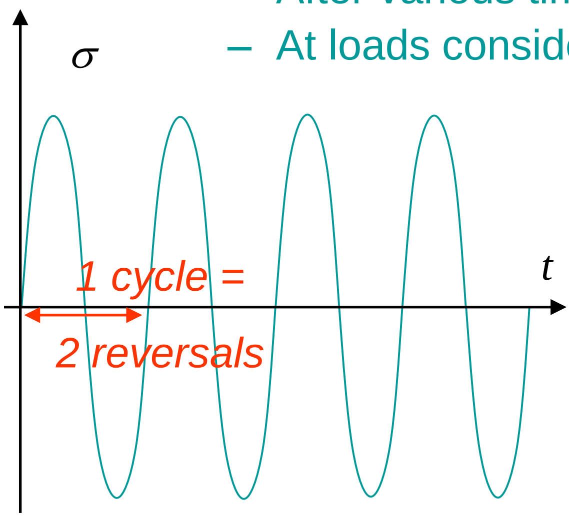
$$\sigma_{\mathrm{TS}}\sqrt{a} \div \sqrt{E\left(2\gamma_s + W_{\mathrm{pl}}\right)}$$

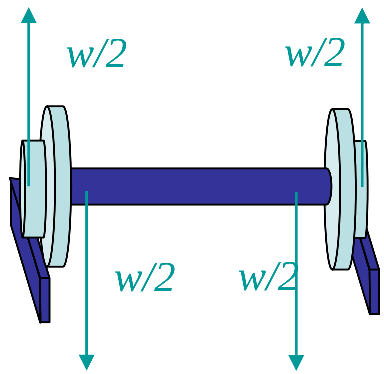






- In static: design with stresses lower than
  - Elastic limit (σ_p^0) or
  - Tensile strength (σ_{TS})
- ~1860, Wöhler
  - Technologist in the German railroad system
  - Studied the failure of railcar axles
    - Failure occurred
      - After various times in service
      - At loads considerably lower than expected

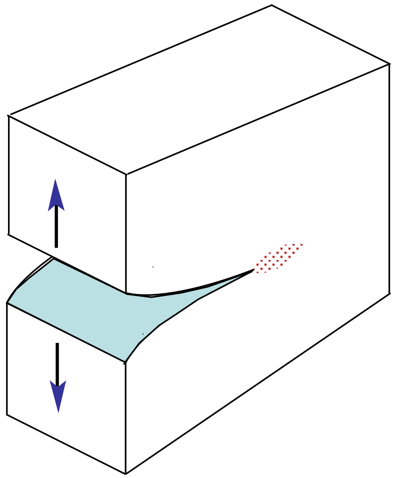




    - Failure due to cyclic loading/unloading
  - « Total life » approach
    - **Empirical** approach of fatigue

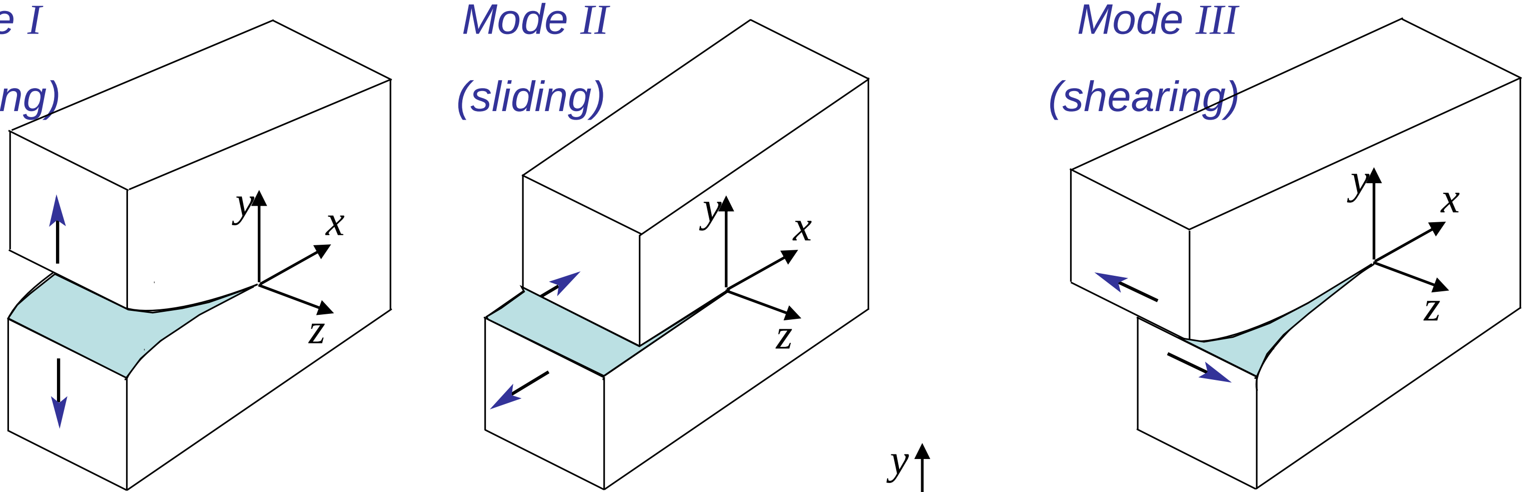
- Definition of elastic fracture
  - Strictly speaking:
    - During elastic fracture, the only changes to the material are atomic separations
  - As it never happens, the pragmatic definition is
    - The process zone, which is the region where the inelastic deformations
      - Plastic flow,
      - Micro-fractures,
      - Void growth, …

      happen, is a small region compared to the specimen size, and is at the crack tip
  - Valid for brittle failure and confined plasticity (Small Scale Yielding)

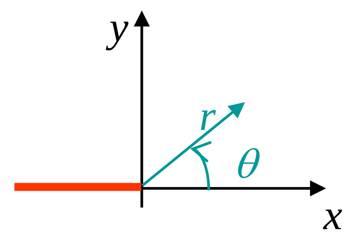


- Singularity at crack tip for linear and elastic materials
  - 1957, Irwin, 3 fracture modes

Mode I *(opening)* — *Mode II* *(sliding)* — *Mode III* *(shearing)*



- Boundary conditions



Mode I

$$\begin{cases} \boldsymbol{\sigma}_{zz} = 0 \quad \text{or } \boldsymbol{\varepsilon}_{zz} = 0 \\ \boldsymbol{\sigma}_{yy}(\theta = \pm\pi) = 0 \\ \boldsymbol{\sigma}_{xy}(\theta = \pm\pi) = 0 \\ \boldsymbol{u}_x(\theta > 0) = \boldsymbol{u}_x(\theta < 0) \\ \boldsymbol{u}_y(\theta > 0) = -\boldsymbol{u}_y(\theta < 0) \end{cases}$$

Mode II

$$\begin{cases} \boldsymbol{\sigma}_{zz} = 0 \quad \text{or } \boldsymbol{\varepsilon}_{zz} = 0 \\ \boldsymbol{\sigma}_{yy}(\theta = \pm\pi) = 0 \\ \boldsymbol{\sigma}_{xy}(\theta = \pm\pi) = 0 \\ \boldsymbol{u}_x(\theta > 0) = -\boldsymbol{u}_x(\theta < 0) \\ \boldsymbol{u}_y(\theta > 0) = \boldsymbol{u}_y(\theta < 0) \end{cases}$$

Mode III

$$\begin{cases} \boldsymbol{\sigma}_{xx} = \boldsymbol{\sigma}_{xy} = \boldsymbol{\sigma}_{yy} = \boldsymbol{\sigma}_{zz} = 0 \\ \boldsymbol{u}_y = \boldsymbol{u}_x = 0 \\ \boldsymbol{u}_z(\theta > 0) = -\boldsymbol{u}_z(\theta < 0) \end{cases}$$

- Singularity at crack tip for linear and elastic materials (3)
  - Asymptotic solutions (Airy functions)

Mode I

$$\boldsymbol{\sigma}_{yy} = \frac{C}{\sqrt{r}}\cos\frac{\theta}{2}\left[1+\sin\frac{3\theta}{2}\sin\frac{\theta}{2}\right] + \cancel{\mathcal{O}(r^0)}$$

Mode II

$$\boldsymbol{\sigma}_{xy} = \frac{C}{\sqrt{r}}\cos\frac{\theta}{2}\left[1-\sin\frac{3\theta}{2}\sin\frac{\theta}{2}\right] + \cancel{\mathcal{O}(r^0)}$$

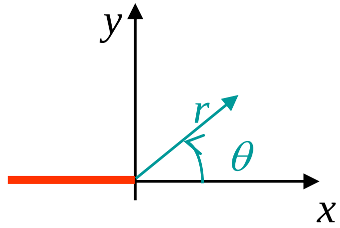
Mode III

$$\boldsymbol{\sigma}_{yz} = \frac{C}{\sqrt{r}}\cos\frac{\theta}{2} + \cancel{\mathcal{O}(r^0)}$$

  - Introduction of the Stress Intensity Factors - SIF (Pa $\text{m}^{1/2}$)

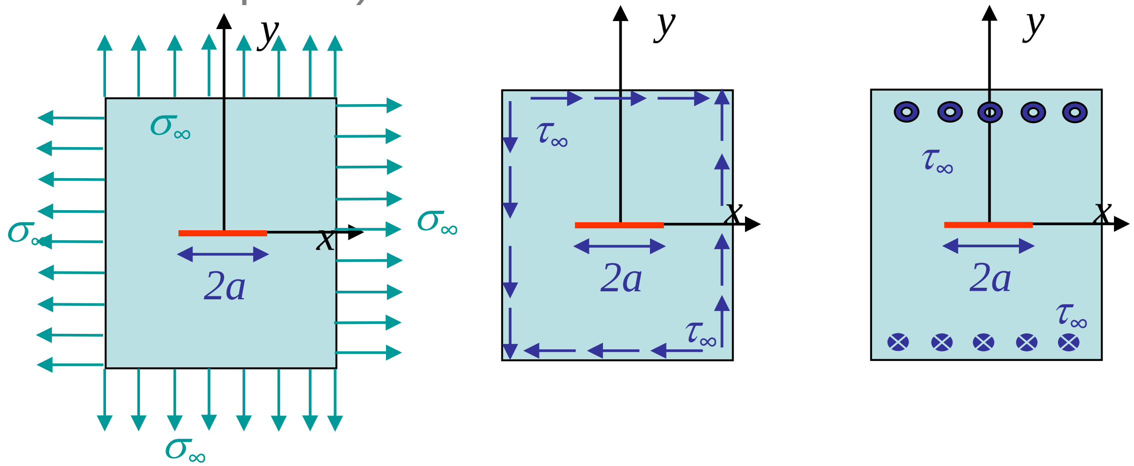
$$\begin{cases} K_I = \lim\limits_{r\to 0}\left(\sqrt{2\pi r}\,\boldsymbol{\sigma}_{yy}^{\text{mode I}}\,|_{\theta=0}\right) = C\sqrt{2\pi} \\ K_{II} = \lim\limits_{r\to 0}\left(\sqrt{2\pi r}\,\boldsymbol{\sigma}_{xy}^{\text{mode II}}\,|_{\theta=0}\right) = C\sqrt{2\pi} \\ K_{III} = \lim\limits_{r\to 0}\left(\sqrt{2\pi r}\,\boldsymbol{\sigma}_{yz}^{\text{mode III}}\,|_{\theta=0}\right) = C\sqrt{2\pi} \end{cases} \Longrightarrow \begin{cases} \boldsymbol{\sigma}^{\text{mode i}} = \dfrac{K_i}{\sqrt{2\pi r}}\mathbf{f}^{\text{mode i}}(\theta) \\ \boldsymbol{u}^{\text{mode i}} = K_i\sqrt{\dfrac{r}{2\pi}}\boldsymbol{g}^{\text{mode i}}(\theta) \end{cases}$$

  - **K_i are dependent on both**
    - **Loading &**
    - **Geometry**



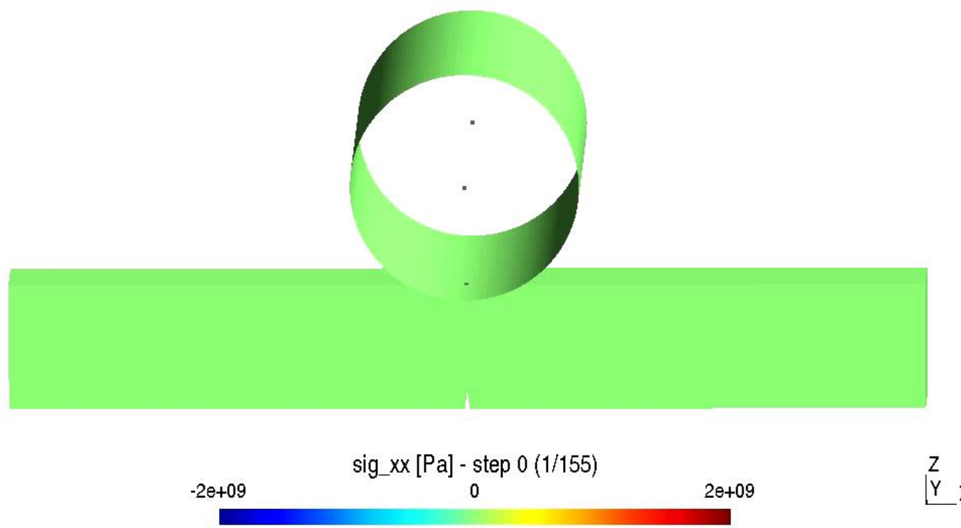
- Evaluation of the stress Intensity Factor (SIF)
  - Analytical (crack *2a* in an infinite plane)

$$\begin{cases} K_I = \sigma_\infty \sqrt{\pi a} \\ K_{II} = \tau_\infty \sqrt{\pi a} \\ K_{III} = \tau_\infty \sqrt{\pi a} \end{cases}$$



  - Numerical

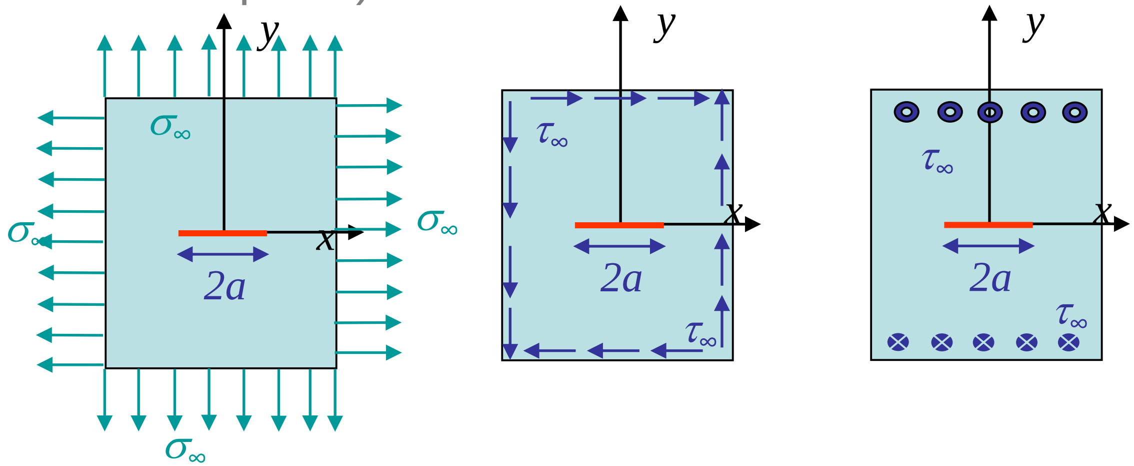
$$\begin{cases} K_I = \beta_I \sigma_\infty \sqrt{\pi a} \\ K_{II} = \beta_{II} \tau_\infty \sqrt{\pi a} \\ K_{III} = \beta_{III} \tau_\infty \sqrt{\pi a} \end{cases}$$



    - β_i depends on
      - Geometry
      - Crack length

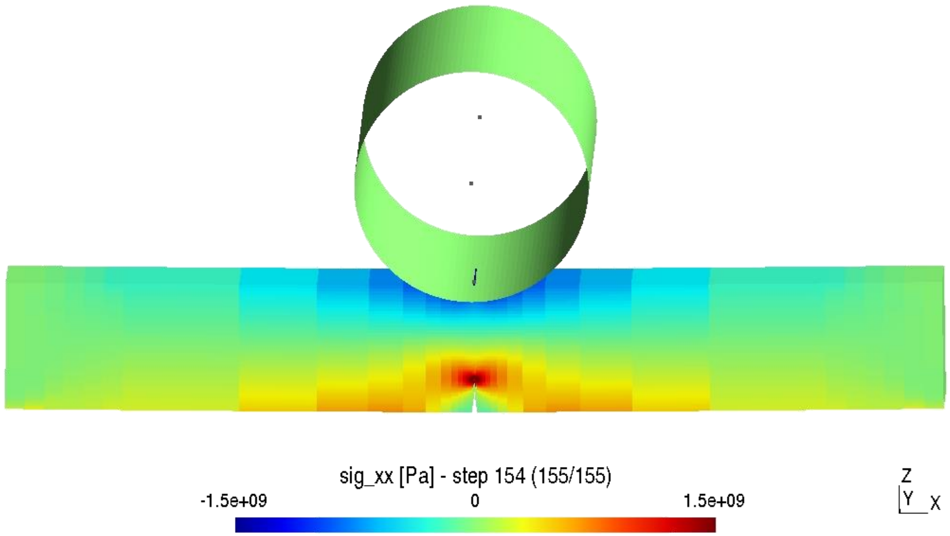
- Evaluation of the stress Intensity Factor (SIF)
  - Analytical (crack $2a$ in an infinite plane)

$$\begin{cases} K_I = \sigma_\infty \sqrt{\pi a} \\ K_{II} = \tau_\infty \sqrt{\pi a} \\ K_{III} = \tau_\infty \sqrt{\pi a} \end{cases}$$



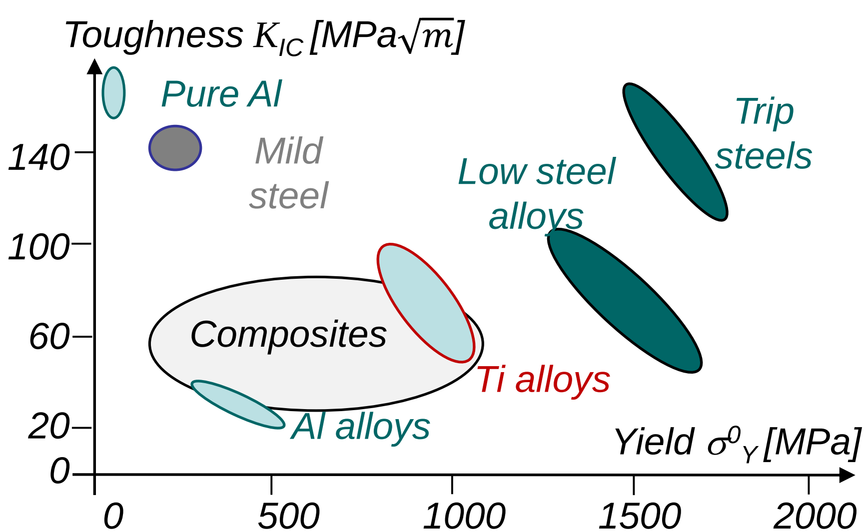
  - Numerical

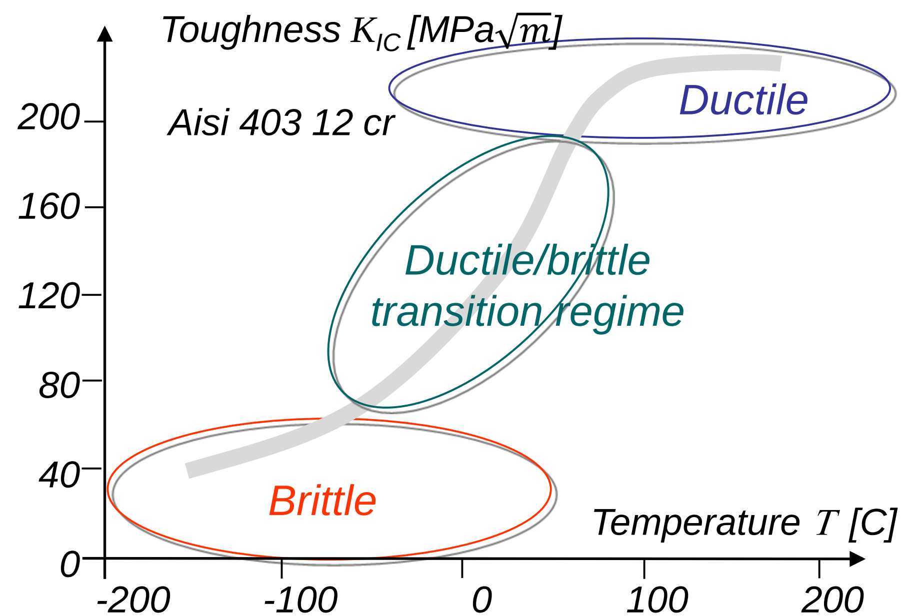
$$\begin{cases} K_I = \beta_I \sigma_\infty \sqrt{\pi a} \\ K_{II} = \beta_{II} \tau_\infty \sqrt{\pi a} \\ K_{III} = \beta_{III} \tau_\infty \sqrt{\pi a} \end{cases}$$



