Fracture Mechanics, Damage and Fatigue
Non Linear Fracture Mechanics: Numerical Methods

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Numerical Methods

- **LEFM**
  - Crack propagation
  - Cohesive models
  - XFEM

- **Ductile material**
  - Extension to the brittle methods
  - Damage models

- **Multiscale methods**
  - Atomistic models
• **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

• **Therefore**
  – Linear elastic stress analysis describes the fracture process with accuracy

\[ \sigma_{\text{mode } i} = \frac{K_i}{\sqrt{2\pi r}} f_{\text{mode } i}(\theta) \]

\[ u_{\text{mode } i} = K_i \sqrt{\frac{r}{2\pi}} g_{\text{mode } i}(\theta) \]
• SIF \((K_I, K_{II}, K_{III})\): asymptotic solution in linear elasticity

• Crack closure integral
  – Energy required to close the crack by an infinitesimal \(da\)
  – If an internal potential exists
    \[ G = -\partial_A (E_{\text{int}} - W_{\text{ext}}) = -\partial_A \Pi_T \]
  with
  \[ \Delta \Pi_T = \int_{\Delta A} \int_{\Delta [u]} t([u']) \cdot [d\mathbf{u}'] d\Delta A \]
  • AND if linear elasticity
    \[ G = -\partial_A \Delta \Pi_T = -\lim_{\Delta A \to 0} \frac{1}{\Delta A} \int_{\Delta A} \frac{1}{2} t \cdot [\Delta \mathbf{u}] d\partial A \]
  – AND if straight ahead growth

• \(J\) integral
  – Energy that flows toward crack tip
  – If an internal potential exists
    \[ J = \int_{\Gamma} [U(\mathbf{\varepsilon}) \mathbf{n}_x - \mathbf{u}_x \cdot \mathbf{T}] d\mathbf{l} \]
    • Is path independent if the contour \(\Gamma\) embeds a straight crack tip
    • BUT no assumption on subsequent growth direction
    • If crack grows straight ahead:
      \[ G = J \]
    • If linear elasticity:
      \[ J = \frac{K_I^2}{E'} + \frac{K_{II}^2}{E'} + \frac{K_{III}^2}{2\mu} \]
    • Can be extended to plasticity if no unloading (power law)
LEFM

• **Crack growth criteria**
  - Crack growth criterion is \( G \geq G_C \)
  - Stability of the crack is reformulated (in 2D)
    - Stable crack growth if \( \partial_a G \leq \partial_a R_C \)
    - Unstable crack growth if \( \partial_a G > \partial_a R_C \)
  - Crack growth direction
    - Method of the maximum hoop stress
      - Crack criterion
        \[
        \left( \sqrt{2\pi r} \sigma_{\theta\theta} (r, \theta^*) \right) \geq K_C
        \]
        with \( \partial_{\theta} \sigma_{\theta\theta} \mid_{\theta^*} = 0 \) \& \( \partial^2_{\theta\theta} \sigma_{\theta\theta} \mid_{\theta^*} < 0 \)
      - In case of mixed loading
        \[
        \cot \beta^* = \frac{K_{II}}{K_I}
        \]
      - This corresponds to
        \[
        \begin{cases}
        K_C = \sqrt{2\pi r} \sigma_{\theta\theta} \mid_{\theta^*} = K_I \cos^3 \frac{\theta^*}{2} - \frac{3K_{II}}{2} \sin \theta^* \cos \frac{\theta^*}{2} \\
        2 \tan \left( \frac{\theta^*}{2} \right) - \cot \left( \frac{\theta^*}{2} \right) = \tan \beta^* = \frac{K_I}{K_{II}}
        \end{cases}
        \]
Crack propagation

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

- 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 $K_i$ (see lecture on SIF)
  - Use criterion on crack propagation
    - Example: the maximal hoop stress criterion
      \[
      \left( \sqrt{2\pi r} \sigma_{\theta\theta}(r, \theta^*) \right) \geq K_c
      \]
      with crack propagation direction obtained by
      \[
      \partial_\theta \sigma_{\theta\theta} \big|_{\theta^*} = 0 \quad \& \quad \partial^2_{\theta\theta} \sigma_{\theta\theta} \big|_{\theta^*} < 0
      \]
  - If the crack propagates
    - Move crack tip by $\Delta a$ in the $\theta^*$-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
Cohesive elements

• 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 $\delta_t$, there are attractive forces (see overview lecture)

  – For elasticity $J = \int_0^{\delta_t} \sigma_y(\delta) d\delta$ (recall lecture on cohesive zone)
    • So the area below the $\sigma$-$\delta$ curve corresponds to $G_C$ if crack grows straight ahead