    - β_i depends on
      - Geometry
      - Crack length

- 1957, Irwin, new failure criterion
  - $\sigma_{max} \rightarrow \infty$ ⟹ σ is irrelevant
  - Compare the SIFs (dependent on loading and geometry) to a new material property: the toughness
    - If $K_i = K_{iC}$ ⟹ crack growth
    - Toughness (ténacité) K_{Ic}
      - Steel, Al, … : see figures
      - Concrete: 0.2 - 1.4 $\text{MPa m}^{1/2}$

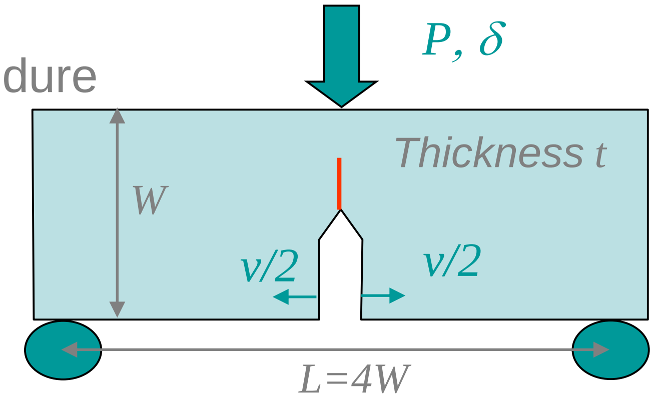


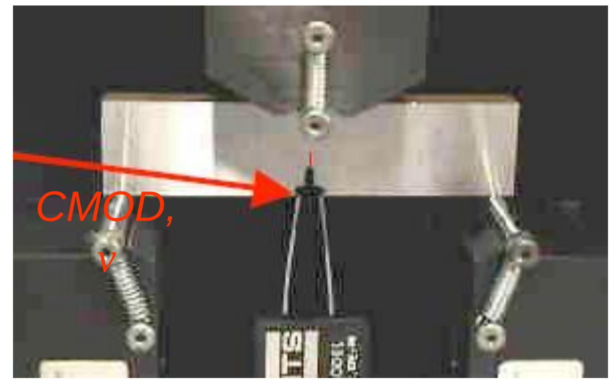


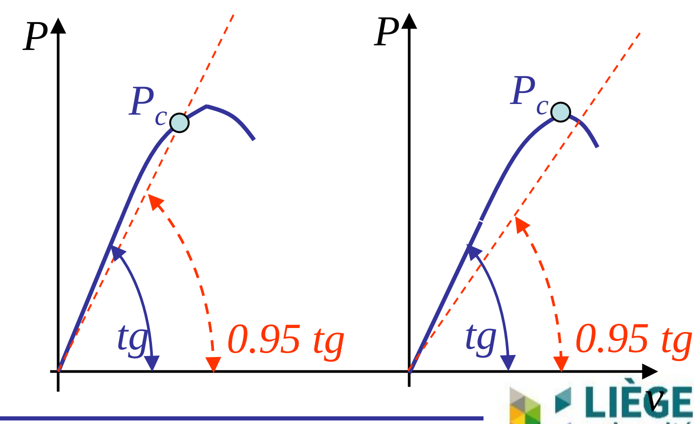
- Measuring K_{Ic}
  - Done by strictly following the ASTM E399 procedure
  - Preparation
    - A possible specimen is the Single Edge Notch Bend (SENB)
      - Plane strain constraint (thick enough specimen) ⇒ conservative
      - Specimen machined with a V-notch in order to start a sharp crack
    - Cyclic loading to initiate a fatigue crack
  - Toughness test performed
    - Calibrated P - δ recording equipment
    - The Crack Mouth Opening Displacement (CMOD=v) is measured with a clipped gauge
    - P_c is obtained on P-v curves
      - either the 95% offset value or
      - the maximal value reached before
    - K_{Ic} is deduced from P_c using

$$K_I = \frac{PL}{tW^{\frac{3}{2}}} f\left(\frac{a}{W}\right)$$

      - $f(a/W)$ depends on the test (SENB, …)







- Energy evolution during crack growth
  - Assuming the crack propagates
    - Example: body subjected to Q constant
    - As the crack grows, there is a displacement δu

$$\Rightarrow \delta W_{\text{ext}} = Q\delta u$$

  - Energy release rate G for Q constant
    - Change in energy system for a crack growth δA

$$\delta E_{\text{int}} = Q\delta u - G\delta A = \delta\left(Qu\right) - G\delta A$$

$$\Rightarrow G = -\partial_A\left(E_{\text{int}} - Qu\right)$$

    - The internal (elastic) energy thus reads

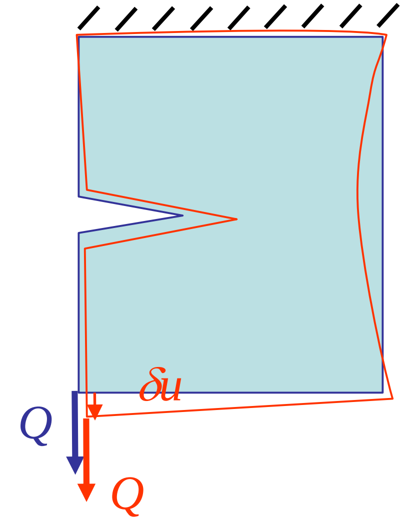
$$E_{\text{int}} = E_{\text{int}}\left(Q, A\right)$$

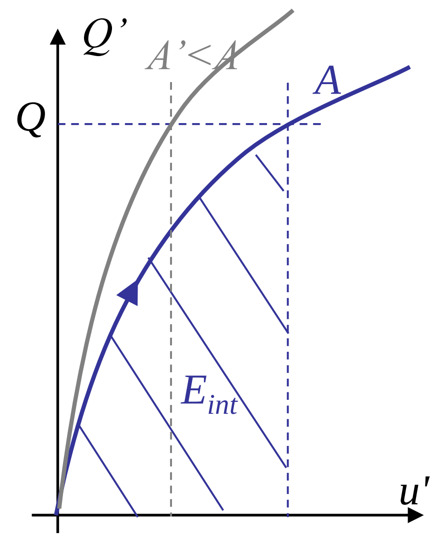
    - From complementary energy

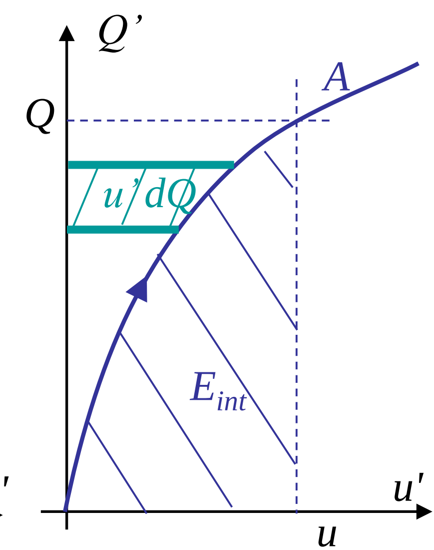
$$u\left(Q,\, A\right) = -\partial_Q\left(E_{\text{int}} - Qu\right)$$

$$\Rightarrow \partial_Q G = \partial_A u$$

$$\Rightarrow G = \int_0^Q \partial_A u\left(Q',\, A\right) dQ'$$

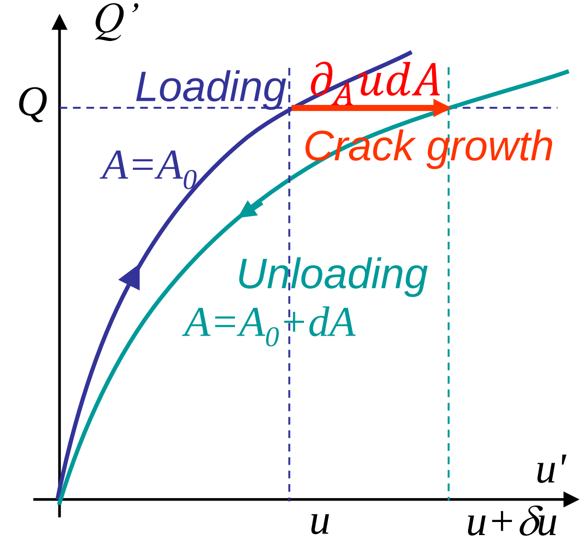






- Energy release rate interpretation

$$\begin{cases} G = -\partial_A \left(E_{\text{int}} - Qu\right) \\ G = \int_0^Q \partial_A u \left(Q',\, A\right) dQ' \end{cases}$$



  - Can be measured by conducting experiments
    - Body with crack surface A_0 loaded up to Q^*
    - Crack growth dA at constant load ⇒ the specimen becomes more flexible ⇒ displacement increment $\partial_A u dA$
    - Unload to zero
    - The area between the 2 curves is then $G\,dA$

- Link with the stress intensity factor
  - In linear elasticity & crack growing straight ahead

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

⇒ The energy release rate can also be used to assess crack growth

- Critical energy release rate
  - If $\Pi_T = E_{\text{int}} - Qu$ is the potential energy of the specimen

$$G = -\partial_A \left(E_{\text{int}} - W_{\text{ext}}\right) = -\partial_A \Pi_T$$

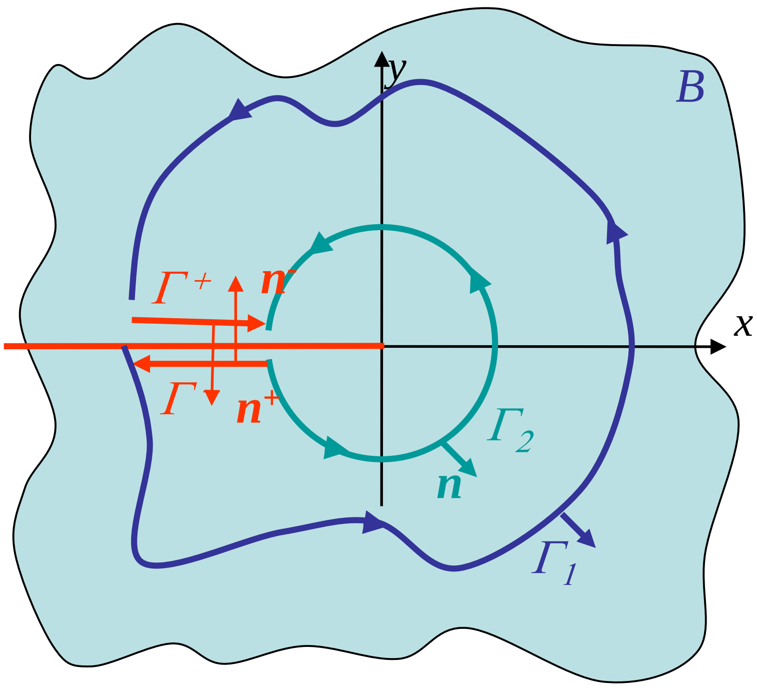
  - Total energy has to be conserved
    - Total energy $E = \Pi_T + \Gamma$
    - Γ is the energy required to create a crack of surface *A*
    - There is crack growth when $G = G_c = \partial_A \Gamma$
      - Brittle materials $G_c = 2\gamma_s$
        - » γ_s is the surface energy, a crack creates 2 surfaces
      - For other materials (ductile, composite, polymers, …) this energy depends on the failure process (void coalescence, debonding, …)

$$\Longrightarrow G_c = 2\gamma_s + W_{\text{pl}}$$

  - Crack growth criterion is $G \geq G_C$
- Link with toughness
  - Since $G = \frac{K_I^2}{E'} + \frac{K_{II}^2}{E'} + \frac{K_{III}^2}{2\mu} \Longrightarrow G_C = \frac{K_{IC}^2}{E'^2}$

- J-integral
  - Assuming stress-free lips
  - Energy that flows toward the crack tip by

$$J = \int_{\Gamma_1} \left[U(\boldsymbol{\varepsilon})\, \boldsymbol{n}_x - \boldsymbol{u}_{,x} \cdot \boldsymbol{T} \right] dl$$
$$= \int_{\Gamma_2} \left[U(\boldsymbol{\varepsilon})\, \boldsymbol{n}_x - \boldsymbol{u}_{,x} \cdot \boldsymbol{T} \right] dl$$



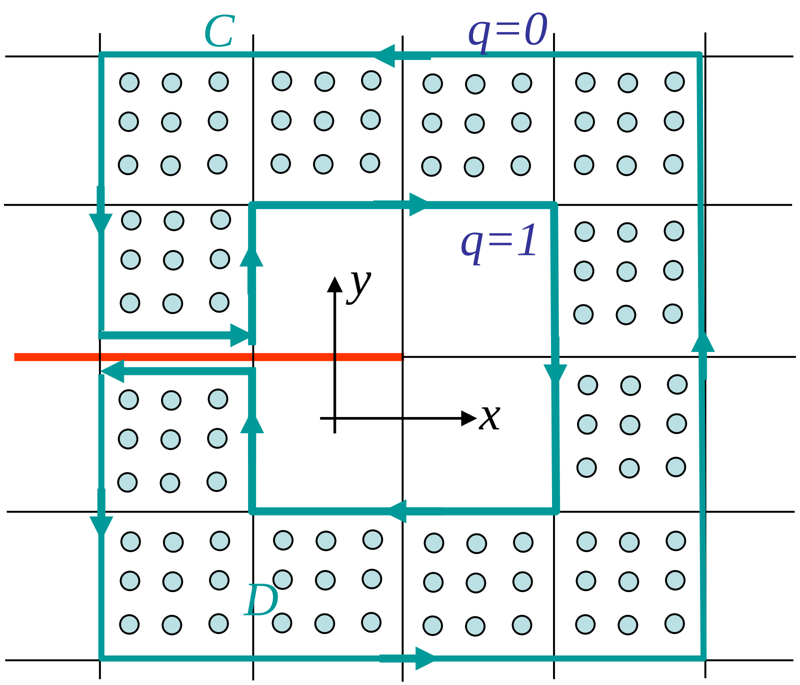
    - It is path independent
    - No assumption on linearity required
    - Does not depend on subsequent crack growth direction
  - For linear elasticity and for any contour Γ embedding a straight crack

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

- Finite element model: J-integral by domain integration
  - Can be rewritten

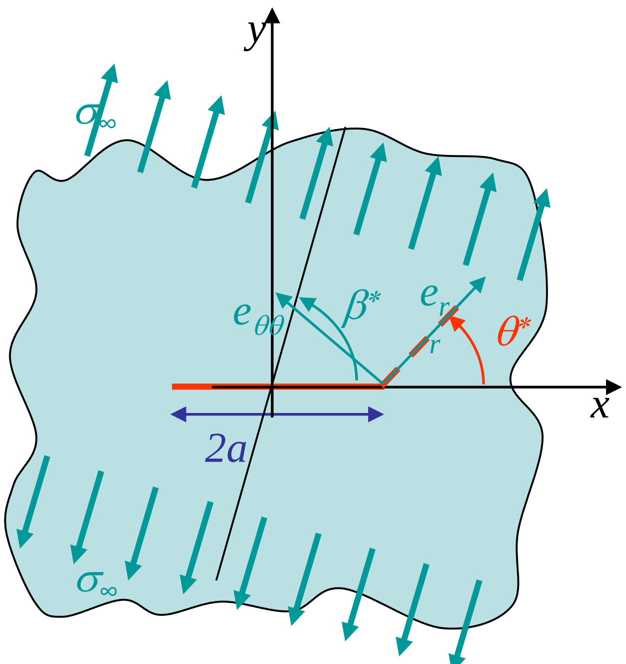
$$J = \int_D \left[\boldsymbol{\sigma}_{ij}\boldsymbol{u}_{i,x}q_{,j} - Uq_{,x}\right] dA$$

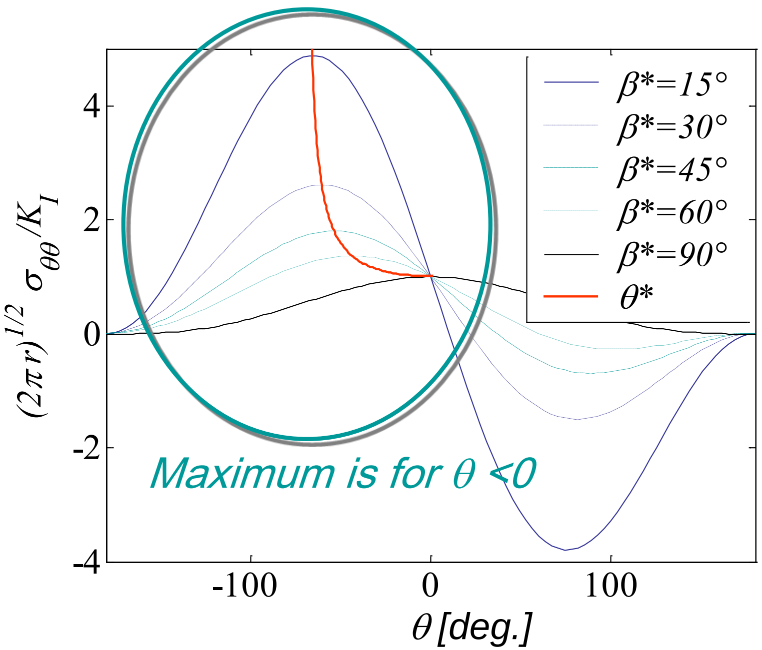
    - q is discretized using the same shape functions than the elements
  - This integral is valid for any region around the crack tip
    - As long as the crack lips are straight
  - Efficient for finite element method



- Direction of crack grow
  - Assumptions: the crack will grow in the direction where the SIF related to mode I in the new frame is maximal
    - Crack growth if $\left(\sqrt{2\pi r}\boldsymbol{\sigma}_{\theta\theta}\left(r,\ \theta*\right)\right) \geq K_C$ with $\partial_\theta \boldsymbol{\sigma}_{\theta\theta}|_{\theta*} = 0$
  - From direction of loading, one can compute the propagation direction

$$\cot\beta^* = \frac{K_{II}}{K_I} \Longrightarrow \boldsymbol{\sigma}_{\theta\theta} = \frac{K_I}{\sqrt{2\pi r}}\left[\cos^3\frac{\theta}{2} - \frac{3\cot\beta^*}{2}\sin\theta\cos\frac{\theta}{2}\right]$$





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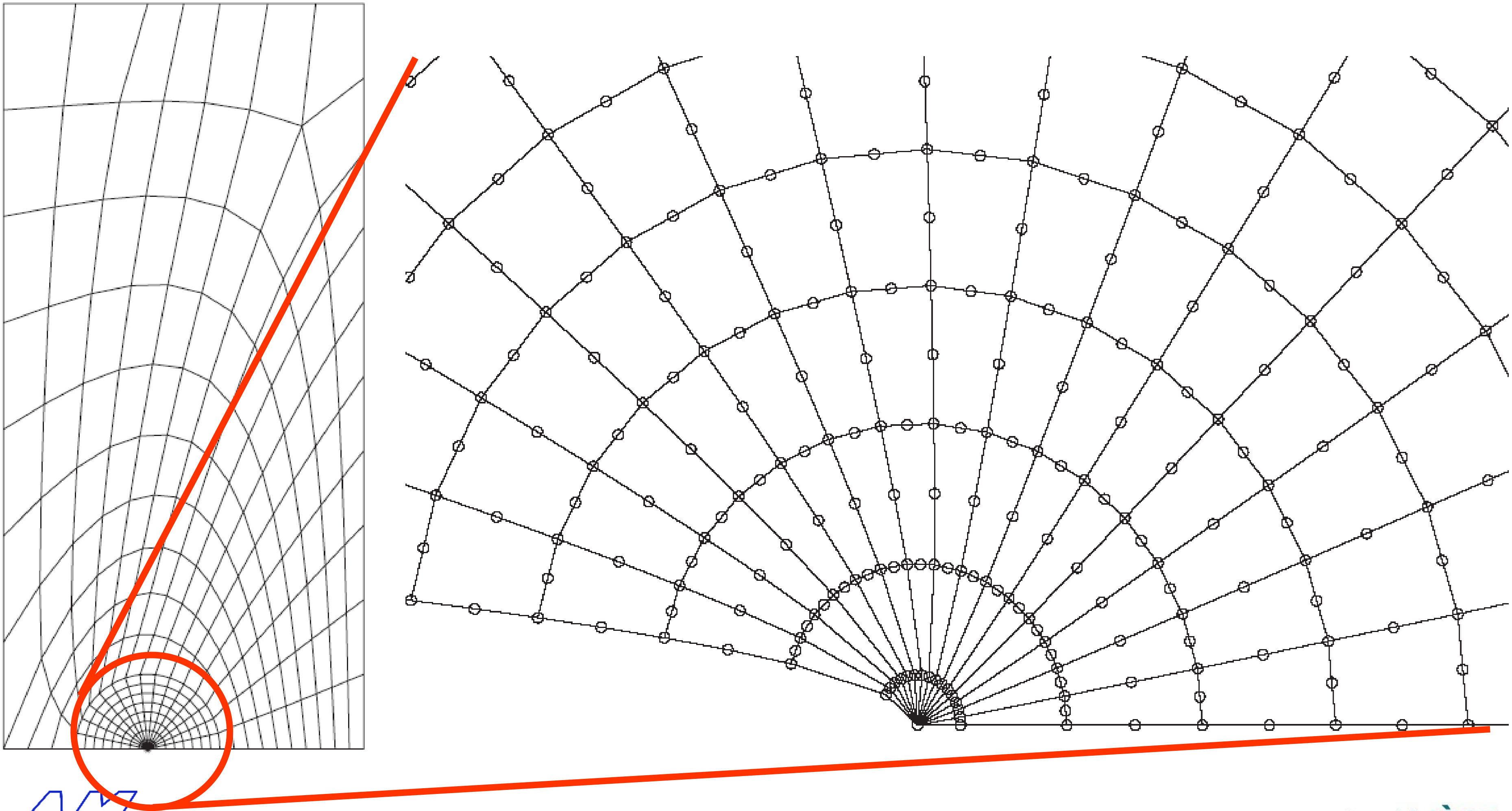
Crack propagation

- A simple method is a FE simulation where the crack is used as BCs
  - The mesh is conforming with the crack lips



- Finite element model: J-integral by domain integration

$$J = \int_{\Gamma_1} \left[U(\boldsymbol{\varepsilon})\, \boldsymbol{n}_x - \boldsymbol{u}_{,x} \cdot \boldsymbol{T} \right] dl$$

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

  – Can be rewritten

$$J = \int_D \left[\boldsymbol{\sigma}_{ij} \boldsymbol{u}_{i,x} q_{,j} - U q_{,x} \right] dA$$

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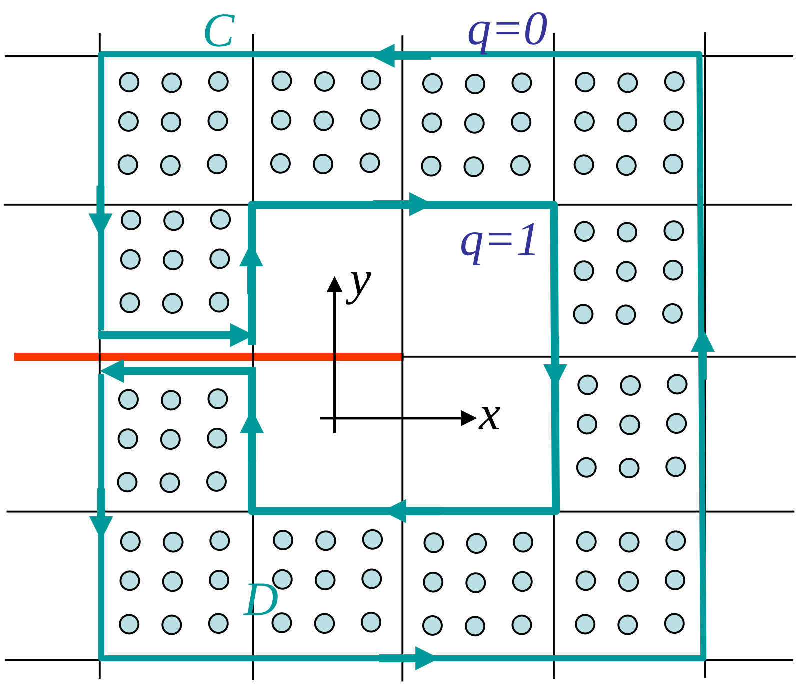
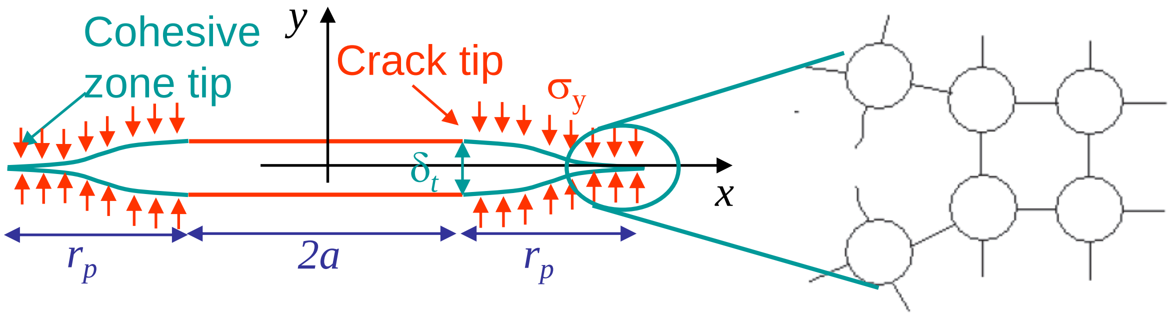
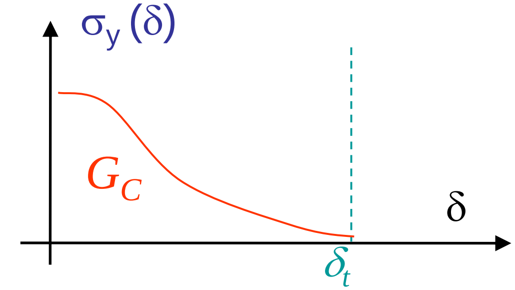


- A simple method is a FE simulation where the crack is used as BCs (2)
  - Mesh the structure in a conforming way with the crack
  - Extract SIFs K_i (different methods, but J-integral is common)
  - Use criterion on crack propagation
    - Example: the maximal hoop stress criterion $\left(\sqrt{2\pi r}\boldsymbol{\sigma}_{\theta\theta}\left(r,\,\theta*\right)\right) \geq K_C$

      with crack propagation direction obtained by $\partial_\theta \boldsymbol{\sigma}_{\theta\theta}\big|_{\theta*} = 0$ & $\partial^2_{\theta\theta} \boldsymbol{\sigma}_{\theta\theta}\big|_{\theta*} < 0$
  - If the crack propagates
    - Move crack tip by Δa in the θ*-direction
    - A new mesh is required as the crack has changed (since the mesh has to be conforming)
      - Involves a large number of remeshing operations (time consuming)
      - Is not always fully automatic
      - Requires fine meshes and Barsoum elements
  - Not used

- The cohesive method is based on Barenblatt model
  - This model is an idealization of the brittle fracture mechanisms
    - Separation of atoms at crack tips (cleavage)
    - As long as the atoms are not separated by a distance δ_t, there are attractive forces (see overview lecture)

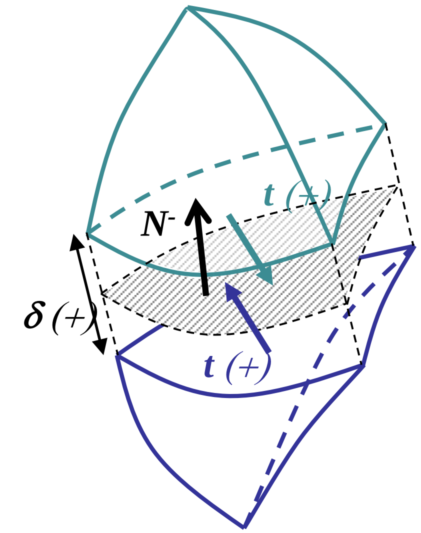


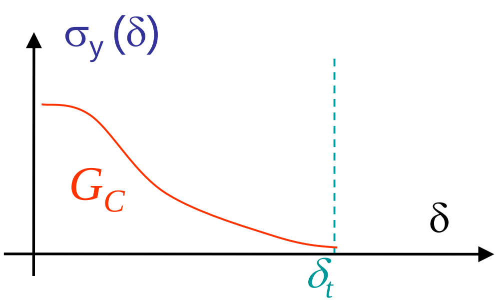


  - For elasticity $G_C = \int_0^{\delta_t} \sigma_y(\delta) d\delta$
    - So the area below the σ-δ curve corresponds to G_C if crack grows straight ahead
  - This model requires only 2 parameters
    - Peak cohesive traction σ_{max} (spall strength)
    - Fracture energy G_C (typically from K_{IC})
    - Shape of the curves has no importance as long as it is monotonically decreasing

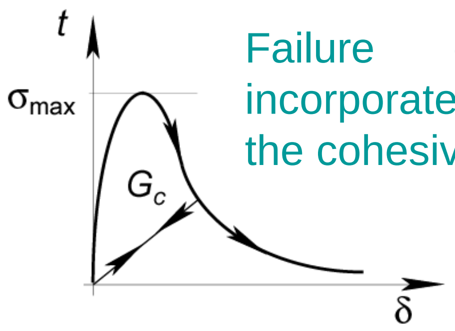
- Insertion of cohesive elements
  - Between 2 volume elements
  - Computation of the opening (cohesive element)
    - Normal to the interface in the deformed configuration $\boldsymbol{N}^-$
    - Normal opening $\delta_n = \max([\![\boldsymbol{u}]\!] \cdot \boldsymbol{N}^-,\, 0)$
    - Sliding $\boldsymbol{\delta}_s = [\![\boldsymbol{u}]\!] - [\![\boldsymbol{u}]\!] \cdot \boldsymbol{N}^- \boldsymbol{N}^-$
    - Resulting opening $\delta = \sqrt{\delta_n^2 + \beta_c^2 \left\|\boldsymbol{\delta}_s\right\|^2}$

      with β_c the ratio between the shear and normal critical tractions
  - Definition of a potential
    - Potential $\phi = \phi(\delta)$ to match the traction separation law (TSL) curve
    - Traction (in the deformed configuration) derives from this potential $\boldsymbol{t} = \frac{\partial \phi}{\partial \boldsymbol{\delta}} = \frac{\partial \phi}{\partial \delta_n} \boldsymbol{N}^- + \frac{\partial \phi}{\partial \delta_s} \frac{\boldsymbol{\delta}_s}{\delta_s}$



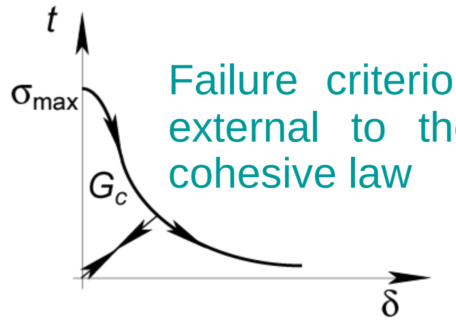


- Computational framework
  - How are the cohesive elements inserted?
  - First method: intrinsic Law
    - Cohesive elements inserted from the beginning
    - So the elastic part prior to crack propagation is accounted for by the TSL
    - Drawbacks:
      - Requires a priori knowledge of the crack path to be efficient
      - Mesh dependency [Xu & Needelman, 1994]
      - Initial slope that modifies the effective elastic modulus
        - » Alteration of a wave propagation
      - This slope should tend to infinity [Klein et al. 2001]
        - » Critical time step is reduced



Failure criterion incorporated within the cohesive law

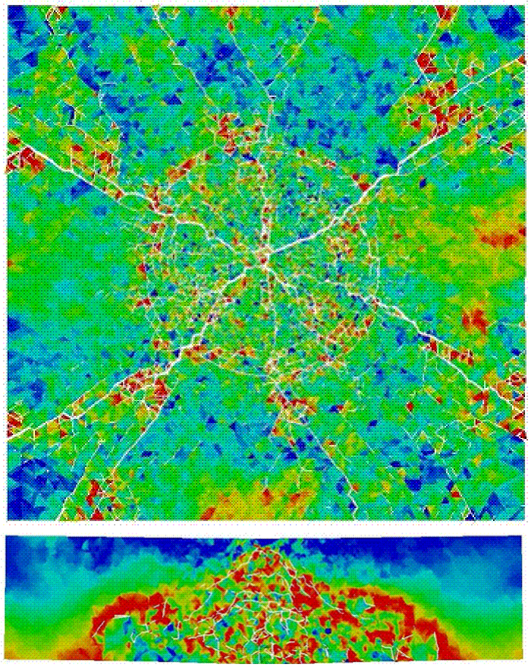
  - Second method: extrinsic law
    - Cohesive elements inserted on the fly when failure criterion ($\sigma>\sigma_{max}$) is verified [Ortiz & Pandolfi 1999]
    - Drawback:
      - Complex implementation in 3D especially for parallelization

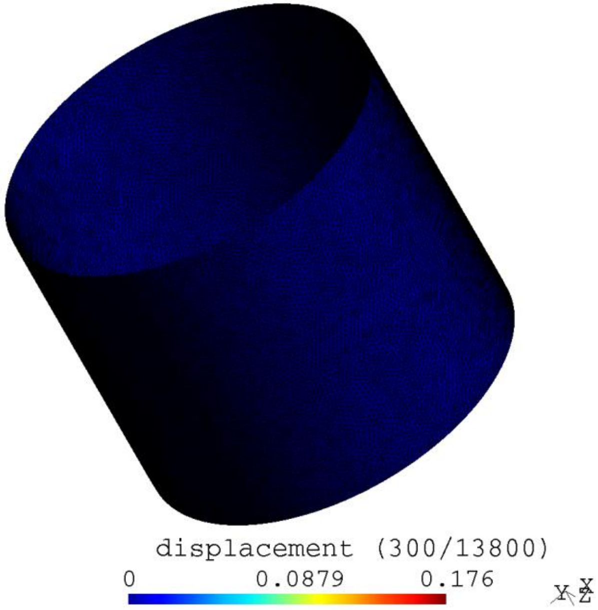


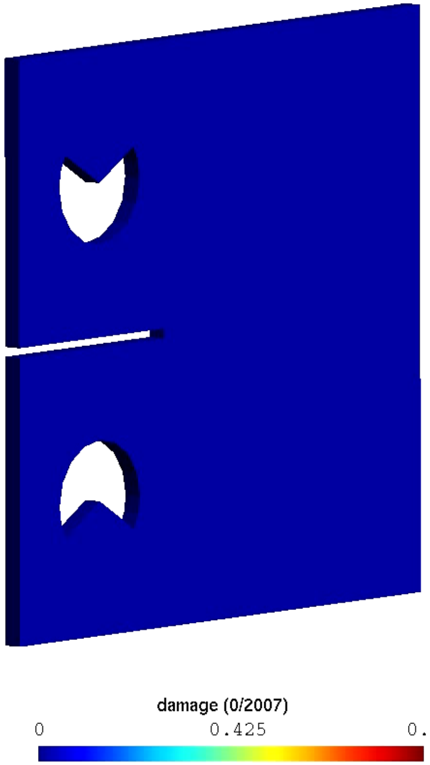
Failure criterion external to the cohesive law

Cohesive elements

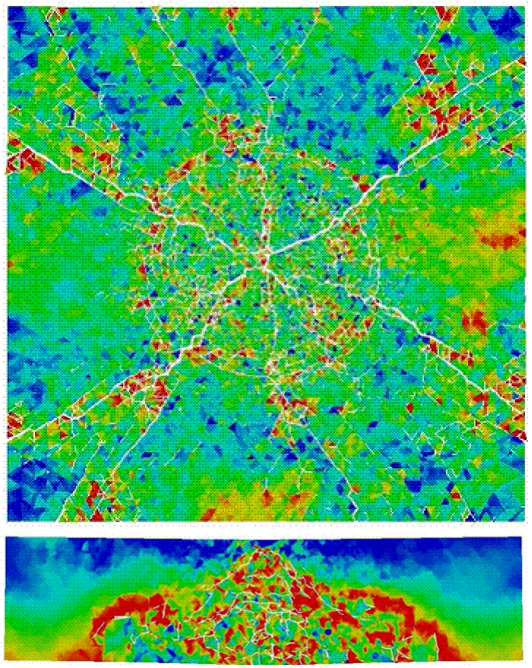
- Examples

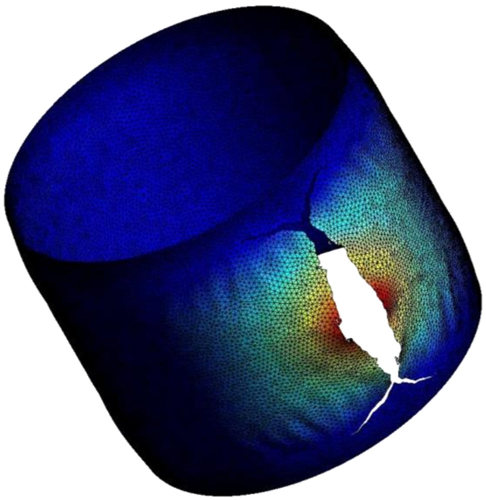


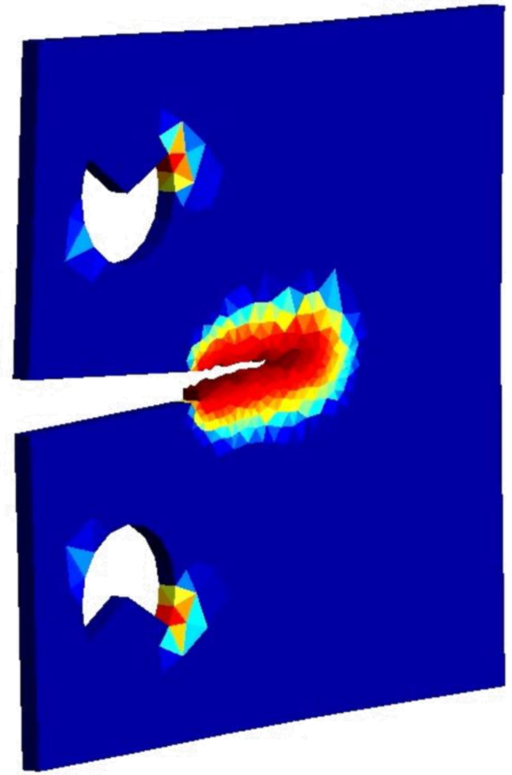


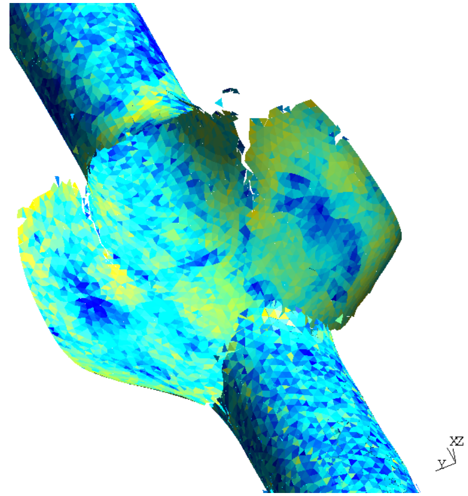


- Examples





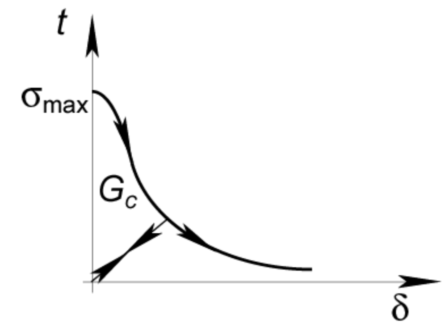


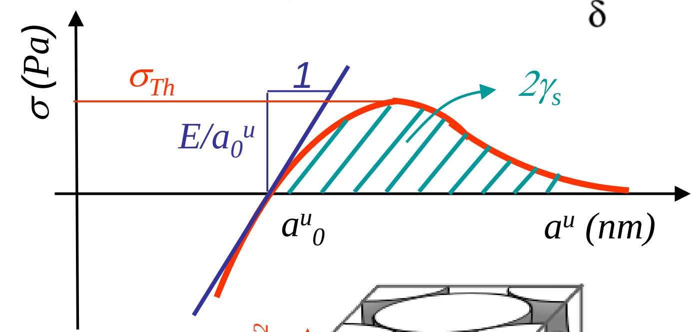


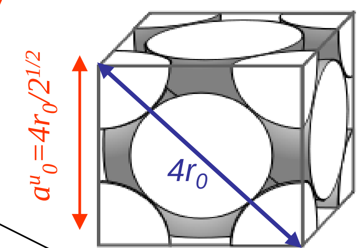
- Experimental characterization of the parameters
  - Critical energy release rate G_C
    - From toughness tests $G_C = \frac{K_{IC}^2}{E'^2}$
  - Spall strength σ_{max}
    - For perfect crystal ⟹ analytical value

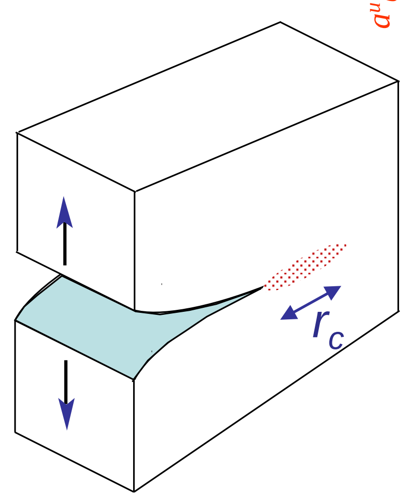
$$\sigma_{\mathrm{Th}} = \sqrt{\frac{E\gamma_s}{a_0^u}}$$

    - For non-perfect materials
      - Could be a measured stress at distance r_C
      - Delicate to put in place
    - In practice calibration (see next slide)