  – This model requires only 2 parameters
    • Peak cohesive traction $\sigma_{\text{max}}$ (spall strength)
    • Fracture energy $G_C$
    • Shape of the curves has no importance as long as it is monotonically decreasing
Cohesive elements

- **Insertion of cohesive elements**
  - Between 2 volume elements
  - Computation of the opening (cohesive element)
    - Normal to the interface in the deformed configuration \( N^- \)
    - Normal opening \( \delta_n = \max([u] \cdot N^-, 0) \)
    - Sliding \( \delta_s = [u] - [u] \cdot N^- N^- \)
    - Resulting opening \( \delta = \sqrt{\delta_n^2 + \beta_c^2 \| \delta_s \|^2} \)
      with \( \beta_c \) 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
      \[
      t = \frac{\partial \phi}{\partial \delta} = \frac{\partial \phi}{\partial \delta_n} N^- + \frac{\partial \phi}{\partial \delta_s} \delta_s
      \]
Cohesive elements

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

- Examples
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
    • So parallelization is mandatory
  – Could be mesh dependant
eXtended Finite Element Method

• How to get rid of conformity requirements?
• Key principles
  – For a FE discretization, the displacement field is approximated by
    \[ u_h(\xi^i) = \sum_{a \in I} N^a(\xi^i) u^a \]
    - Sum on nodes \( a \) in the set \( I \) (11 nodes here)
    - \( u^a \) are the nodal displacements
    - \( N^a \) are the shape functions
    - \( \xi^i \) are the reduced coordinates
  – XFEM
    - New degrees of freedom are introduced to account for the discontinuity
    - It could be done by inserting new nodes (\( \times \)) 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 (\( \circ \))
Key principles (2)

- New degrees of freedom are introduced to account for the discontinuity

\[ u_h (\xi^i) = \sum_{a \in I} N^a (\xi^i) u^a + \sum_{a \in J} N^a (\xi^i) F^a (\xi^i) u^{*a} \]

  - \( J \), 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 \( \text{lsn}(\xi^i, \xi^{i*}) \) is the signed distance between a point \( \xi^i \) of the solid and its projection \( \xi^{i*} \) on the crack

\[ u_h (\xi^i) = \sum_{a \in I} N^a (\xi^i) u^a + \sum_{a \in J} N^a (\xi^i) H \left( \text{lsn} \left( \xi^i, \xi^{i*} \right) \right) u^{*a} \]

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

\[
\mathbf{u}_h (\xi^i) = \sum_{a \in I} N^a (\xi^i) \mathbf{u}^a + \sum_{a \in J} N^a (\xi^i) H \left( \ln \left( \xi^i, \xi'^i \right) \right) \mathbf{u}^*a \\
+ \sum_{a \in K} N^a (\xi^i) \sum_b \Psi_b (\xi^i) \psi_b^a
\]

• LEFM solution is asymptotic \(\rightarrow\) only nodes close to crack tip can be enriched
• $\psi_b^a$ is the new degree $b$ at node $a$ (more than one see next slide)
• $\Psi_b$ is the new shape function $b$ (more than one see next slide)
eXtended Finite Element Method

• Key principles (4)
  
  – New enrichment with LEFM solution (2)

\[
\mathbf{u}_h(\xi^i) = \sum_{a \in I} N^a(\xi^i) \mathbf{u}^a + \sum_{a \in J} N^a(\xi^i) H\left(\ln\left(\xi^i, \xi^{i*}\right)\right) \mathbf{u}^{*a} \\
\quad + \sum_{a \in K} N^a(\xi^i) \sum_b \Psi_b(\xi^i) \psi_b^a
\]

  – \( \Psi_b \) and \( \psi_b^a \) from LEFM solutions

\[
\mathbf{u}_{x'} = \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ K_I \cos\frac{\theta}{2} \left[ \kappa - 1 + 2 \sin^2\frac{\theta}{2} \right] + K_{II} \sin\frac{\theta}{2} \left[ \kappa + 1 + 2 \cos^2\frac{\theta}{2} \right] \right\}
\]

\[
\mathbf{u}_{y'} = \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ K_I \sin\frac{\theta}{2} \left[ \kappa + 1 - 2 \cos^2\frac{\theta}{2} \right] + K_{II} \cos\frac{\theta}{2} \left[ 1 - \kappa + 2 \sin^2\frac{\theta}{2} \right] \right\}
\]

\[
\mathbf{u}_{z'} = \frac{2K_{III}(1+\nu)}{E} \sqrt{\frac{2r}{\pi}} \sin\frac{\theta}{2}
\]
Key principles (5)