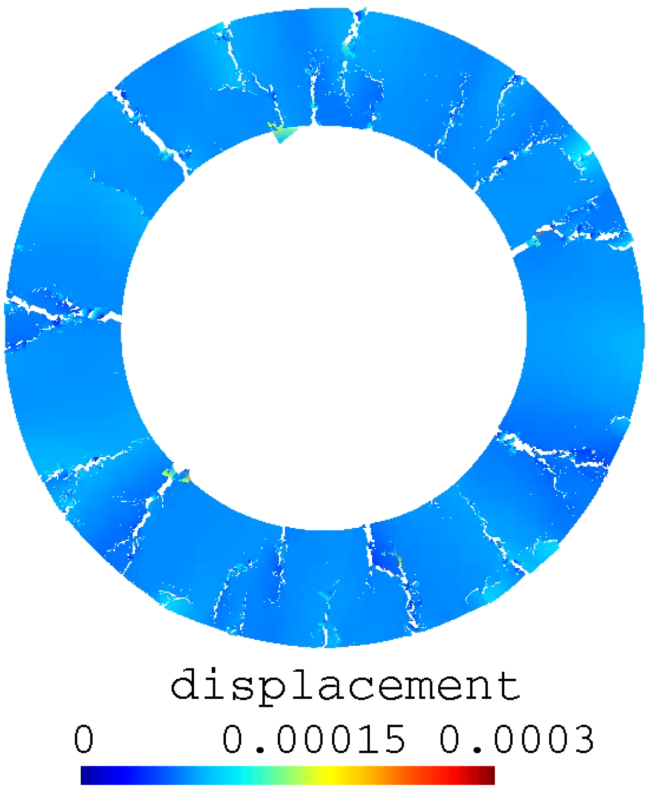


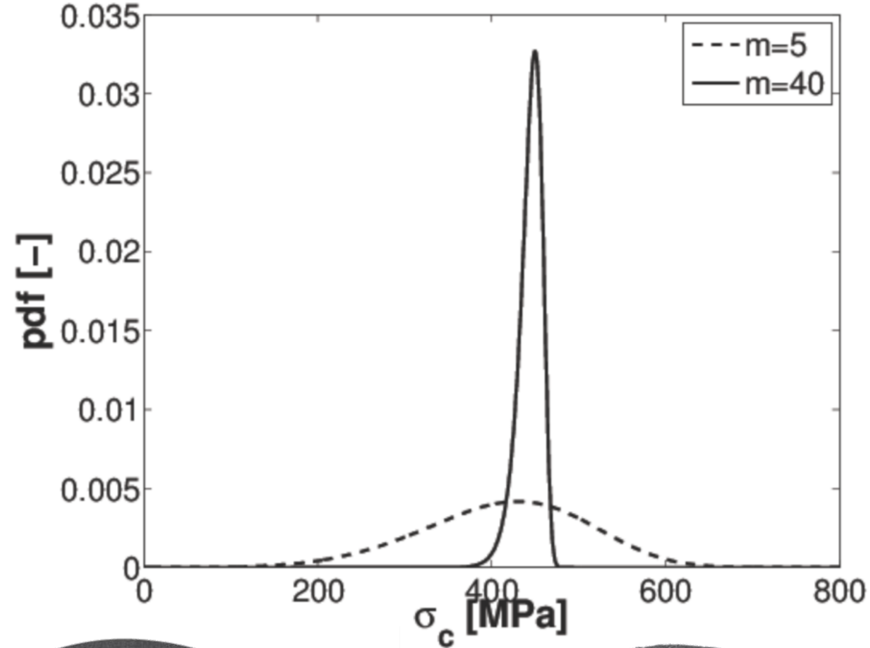


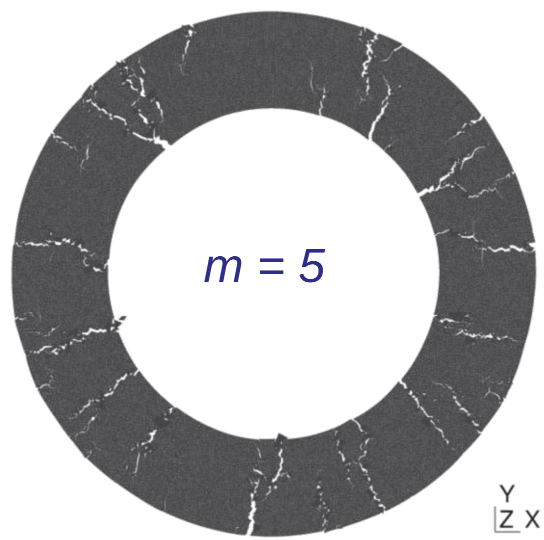


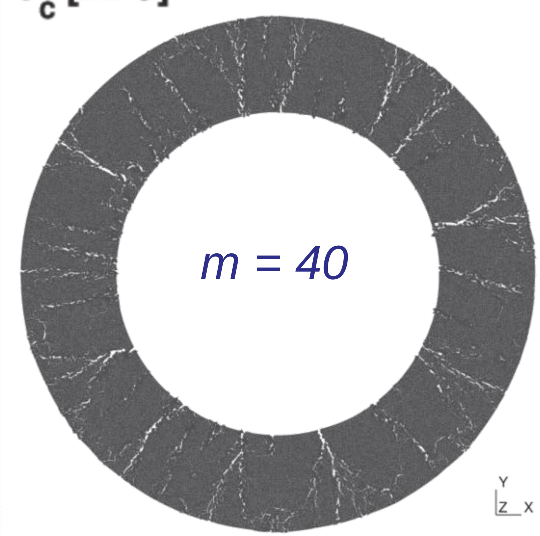
Cohesive elements

- Effect of the spall strength σ_{max}
  - It should cover the stochastic effect of material discrepancies
  - Use of Weibull function



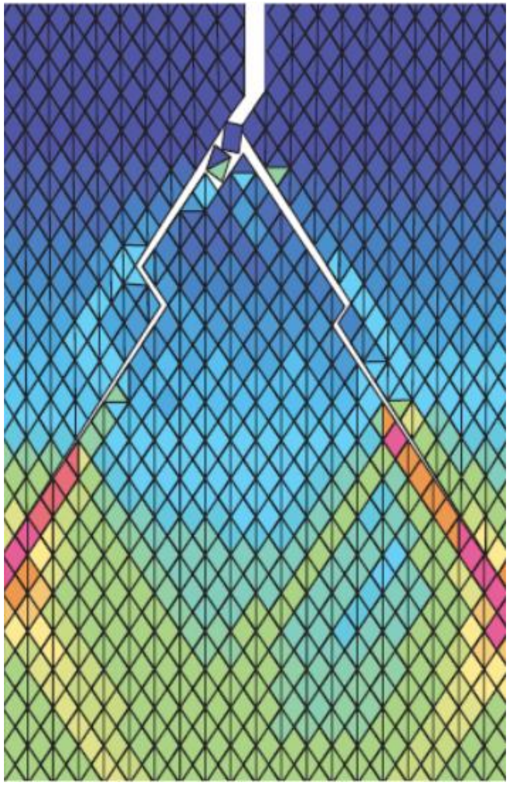




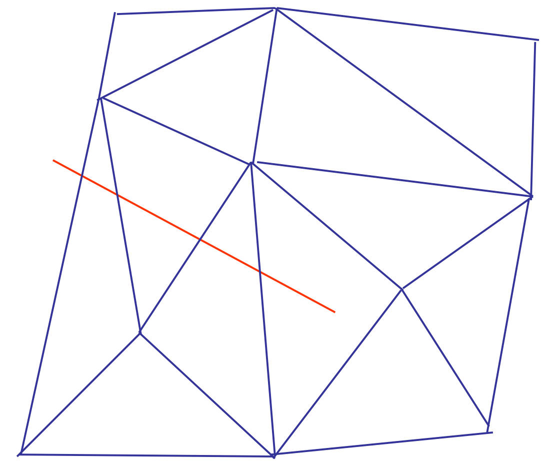


Cohesive elements

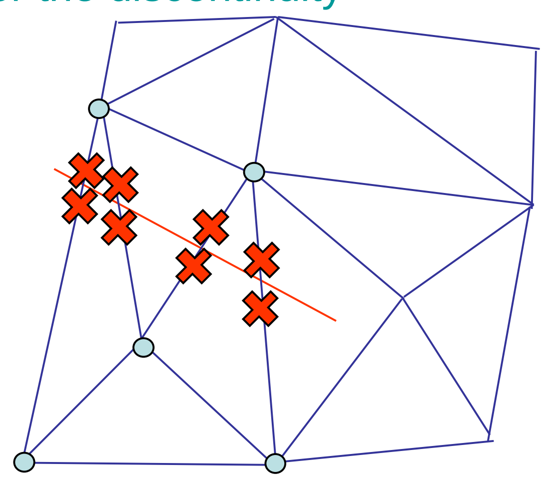
- Advantages of the method
  - Can be mesh independent (non regular meshes)
  - Can be used for large problem size
  - Automatically accounts for time scale [Camacho & Ortiz, 1996]
    - Fracture dynamics has not been studied in these classes
  - Really useful when crack path is already known
    - Debonding of fibers
    - Delamination of composite plies
    - …
  - No need for an initial crack
    - The method can detect the initiation of a crack
- Drawbacks
  - Still requires a conforming mesh
  - Requires fine meshes
    - $h_{\max} = \frac{\pi E G_C}{2(1-\nu^2)\sigma_c^2}$
    - So parallelization is mandatory
  - Could be mesh dependent



- How to get rid of conformity requirements?
- Key principles
  - For a FE discretization, the displacement field is approximated by $\boldsymbol{u}_h\left(\xi^i\right)=\sum_{a\in I} N^a\left(\xi^i\right)\boldsymbol{u}^a$
    - Sum on nodes a in the set I (11 nodes here)
    - u^a are the nodal displacements
    - N^a are the shape functions
    - ξ^i are the reduced coordinates

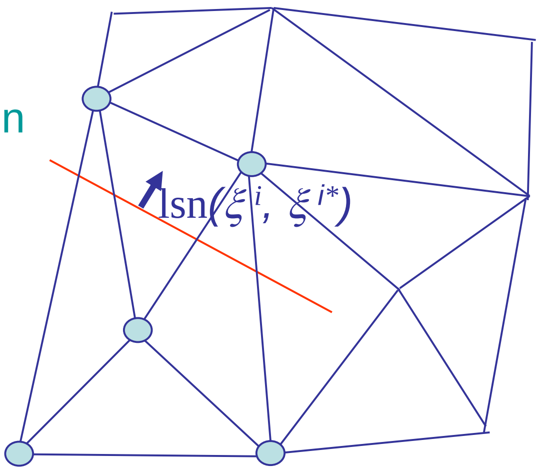


  - XFEM
    - New degrees of freedom are introduced to account for the discontinuity
    - It could be done by inserting new nodes (✖) near the crack tip, but this would be inefficient (remeshing)
    - Instead, shape functions are modified
      - Only shape functions that intersect the crack
      - This implies adding new degrees of freedom to the related nodes (○)



- Key principles (2)
  - New degrees of freedom are introduced to account for the discontinuity

$$\boldsymbol{u}_h\left(\xi^i\right) = \sum_{a\in I} N^a\left(\xi^i\right)\boldsymbol{u}^a + \sum_{a\in J} N^a\left(\xi^i\right) F^a\left(\xi^i\right)\boldsymbol{u}^{*a}$$



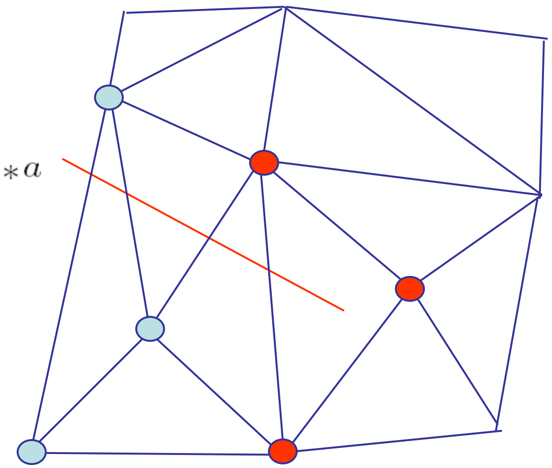
    - J, subset of I, is the set of nodes whose shape-function support is entirely separated by the crack (5 here)
    - u^{*a} are the new degrees of freedom at node a
  - Form of F^a the shape functions related to u^{*a}?
    - Use of Heaviside's function, and we want +1 above and -1 below the crack
    - In order to know if we are above or below the crack, signed-distance has to be computed
    - Normal level set lsn(ξ^i, ξ^{i*}) is the signed distance between a point ξ^i of the solid and its projection ξ^{i*} on the crack

$$\Longrightarrow \boldsymbol{u}_h\left(\xi^i\right) = \sum_{a\in I} N^a\left(\xi^i\right)\boldsymbol{u}^a + \sum_{a\in J} N^a\left(\xi^i\right) H\left(\mathrm{lsn}\left(\xi^i, \xi^{i*}\right)\right)\boldsymbol{u}^{*a}$$

with $H(x) = \pm 1$ if x >< 0

- Key principles (3)
  - Example: removing of a brain tumor (L. Vigneron et al.)
  - At this point
    - A discontinuity can be introduced in the mesh
    - Fracture mechanics is not introduced yet
  - New enrichment with LEFM solution
    - Zone J of Heaviside enrichment is reduced (3 nodes)
    - A zone K of LEFM solution is added to the nodes (●) of elements containing the crack tip

$$\boldsymbol{u}_h\left(\xi^i\right) = \sum_{a\in I} N^a\left(\xi^i\right)\boldsymbol{u}^a + \sum_{a\in J} N^a\left(\xi^i\right) H\left(\text{lsn}\left(\xi^i,\, {\xi^i}^*\right)\right)\boldsymbol{u}^{*a} + \sum_{a\in K} N^a\left(\xi^i\right)\sum_b \Psi_b\left(\xi^i\right)\boldsymbol{\psi}_b^a$$



- LEFM solution is asymptotic $\Longrightarrow$ only nodes close to crack tip can be enriched
- $\psi_b{}^a$ is the new degree b at node a
- Ψ_b is the new shape function b

- Crack propagation criterion
  - Requires the values of the SIFs (2)
    - A more accurate solution is to compute J
      - But K_I, K_{II} & K_{III} have to be extracted from $J = \frac{K_I^2}{E'} + \frac{K_{II}^2}{E'} + \frac{K_{III}^2}{2\mu}$
        - » Define an adequate auxiliary field u^{aux}
        - » Compute $J^{aux}(u^{aux})$ and $J^{s}(u+u^{aux})$
        - » On can show that the interaction integral (see lecture on SIFs)

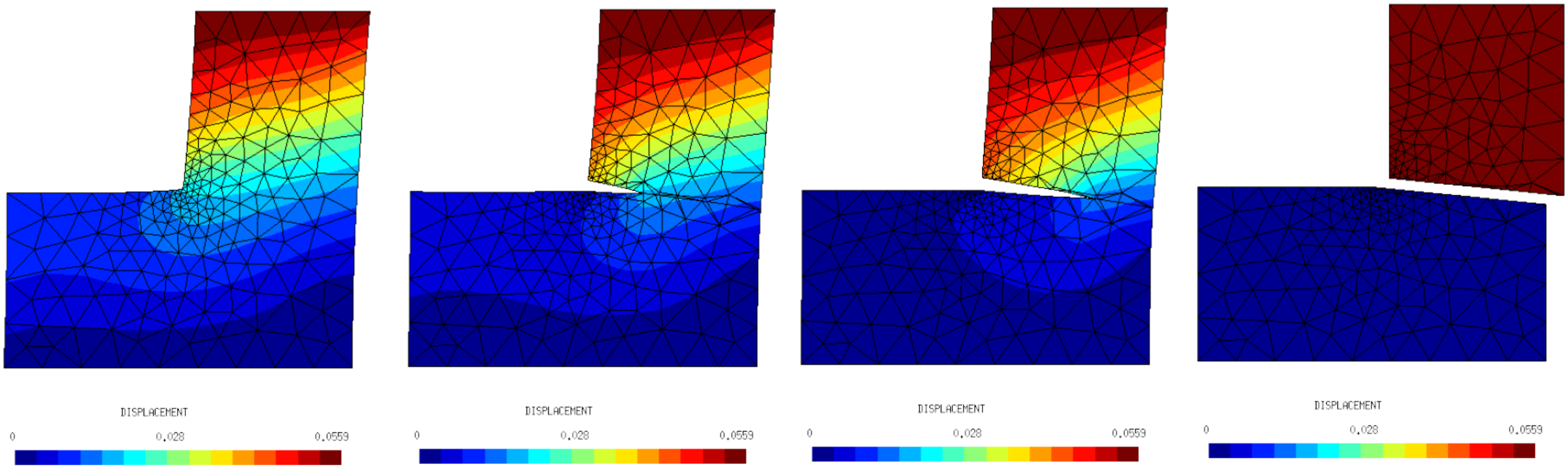
$$I^s = J^s - J - J^{aux} = \frac{2}{E'}\left(K_I K_I^{aux} + K_{II} K_{II}^{aux}\right) + \frac{1}{\mu} K_{III} K_{III}^{aux}$$

        - » If u^{aux} is chosen such that only $K_i^{aux} \neq 0$, K_i is obtained directly
  - Then the maximum hoop stress criterion can be used

$$\left(\sqrt{2\pi r}\boldsymbol{\sigma}_{\theta\theta}\left(r,\ \theta*\right)\right) \geq K_C \text{ with } \partial_\theta \boldsymbol{\sigma}_{\theta\theta}\big|_{\theta*} = 0 \quad \& \quad \partial^2_{\theta\theta} \boldsymbol{\sigma}_{\theta\theta}\big|_{\theta*} < 0$$

  - The experimental value to determine is thus the toughness K_{IC}

- Numerical example
  - Crack propagation (E. Béchet)

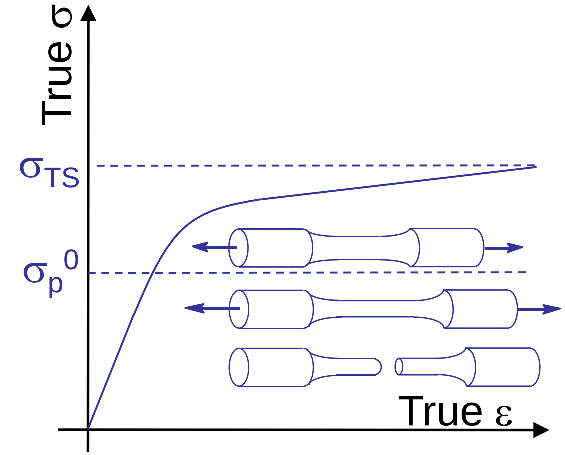


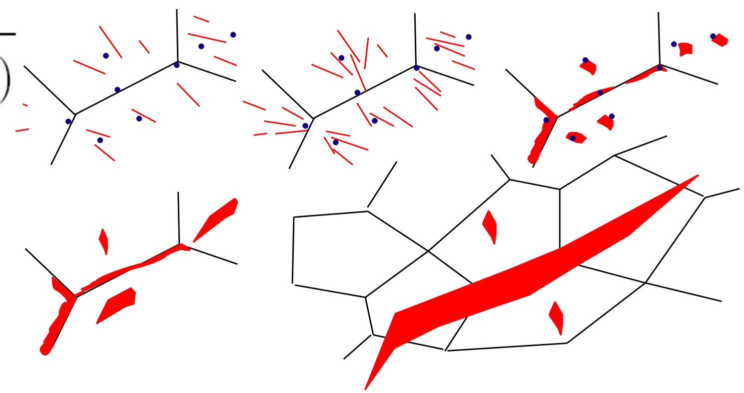
  - Advantages:
    - No need for a conforming mesh (but mesh has still to be fine near crack tip)
    - Mesh independency
    - Computationally efficient
  - Drawbacks:
    - Require radical changes to the FE code
      - New degrees of freedom
      - Gauss integration
      - Time integration algorithm

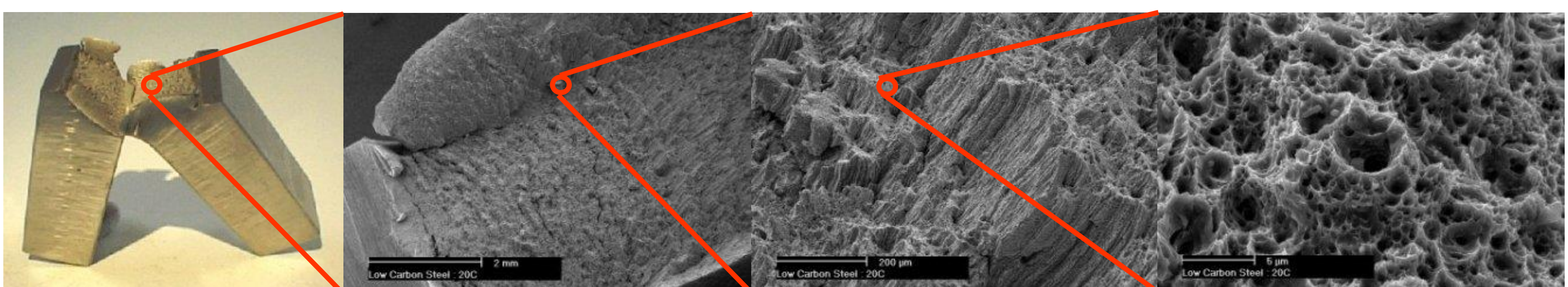
- Some fracture mechanics principles
  - Brittle/ductile materials & Fatigue
  - Linear elastic fracture mechanics
- Computational fracture mechanics for brittle materials
  - Crack propagation
  - Cohesive models
  - XFEM
- Computational fracture mechanics for ductile materials
  - Damage models
- Multiscale methods
  - Composite materials
  - Atomistic models

Damage models

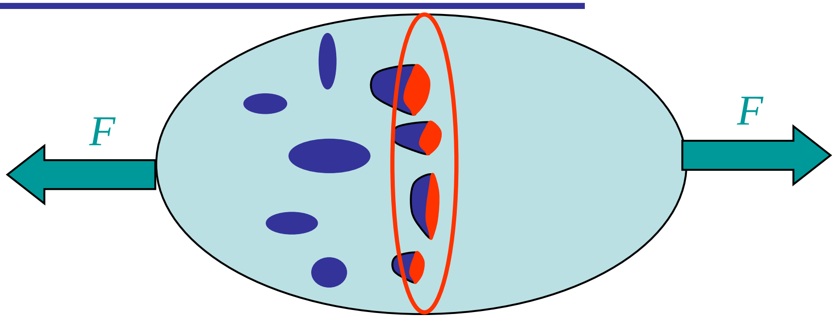
- Failure mechanism
  - Plastic deformations prior to (macroscopic) failure of the specimen
    - Dislocations motion ⟹ void nucleation around inclusions ⟹ micro cavity coalescence ⟹ crack growth
    - Griffith criterion $\sigma_{\text{TS}}\sqrt{a} \div \sqrt{E\,2\gamma_s}$ should be replaced by $\sigma_{\text{TS}}\sqrt{a} \div \sqrt{E\,(2\gamma_s + W_{\text{pl}})}$
  - Numerical models accounting for this failure mode?





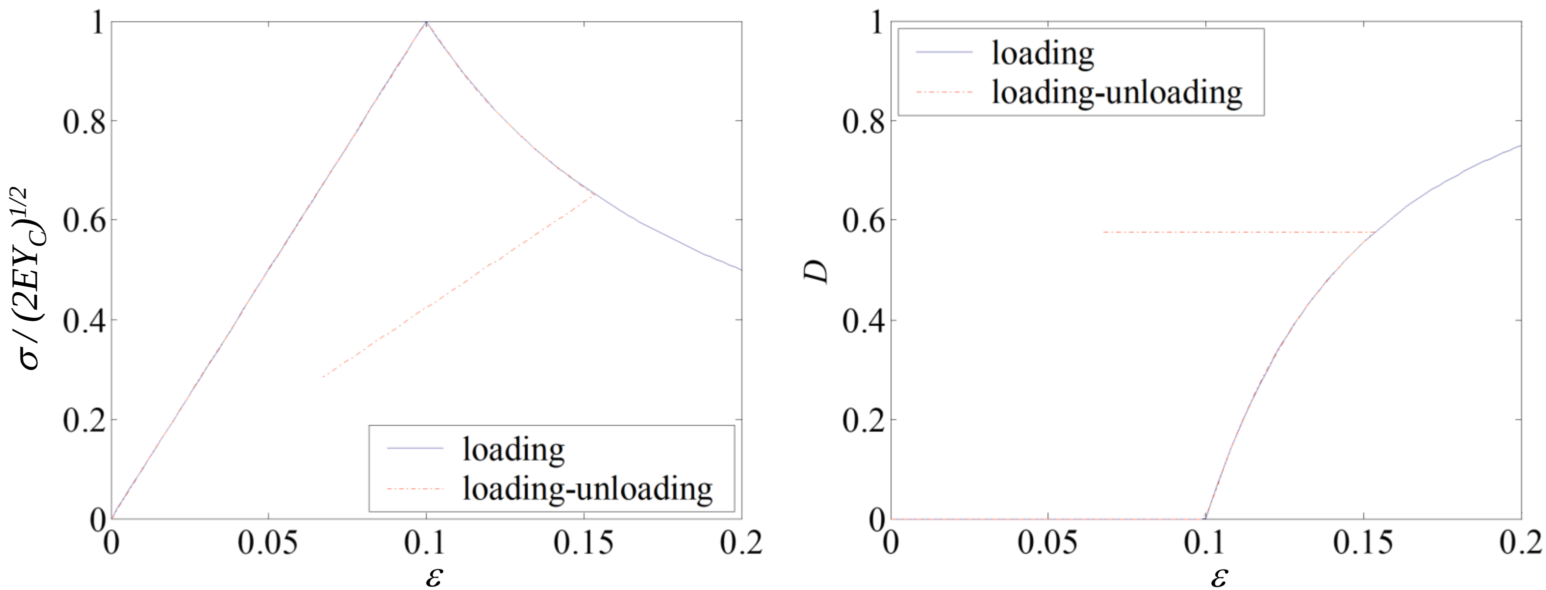


- Introduction to damage (1D)
  - As there are voids in the material, only a reduced surface is balancing the traction



    - Virgin section S $\Longrightarrow$ $\boldsymbol{\sigma}_{xx}^{\text{virgin}} = \frac{F}{S} = \boldsymbol{\sigma}_{xx}$
    - Damage of the surface is defined as $D = \frac{S^{\text{holes}}}{S}$
    - So the effective (or damaged) surface is actually $\hat{S} = S - S^{\text{holes}} = (1 - D)\, S$
    - And so the effective stress is $\hat{\boldsymbol{\sigma}}_{xx} = \frac{F}{S\,(1-D)} = \frac{\boldsymbol{\sigma}_{xx}}{1-D}$
  - Resulting deformation
    - Hooke's law is still valid if it uses the effective stress $\boldsymbol{\varepsilon}_{xx} = \frac{\hat{\boldsymbol{\sigma}}}{E} = \frac{\boldsymbol{\sigma}_{xx}}{E\,(1-D)}$
    - So everything is happening as if Hooke's law was multiplied by (1-D)
  - Isotropic 3D linear elasticity $\boldsymbol{\sigma} = (1-D)\,\mathcal{H} : \boldsymbol{\varepsilon}$
  - Failure criterion: D=D_C, with 0 < D_C <1
- But how to evaluate D, and how does it evolve?

- Evolution of damage D for isotropic elasticity
  - Equations
    - Stresses $\boldsymbol{\sigma} = (1 - D)\,\mathcal{H} : \boldsymbol{\varepsilon}$
    - Example of damage criterion $f\,(\boldsymbol{\varepsilon},\, D) = (1 - D)\,\dfrac{\boldsymbol{\varepsilon} : \mathcal{H} : \boldsymbol{\varepsilon}}{2} - Y_C \leq 0$
      - Y_C is an energy related to a deformation threshold
    - There is a time history $f\dot{D} = 0$
      - Either damage is increased if $f = 0$
      - Or damage remains the same if $f < 0$
  - Example for Y_C such that damage appears for $\varepsilon = 0.1$



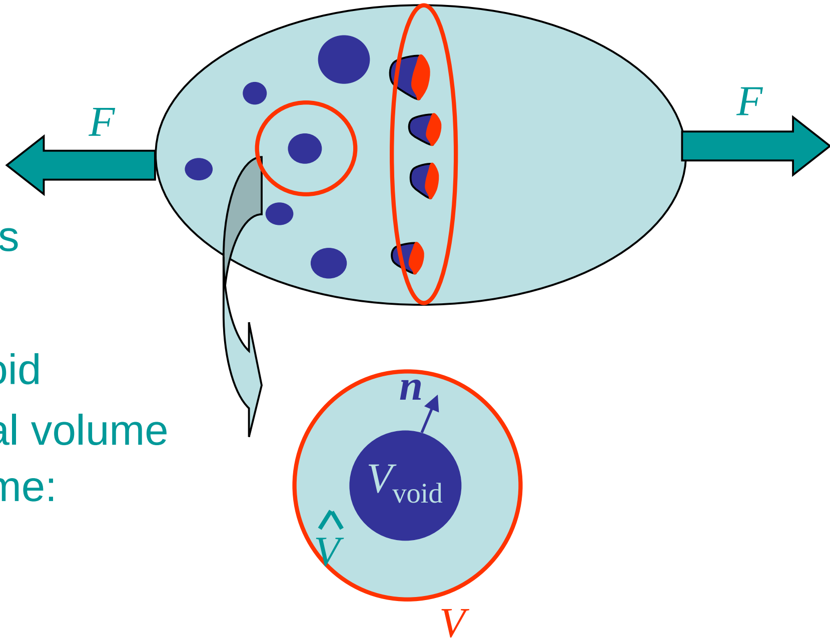
- But for ductile materials plasticity is important as it induces the damage

- Gurson's model, 1977
  - Assumptions
    - Given a rigid-perfectly-plastic material with already existing spherical microvoids
    - Extract a statistically representative sphere V embedding a spherical microvoid
      - Porosity: fraction of voids in the total volume and thus in the representative volume:

$$f_V = \frac{V_{\text{void}}}{V} = 1 - \frac{\hat{V}}{V}$$

with $\hat{V}$ the material part of the volume

      - Material rigid-perfectly plastic ⟹ elastic deformations negligible

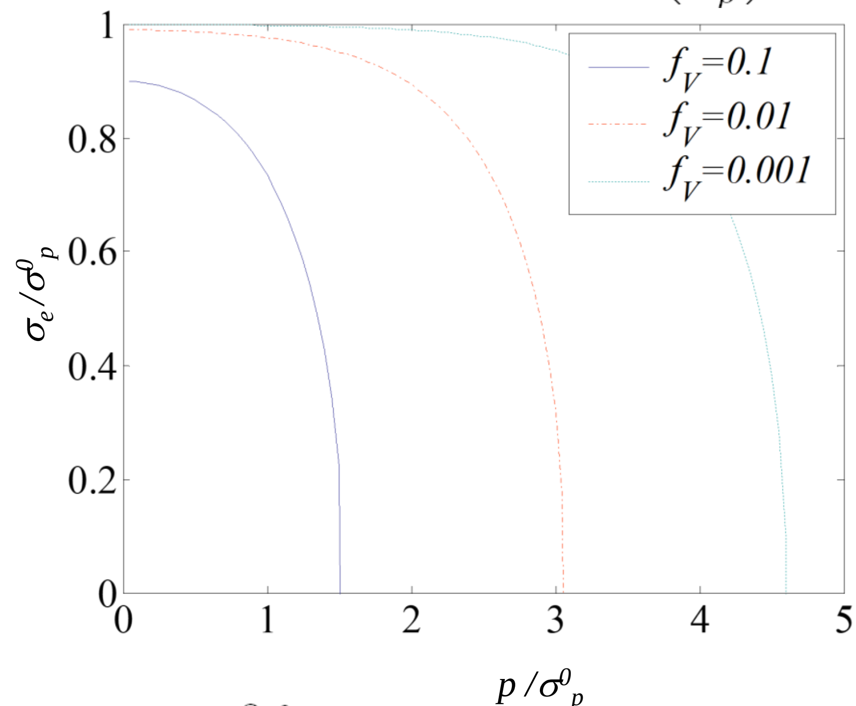


  - Define
    - Macroscopic strains, stresses, potential: $\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$ & W
    - Microscopic strains, stresses, potential: $\hat{\boldsymbol{\varepsilon}}$, $\hat{\boldsymbol{\sigma}}$ & $\hat{W}$

$$\dot{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_V \dot{\hat{\boldsymbol{\varepsilon}}} dV = \frac{1}{V}\int_{\hat{V}} \dot{\hat{\boldsymbol{\varepsilon}}} dV + \frac{1}{V}\int_{V_{\text{void}}} \dot{\hat{\boldsymbol{\varepsilon}}} dV$$

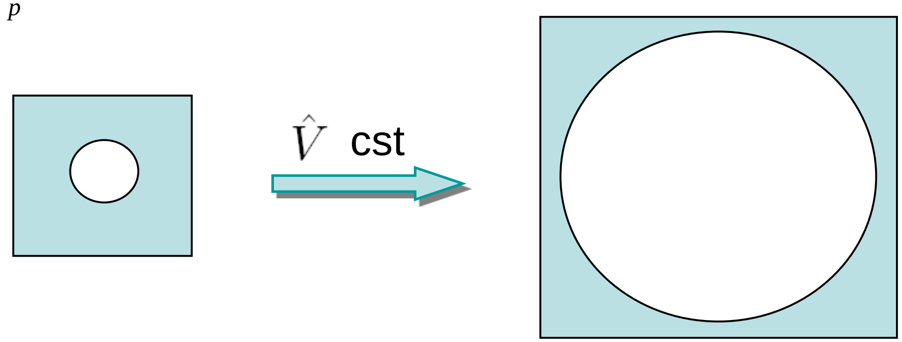
$$\boldsymbol{\sigma} = \frac{\partial \dot{W}}{\partial \dot{\boldsymbol{\varepsilon}}} = \frac{1}{V}\int_{\hat{V}} \frac{\partial \dot{\hat{W}}}{\partial \dot{\hat{\boldsymbol{\varepsilon}}}} : \frac{\partial \dot{\hat{\boldsymbol{\varepsilon}}}}{\partial \dot{\boldsymbol{\varepsilon}}} dV = \frac{1}{V}\int_{\hat{V}} \hat{\boldsymbol{\sigma}} : \frac{\partial \dot{\hat{\boldsymbol{\varepsilon}}}}{\partial \dot{\boldsymbol{\varepsilon}}} dV$$

- Gurson's model, 1977 (4)
  - Shape of the new yield surface $f(\boldsymbol{\sigma}) = \left(\frac{\sigma_e}{\sigma_p^0}\right)^2 + 2 f_V \cosh \frac{\mathrm{tr}(\boldsymbol{\sigma})}{2\sigma_p^0} - f_V^2 - 1 \leq 0$



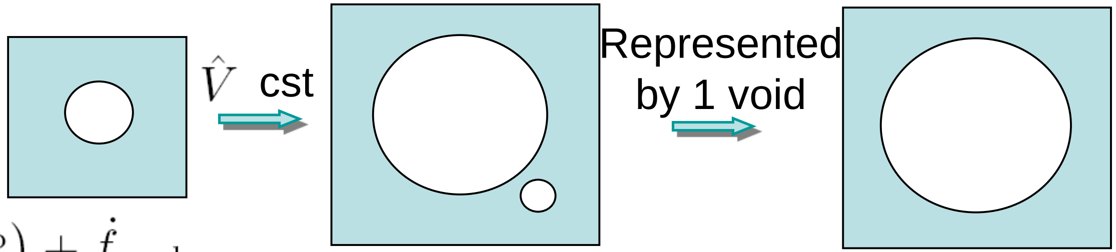
  - Normal flow $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \dot{\lambda}\frac{\partial f}{\partial \boldsymbol{\sigma}}$
  - Evolution of the porosity f_V
    - Assuming isochoric matrix:

$\Rightarrow \dot{f}_V = (1 - f_V)\,\mathrm{tr}\left(\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}\right)$



Damage models

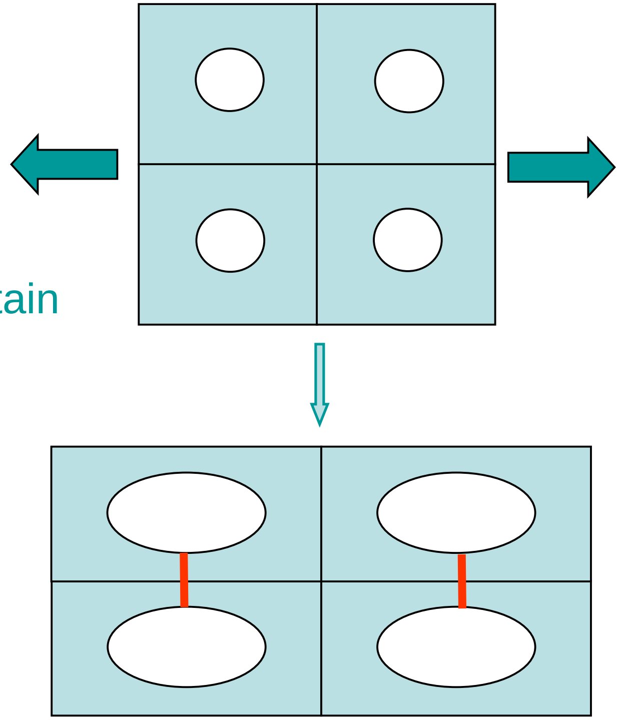
- Hardening
  - Yield criterion $f\left(\boldsymbol{\sigma}\right) = \left(\frac{\sigma_e}{\sigma_p^0}\right)^2 + 2 f_V \cosh \frac{\mathrm{tr}\left(\boldsymbol{\sigma}\right)}{2\sigma_p^0} - f_V^2 - 1 \leq 0$ remains valid but one has to account for the hardening of the matrix $\Longrightarrow \sigma_p^0 \rightarrow \sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right)$
    - In this expression, the equivalent plastic strain of the matrix $\hat{\bar{\varepsilon}}^{\mathrm{p}}$ is used instead of the macroscopic one $\bar{\varepsilon}^{\mathrm{p}}$
  - Values related to the matrix and the macroscopic volume are dependant as the dissipated energies have to match $\Longrightarrow \left(1 - f_V\right) \sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right) \dot{\hat{\bar{\varepsilon}}}^{\mathrm{p}} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$
- Voids nucleation
  - Increase rate of porosity results from
    - Matrix incompressibility
    - Creation of new voids



$\Longrightarrow \dot{f}_V = \left(1 - f_V\right) \mathrm{tr}\left(\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}\right) + \dot{f}_{\mathrm{nucl}}$

- The nucleation rate can be modeled as strain controlled $\Longrightarrow \dot{f}_{\mathrm{nucl}} = A\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right) \dot{\hat{\bar{\varepsilon}}}^{\mathrm{p}}$

- Voids coalescence
  - 1984, Tvergaard & Needleman
    - When two voids are close (f_V ~ f_C), the material loses capacity of sustaining the loading
    - If f_V is still increased, the material is unable to sustain any loading

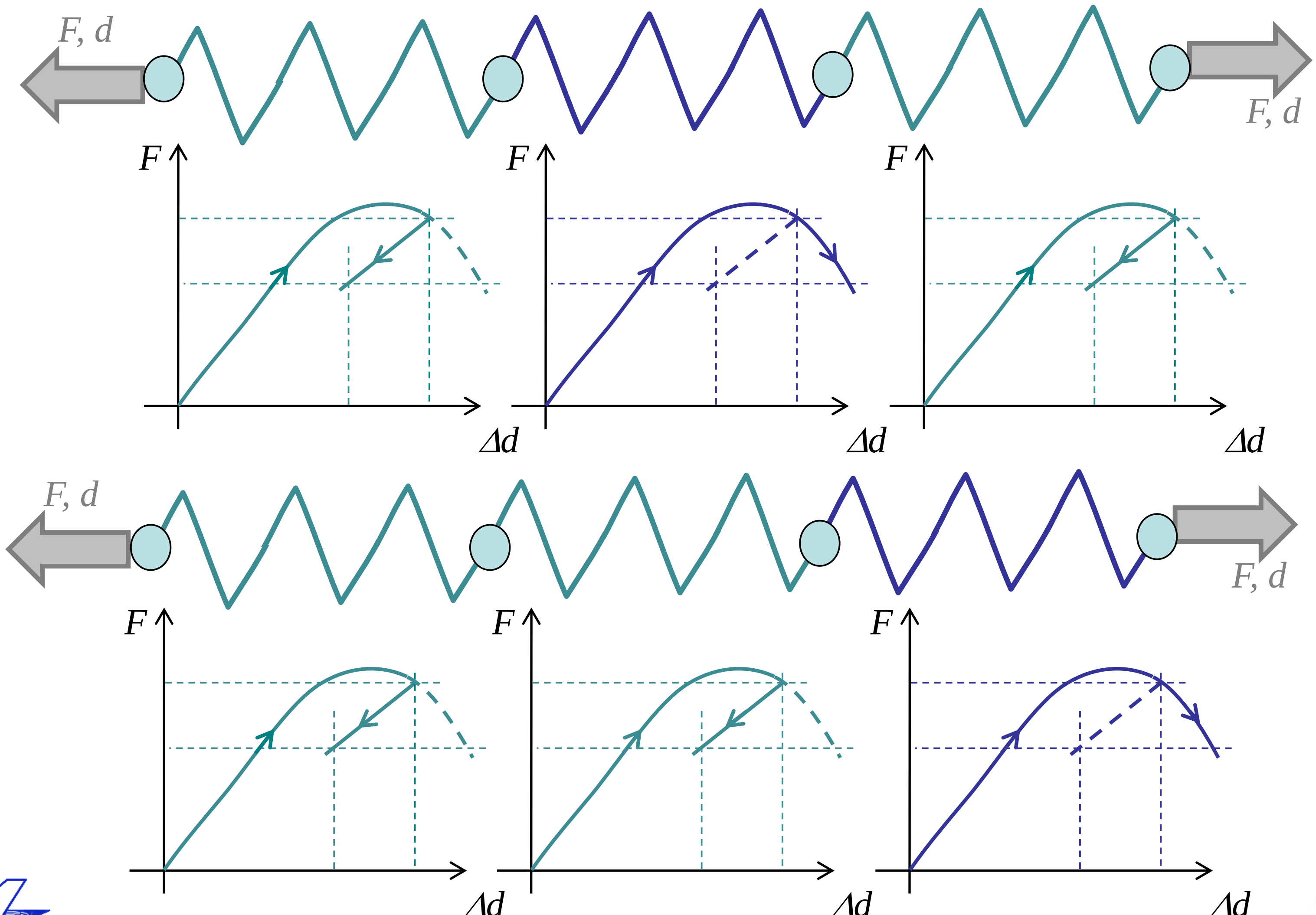


$$f\left(\boldsymbol{\sigma}\right)=\left(\frac{\sigma_e}{\sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right)}\right)^2+2f_V\cosh\frac{\mathrm{tr}\left(\boldsymbol{\sigma}\right)}{2\sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right)}-f_V^2-1\leq 0$$

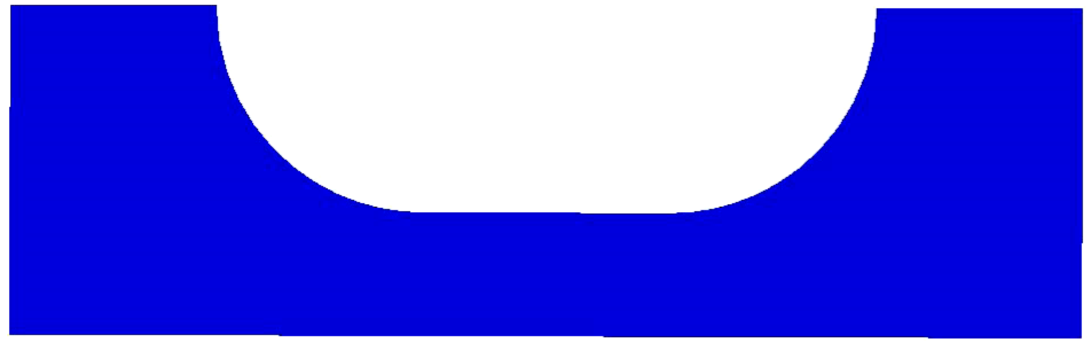
$$f\left(\boldsymbol{\sigma}\right)=\left(\frac{\sigma_e}{\sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right)}\right)^2+2qf_V^*\cosh\frac{\mathrm{tr}\left(\boldsymbol{\sigma}\right)}{2\sigma_p\left(\hat{\bar{\varepsilon}}^{\mathrm{p}}\right)}-q^2{f_V^*}^2-1\leq 0$$

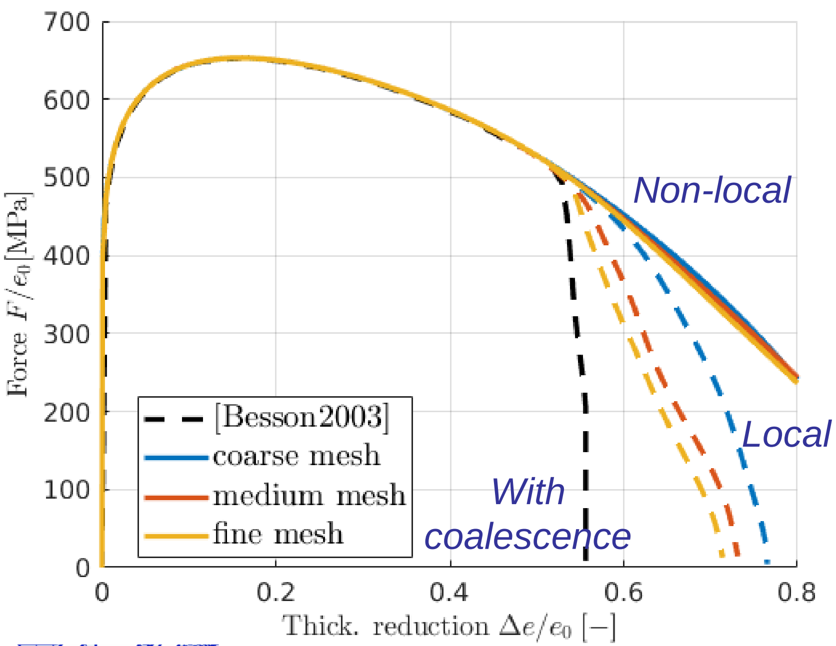
- with $f_V^*=\begin{cases} f_V & \text{if } f_V<f_C \\ f_C+\frac{\frac{1}{q}-f_C}{f_F-f_C}\left(f_V-f_C\right) & \text{if } f_V>f_C \end{cases}$

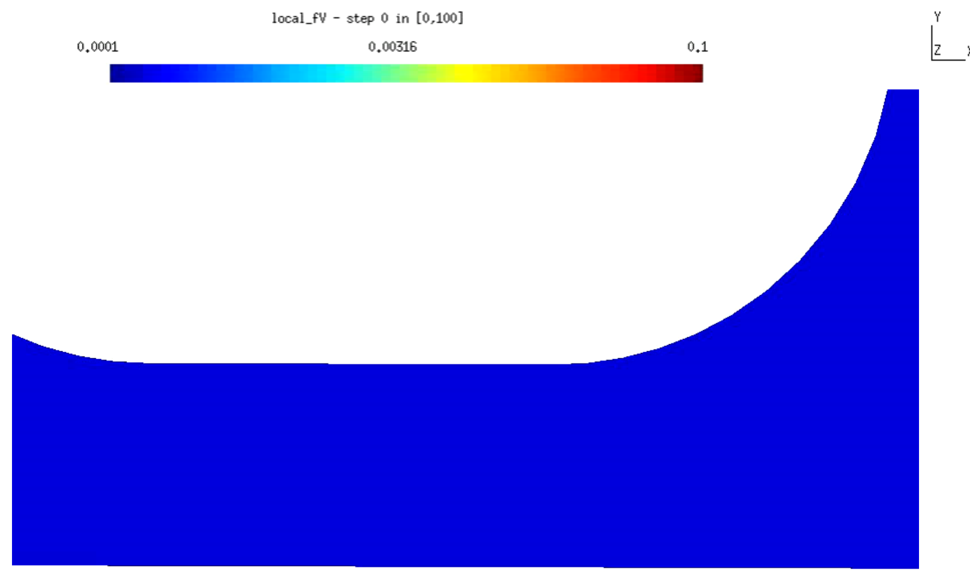
- Softening response
  - Loss of solution uniqueness → mesh dependency



- Softening response (2)
  - Requires non-local models







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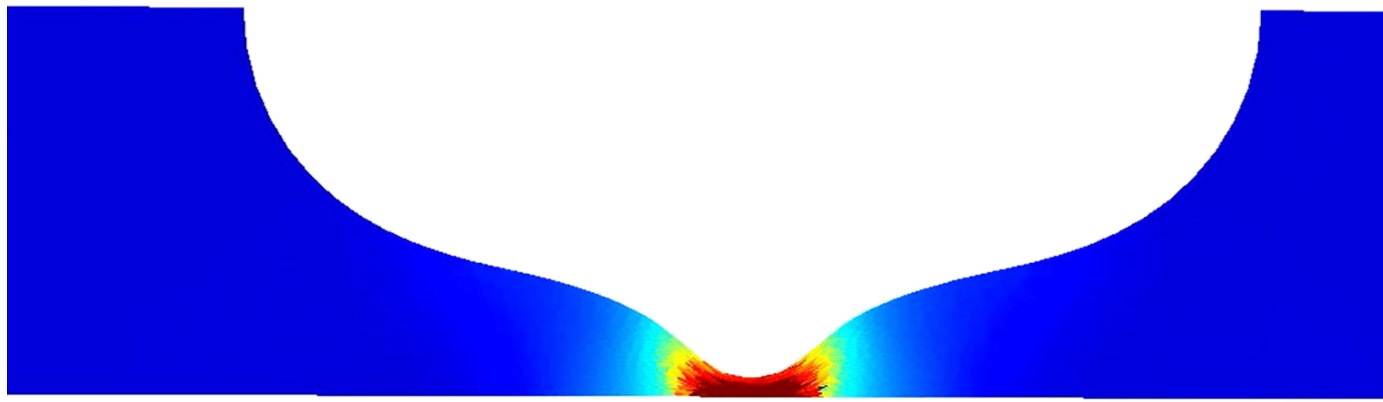
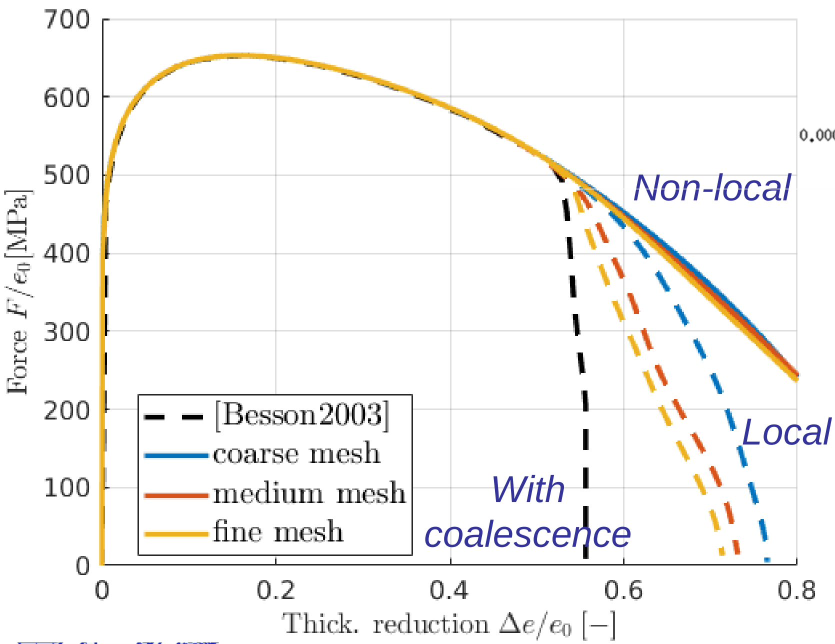
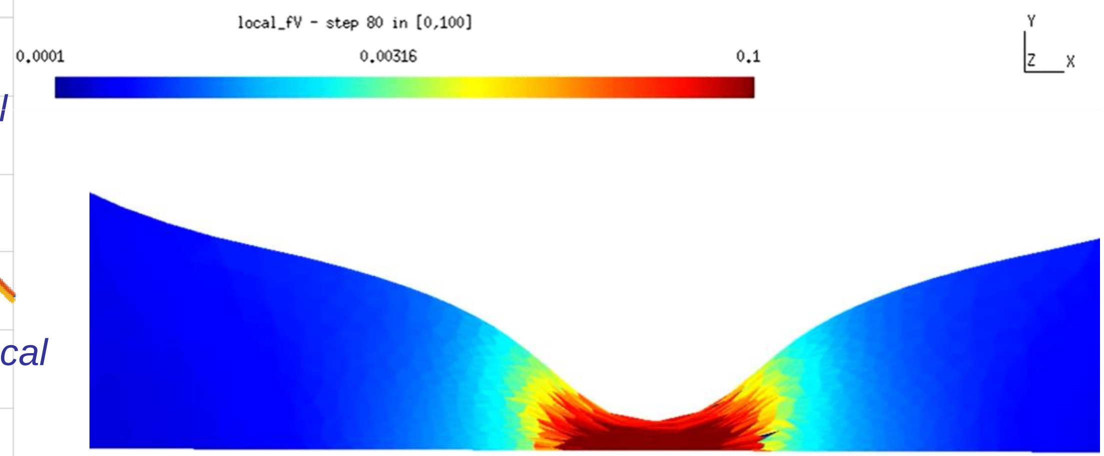
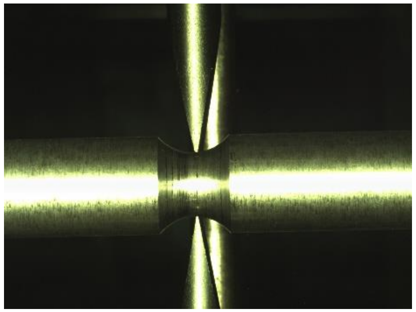
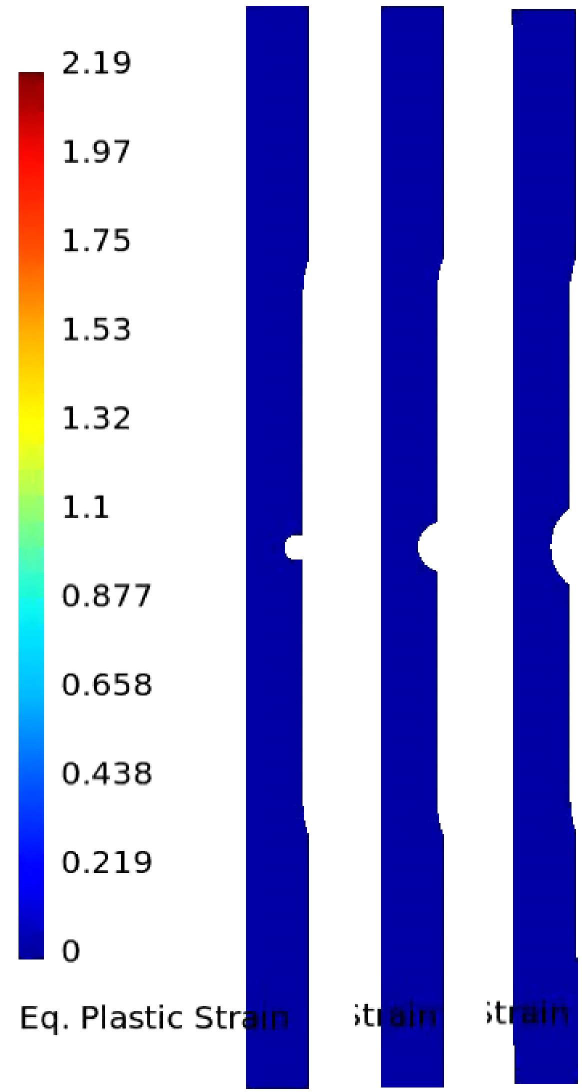




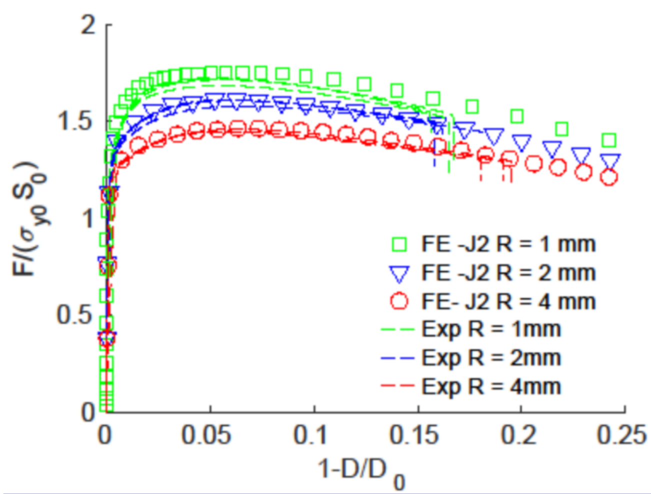


- Complex calibration
  - Experimental tests at different triaxiality states





  - Calibration
    - During plastic localization
    - During voids coalescences
    - For different loading
    - Completed by cell simulations



- Complex calibration
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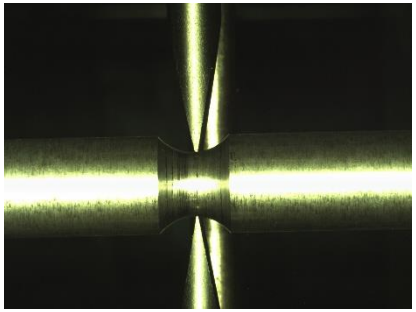

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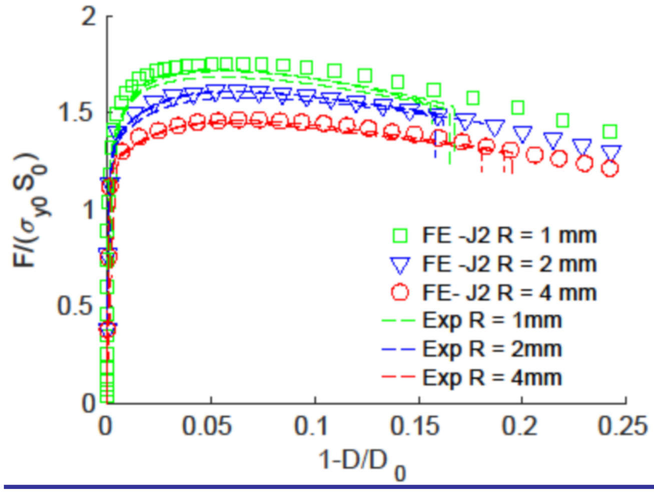
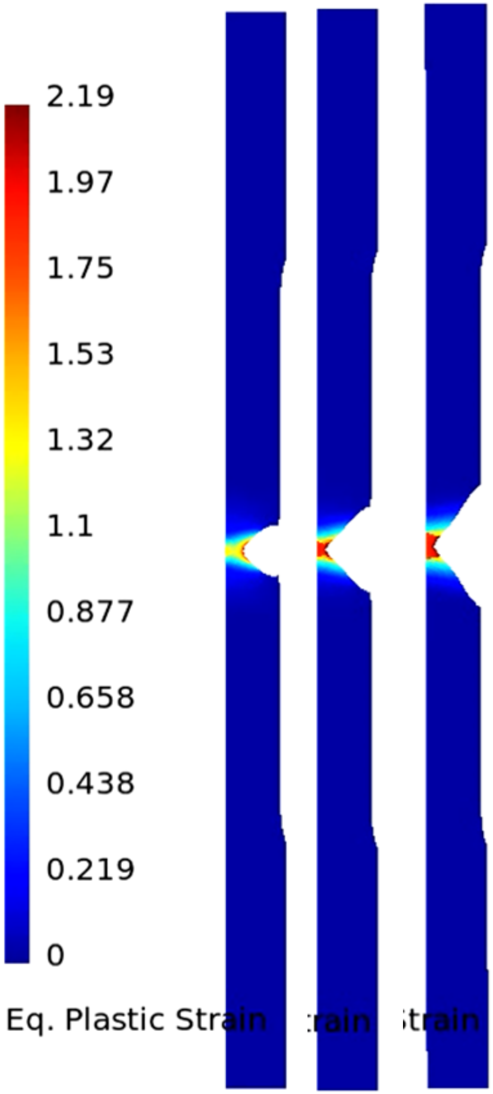
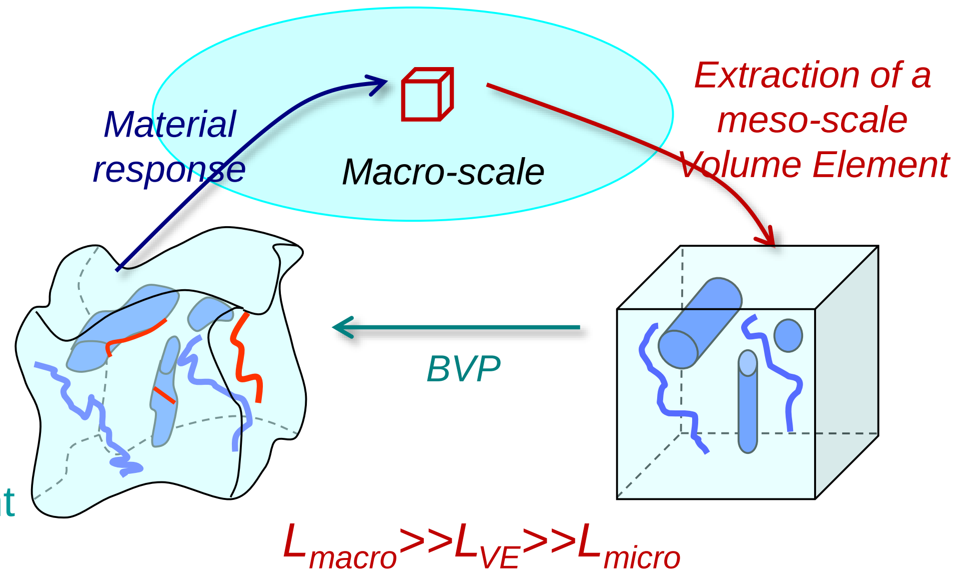


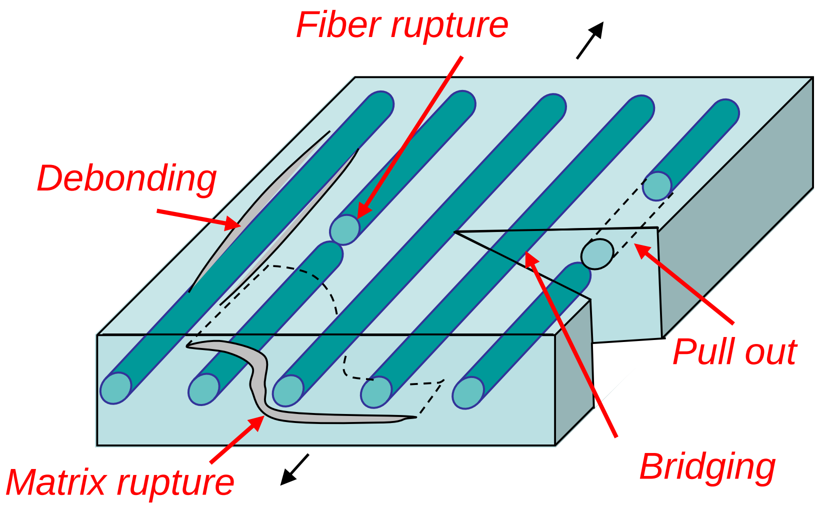


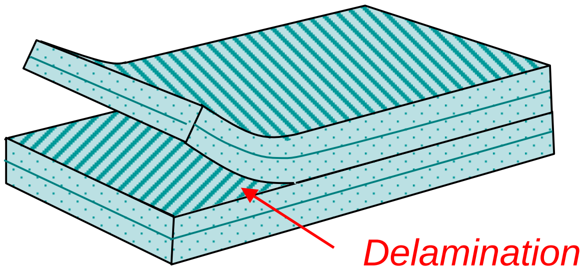
- Some fracture mechanics principles
  - Brittle/ductile materials & Fatigue
  - Linear elastic fracture mechanics
- Computational fracture mechanics for brittle materials
  - Crack propagation
  - Cohesive models
  - XFEM
- Computational fracture mechanics for ductile materials
  - Damage models
- Multiscale methods
  - Composite materials
  - Atomistic models

- Principle
  - Simulate what is happening at small scale with correct physical models
  - 2 BVPs are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)
  - Requires two steps
    - Downscaling: BC of the mesoscale BVP from the macroscale deformation-gradient field
    - Upscaling: The resolution of the mesoscale BVP yields an homogenized macroscale behavior
  - Gurson's model is actually a multiscale model

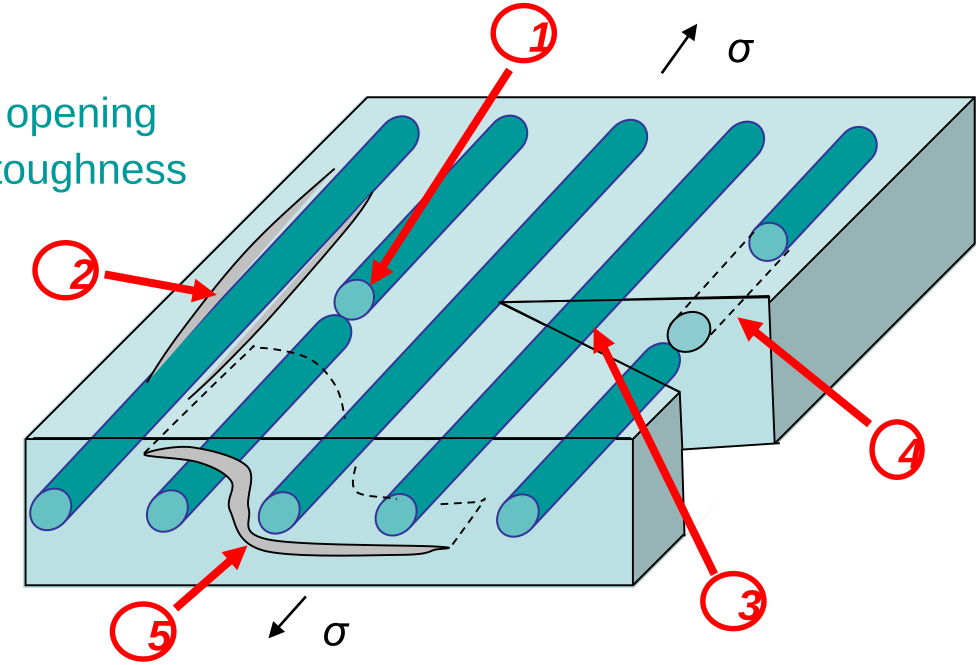


- Example: Failure of composite laminates
  - Heterogeneous materials: failure involves complex mechanisms
  - Failure at different levels
    - Intralaminar failure
    - Delamination

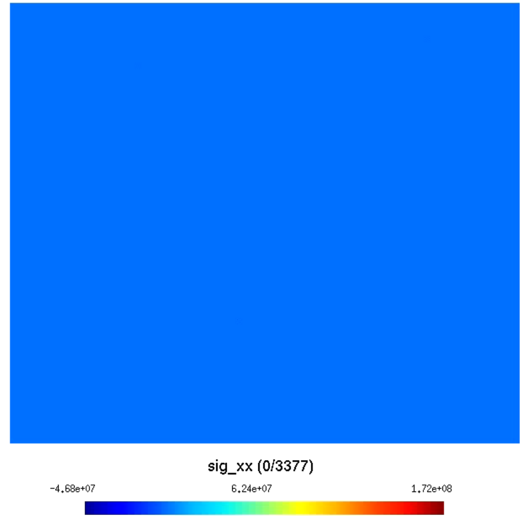


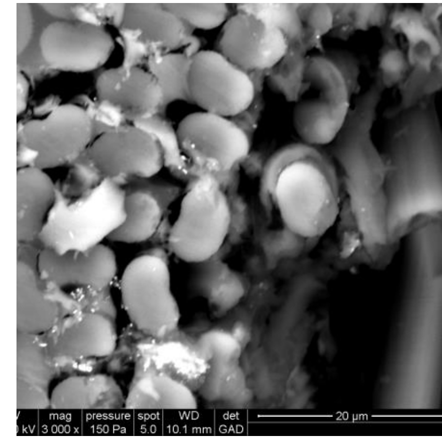


- Intralaminar failure
  - Fiber rupture (1)
    - If no matrix
      - Fiber would not be able to carry any loading
      - Fiber would become useless
    - In reality
      - Matrix transmits the load between the two broken parts
      - Fiber can still (partially) carry the loading
  - Fiber/matrix debonding (2)
  - Fiber bridging (3)
    - Prevents the crack from further opening
    - Corresponds to an increase of toughness
  - Fiber Pullout (4)
  - Matrix cracking (5)
    - Facilitates moisture absorption
    - May initiate delamination between plies
  - Ultimate tensile failure
    - Several of these mechanisms

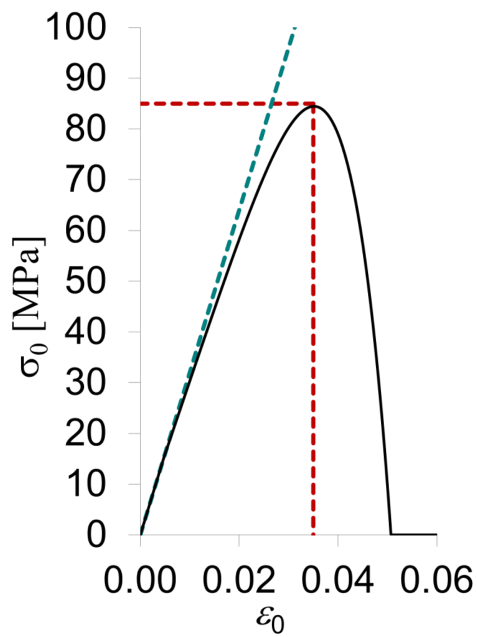


- Intralaminar failure
  - Requires multi-scale approach
    - Micro-Meso damage models
    - Computational homogenization
    - Mean-Field-Homogenization
    - …..
    - A lot of theoretical issues





  - Experimental calibration
    - Complicated because of several modes
    - Ideally from constituents
      - Representative?
    - Ex: 60%-UD Carbon-fiber reinforced epoxy
      - Carbon fiber:
        - » Use of transverse isotropic elastic material
      - Elasto-plastic matrix with damage
        - » Use manufacturer Young's modulus
        - » Use manufacturer strength



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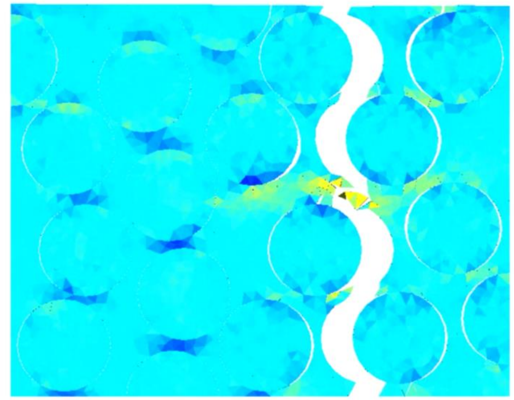

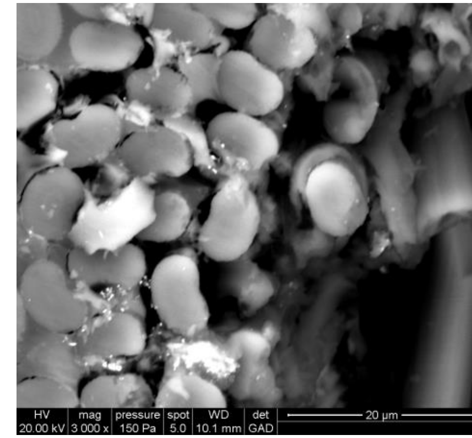

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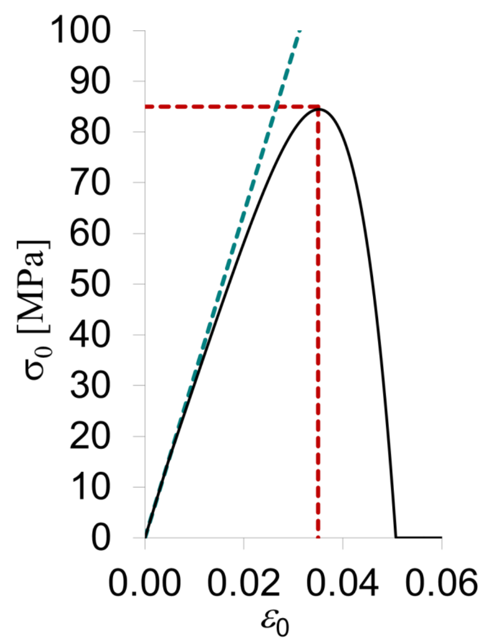
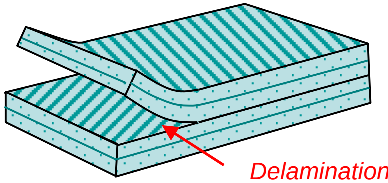
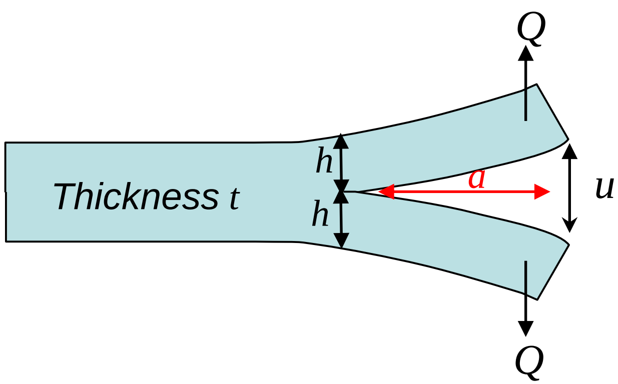
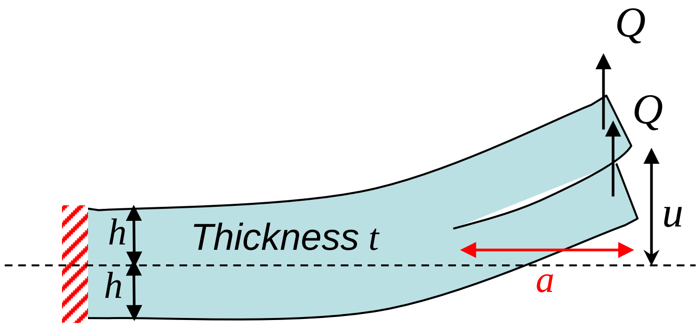


- Interlaminar fracture
  - Due to anisotropy, G_c is not the same in the two directions
    - Mode I and mode II



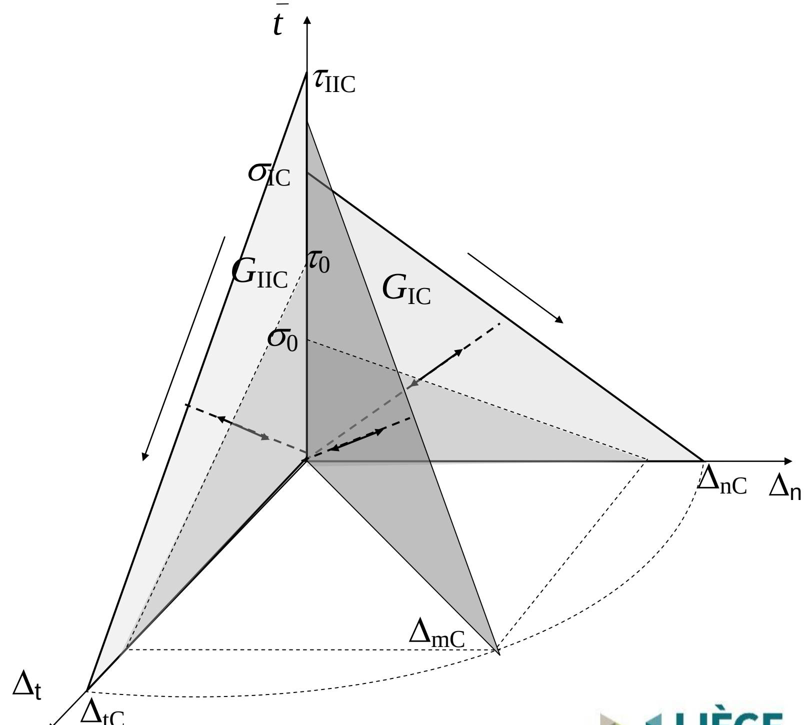




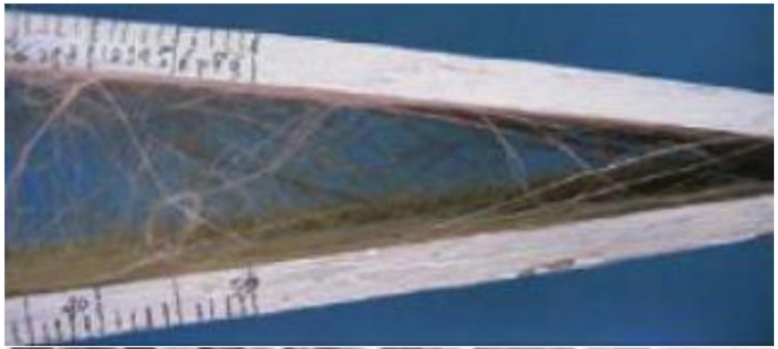
  - Model
    - Cohesive zone model
    - Mixed mode fracture criterion

$$\left(\frac{G_I}{G_{Ic}}\right)^m + \left(\frac{G_{II}}{G_{IIc}}\right)^n = 1$$

where m & n are empirical parameters



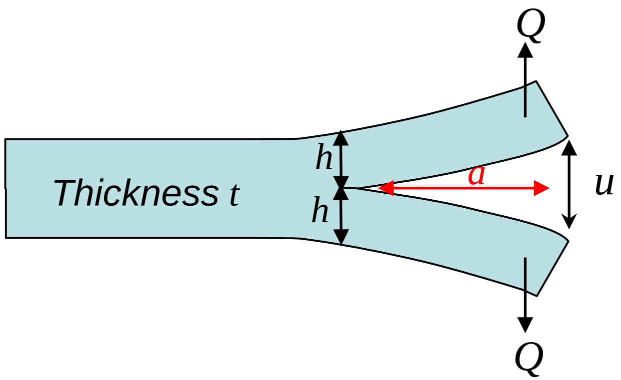
- Interlaminar fracture: Mode I
  - Crack propagates in the matrix (resin)
    - $G_{Ic} = G_c$ of resin?
  - Due to the presence of the fibers
    - $G_{Ic} \neq G_c$ of the pure resin
    - Fiber bridging
      - Increases toughness
    - Fiber/matrix debonding
      - Brittle matrix
        - » Crack surface is not straight as it follows the fibers
        - » More surface created
        - » Higher toughness
      - Tough matrix
        - » Fibers may prevent the damage zone in the matrix from extending far away
        - » Smaller surface created
        - » Lower toughness

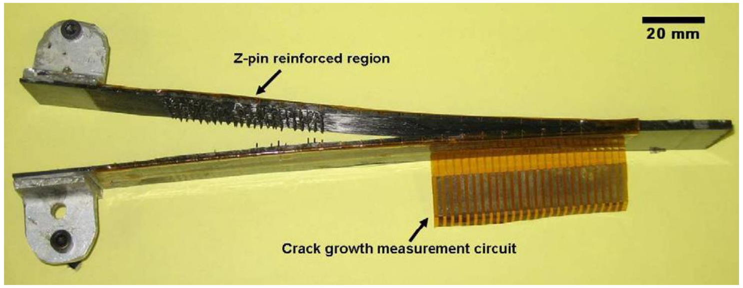


- Interlaminar fracture: Mode I (2)
  - Measure of G_{Ic}
    - DCB

$$\begin{cases} u = \dfrac{8Qa^3}{Eth^3} \\ G = \dfrac{12Q^2a^2}{Et^2h^3} = \dfrac{3u^2Eh^3}{16a^4} = \dfrac{3uQ}{2at} \end{cases}$$

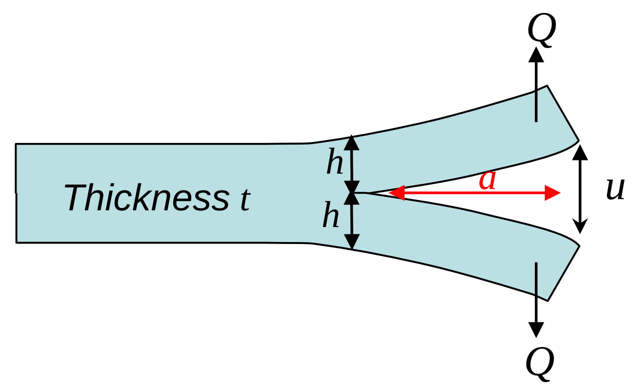
    - At fracture $G_{Ic} = \dfrac{3u_cQ_c}{2at}$
    - The initial delaminated zone is introduced by placing a non-adhesive insert between plies prior to molding

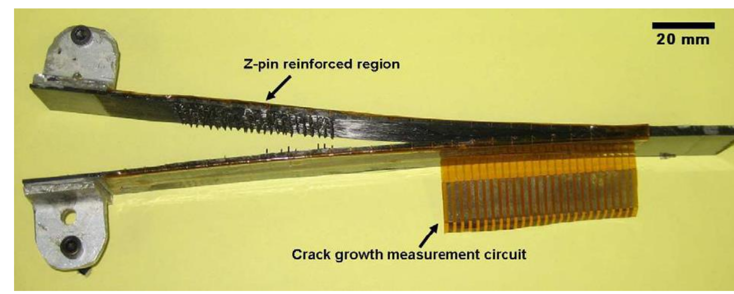




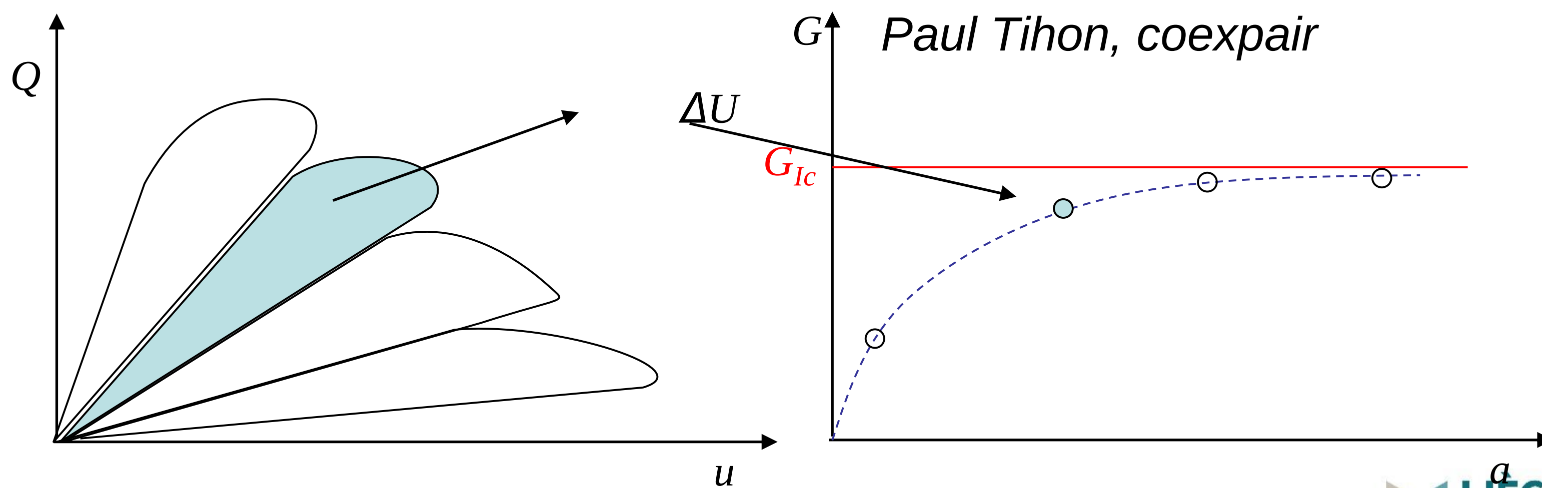
Paul Tihon, coexpair

- Interlaminar fracture: Mode I (3)
  - Measure of G_{Ic} (2)
    - Linear beam theory may give wrong estimates of energy release rate
  - The area method is an alternative solution
    - Periodic loading with small crack propagation increments
      - The loading part is usually nonlinear prior to fracture
    - Since G is the energy released per unit area of crack advance: $G = \frac{\Delta U}{t \Delta a}$

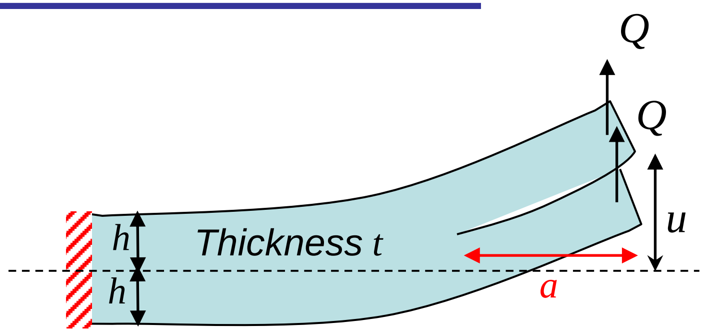




Paul Tihon, coexpair

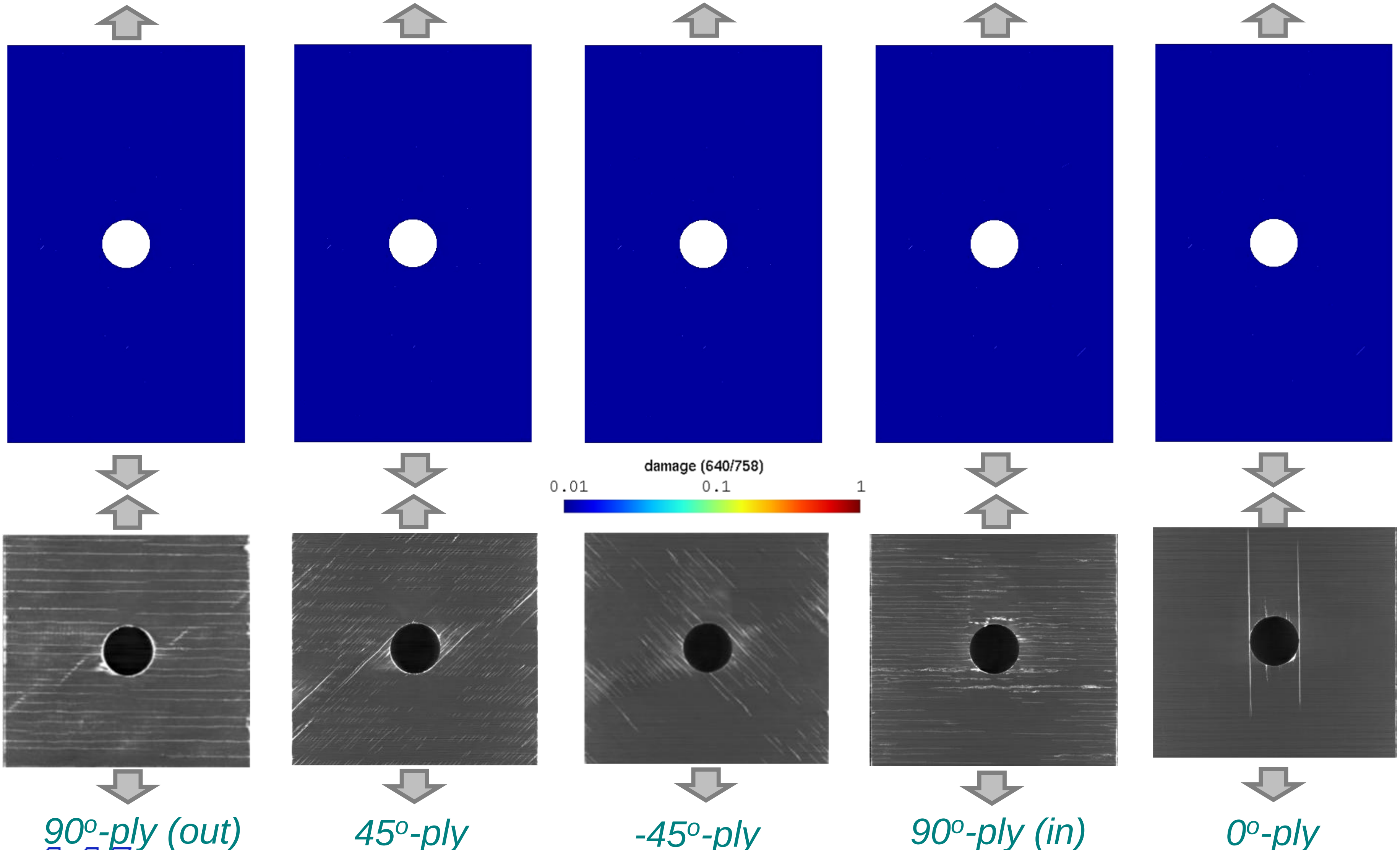


- Interlaminar fracture: Mode II
  - G_{IIc}
    - Usually 2-10 times higher than G_{Ic}
      - Especially for brittle matrix
    - In mode II loading
      - Extended damage zone, containing micro-cracks, forms ahead of the crack tip
      - The formation of this damaged zone is energy consuming
        - » High relative toughness in mode II



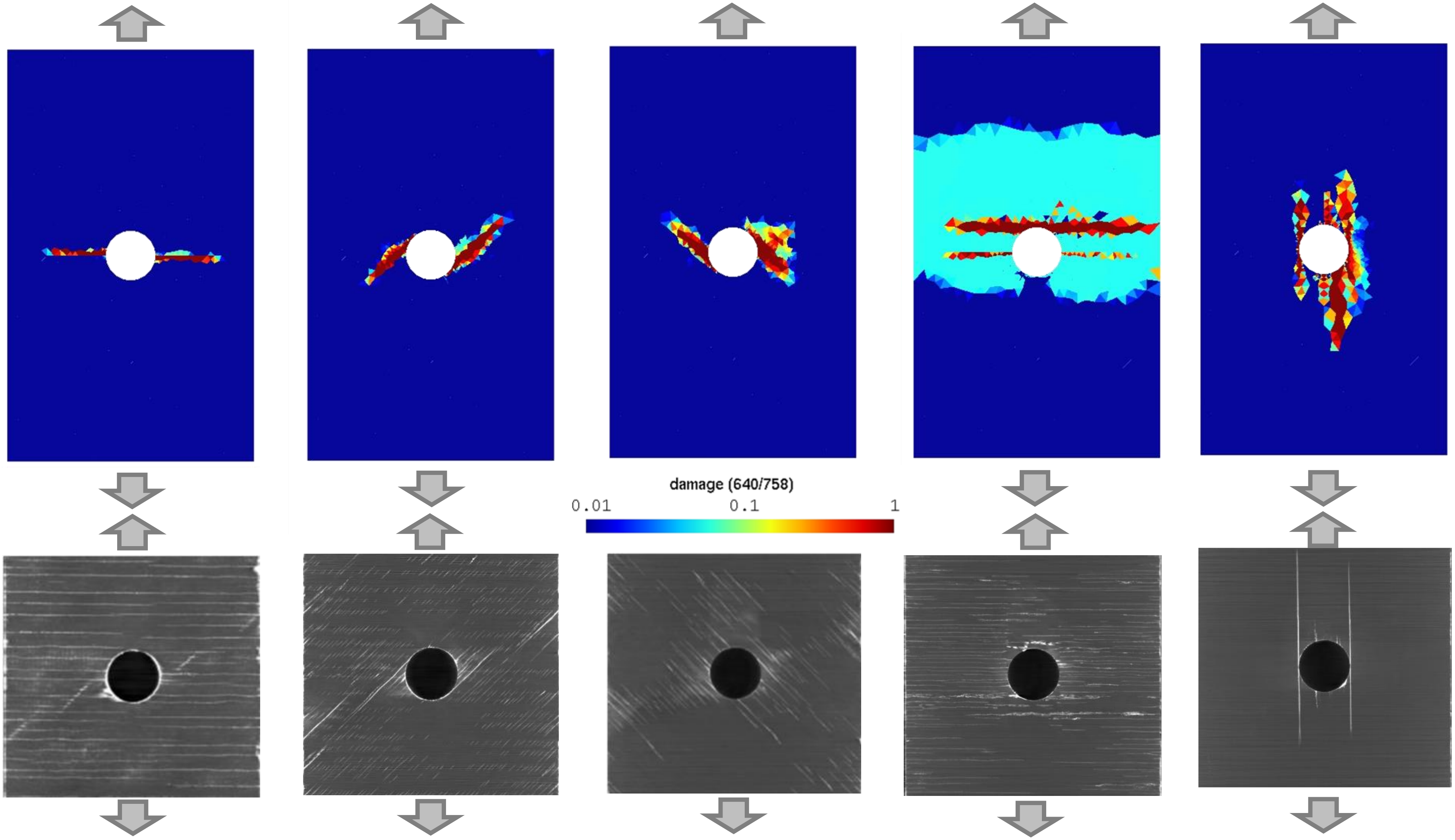
- Note that micro-cracks are 45°-kinked
  - Since pure shearing is involved, this is the direction of maximal tensile stress
  - Thus the micro-cracks are loaded in mode I

- Failure of composite [90º / 45º / -45º / 90º / 0º]$_S$- open hole laminate



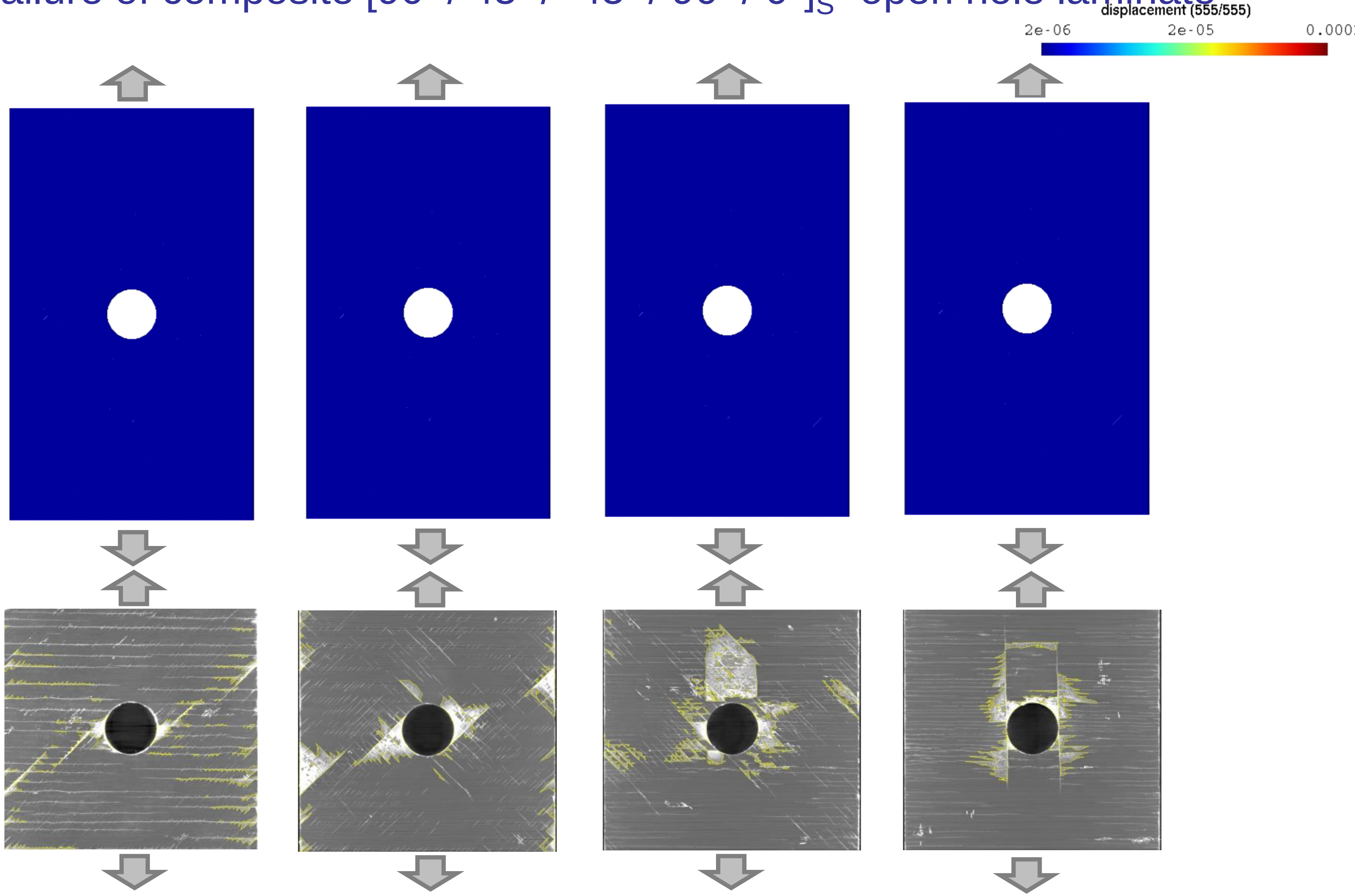
Composite materials

- Failure of composite [90º / 45º / -45º / 90º / 0º]$_S$- open hole laminate



90º-ply (out) | 45º-ply | -45º-ply | 90º-ply (in) | 0º-ply

- Failure of composite [90º / 45º / -45º / 90º / 0º]$_S$- open hole laminate



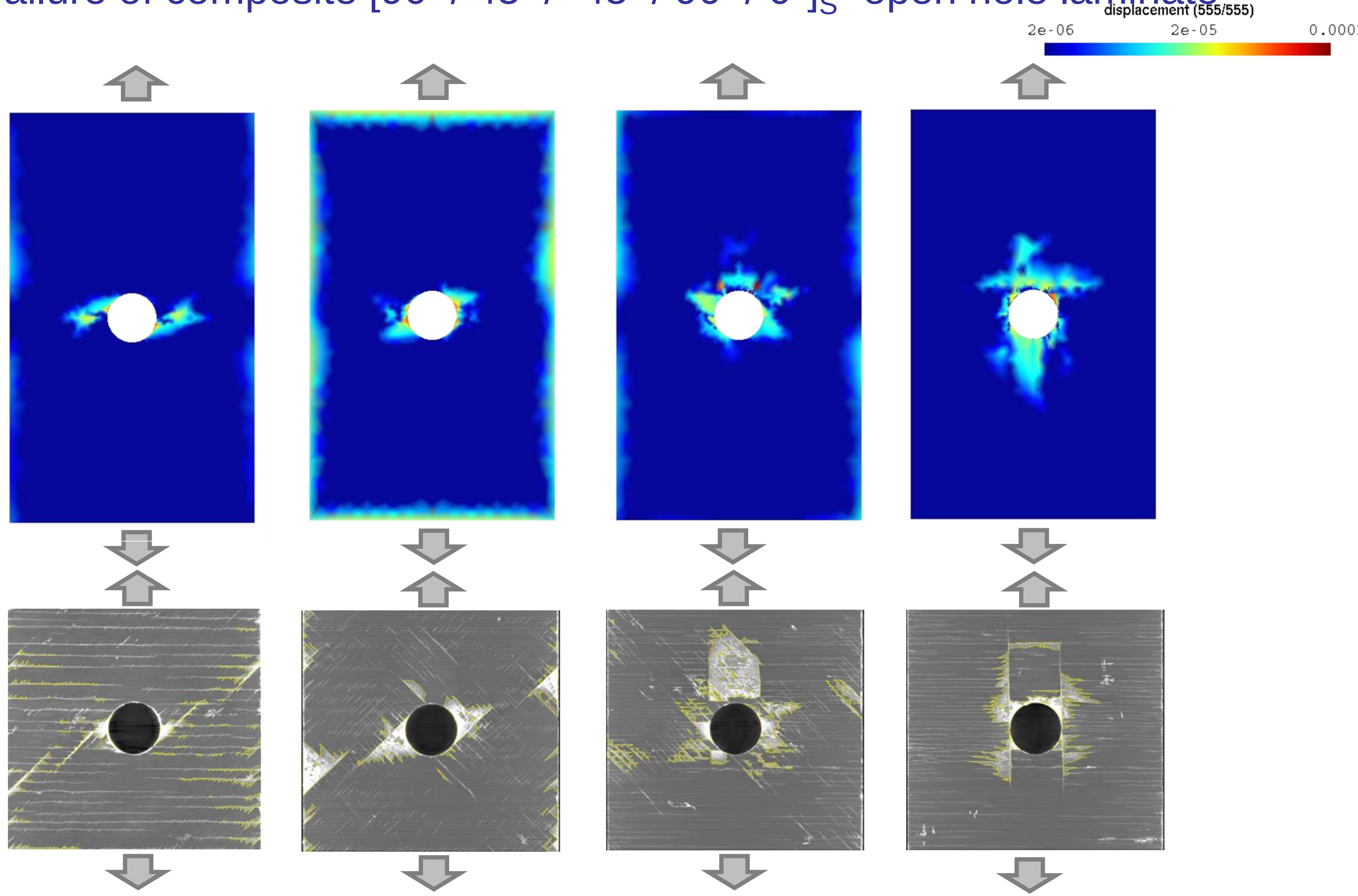
90º (out) / 45º

45º / -45º

-45º / 90º (in)

90º (in) / 0º

- Failure of composite [90º / 45º / -45º / 90º / 0º]$_S$- open hole laminate



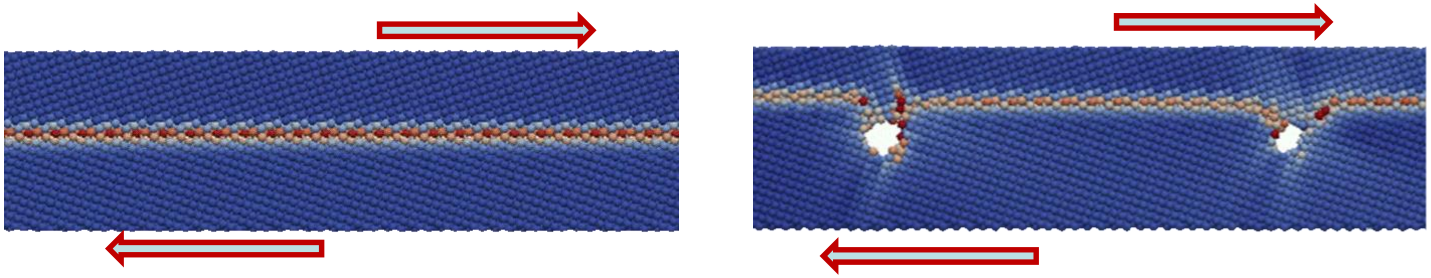
90º (out) / 45º

45º / -45º

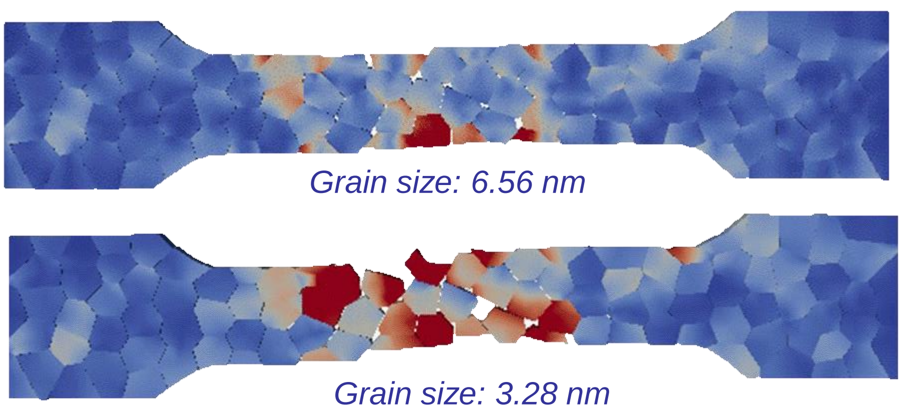
-45º / 90º (in)

90º (in) / 0º

- Example: Failure of polycrystalline materials
  - The mesoscale BVP can also be solved using atomistic simulations



  - Polycrystalline structures can then be studied
    - Finite element for the grains
    - Cohesive elements between the grains
    - Material behaviors and cohesive laws calibrated from the atomistic simulations

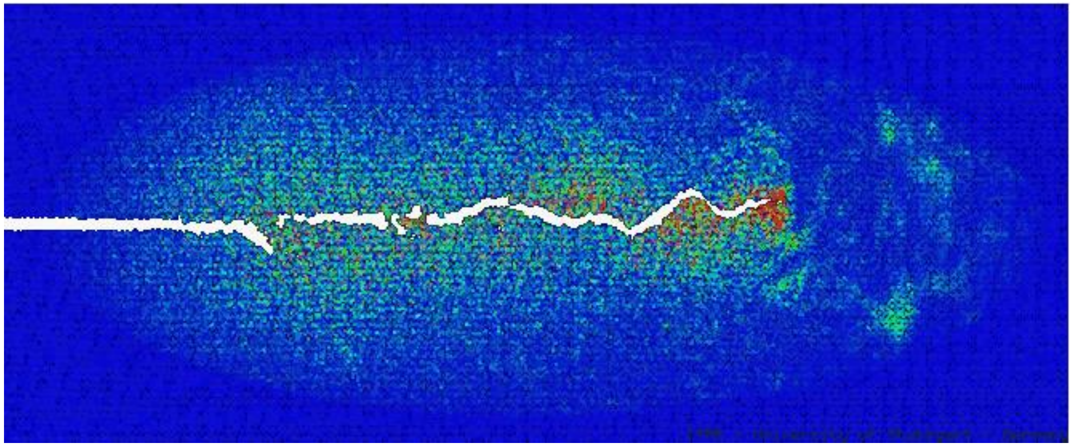


Grain size: 6.56 nm

Grain size: 3.28 nm

Atomistic Methods

- Atomistic models: molecular dynamics
  - Newton equations of motion are integrated for classical particles
  - Particles interact via different types of potentials
    - For metals: Morse-, Lennard-Jones- or Embedded-Atom potentials
    - For liquid crystals: anisotropic Gay-Berne potential
  - The shapes of these potentials are obtained using ab-initio methods
    - Resolution of Schrödinger for a few (<100) atoms
  - Example:
    - Crack propagation in a two dimensional binary model quasicrystal
    - It consists of 250.000 particles and it is stretched vertically
    - Colors represent the kinetic energy of the atoms, that is, the temperature
    - The sound waves, which one can hear during the fracture, can be seen clearly



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References

- *Lecture notes*
  - *Lecture Notes on Fracture Mechanics, Alan T. Zehnder, Cornell University, Ithaca, http://hdl.handle.net/1813/3075*
  - *Fracture Mechanics Online Class, L. Noels, ULg, http://www.ltas-cm3.ulg.ac.be/FractureMechanics*
  - *Fracture Mechanics, Piet Schreurs, TUe, http://www.mate.tue.nl/~piet/edu/frm/sht/bmsht.html*
- *Book*
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