- New enrichment with LEFM solution (3)
  
  But

\[ u_{x'} = \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ K_I \cos \frac{\theta}{2} \left[ \kappa - 1 + 2 \sin^2 \frac{\theta}{2} \right] + K_{II} \sin \frac{\theta}{2} \left[ \kappa + 1 + 2 \cos^2 \frac{\theta}{2} \right] \right\} \]

\[ u_{y'} = \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ K_I \cos \frac{\theta}{2} \left[ \kappa - 1 \right] + K_{II} \sin \frac{\theta}{2} \left[ \kappa + 1 \right] \right\} \]

\[ u_{z'} = \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ K_I \sin \frac{\theta}{2} \left[ \kappa + 1 - 2 \cos^2 \frac{\theta}{2} \right] + K_{II} \cos \frac{\theta}{2} \left[ 1 - \kappa + 2 \sin^2 \frac{\theta}{2} \right] \right\} \]

- We still have \[ u_z' = \frac{2K_{III}}{1 + \nu} \sqrt{\frac{2r}{\pi}} \sin \frac{\theta}{2} \]

We have determined 4 independent shape functions \( \Psi_b \)
• **Key principles (6)**
  – New enrichment with LEFM solution (4)
    • Vectors of unknowns \(\psi_b\) and shape functions \(\Psi_b\) are now defined
      \[
      \begin{align*}
      \mathbf{u}_x &= (\psi_x)_1 \sqrt{r} \sin \frac{\theta}{2} + (\psi_x)_2 \sqrt{r} \cos \frac{\theta}{2} + (\psi_x)_3 \sqrt{r} \sin \frac{\theta}{2} \sin \theta + (\psi_x)_4 \sqrt{r} \cos \frac{\theta}{2} \sin \theta \\
      \mathbf{u}_y &= (\psi_y)_1 \sqrt{r} \sin \frac{\theta}{2} + (\psi_y)_2 \sqrt{r} \cos \frac{\theta}{2} + (\psi_y)_3 \sqrt{r} \sin \frac{\theta}{2} \sin \theta + (\psi_y)_4 \sqrt{r} \cos \frac{\theta}{2} \sin \theta \\
      \mathbf{u}_z &= (\psi_z)_1 \sqrt{r} \sin \frac{\theta}{2} + (\psi_z)_2 \sqrt{r} \cos \frac{\theta}{2} + (\psi_z)_3 \sqrt{r} \sin \frac{\theta}{2} \sin \theta + (\psi_z)_4 \sqrt{r} \cos \frac{\theta}{2} \sin \theta
      \end{align*}
      \]
    • We have 12 new degrees of freedom on the LEFM-enriched nodes
      \[
      \mathbf{u}_h (\xi^i) = \sum_{a \in I} N^a (\xi^i) \mathbf{u}^a + \sum_{a \in J} N^a (\xi^i) H \left( \text{lsn} \left( \xi^i, \xi^i* \right) \right) \mathbf{u}^*\alpha + \sum_{a \in K} N^a (\xi^i) \sum_{b=1}^4 \psi_b (r (\xi^i), \theta (\xi^i)) \psi_b^a
      \]
    • Remark: as \(\Psi_1\) is discontinuous we do not need Heaviside functions for \(K\)-nodes
Key principles (7)

- How are $\Psi_b (r (\xi^i), \theta (\xi^i))$ evaluated?
  - New level sets
    - Normal level set $lsn(\xi^i, \xi^{**})$ is the normal signed distance between a point $\xi^i$ of the solid and the crack tip $\xi^{**}$
    - Tangent level set $lst(\xi^i, \xi^{**})$ is the tangential signed distance between a point $\xi^i$ of the solid and the crack tip $\xi^{**}$

\[
\begin{align*}
  r &= \sqrt{lsn^2(\xi^i, \xi^{**}) + lst^2(\xi^i, \xi^{**})} \\
  \theta &= \pm \arctan \frac{lsn(\xi^i, \xi^{**})}{lst(\xi^i, \xi^{**})}
\end{align*}
\]
• Crack propagation criterion
  – Requires the values of the SIFs
    • Using $\psi^a_b$ as

\[
\begin{align*}
\mathbf{u}_{x'} &= \frac{1 + \nu}{E} \sqrt{\frac{r}{2\pi}} \left\{ \bar{K}_I \cos \frac{\theta}{2} [\kappa - 1] + \bar{K}_I \sin \frac{\theta}{2} \sin \theta + \right. \\
&\quad \left. \bar{K}_{II} \sin \frac{\theta}{2} [\kappa + 1] + \bar{K}_{II} \cos \frac{\theta}{2} \sin \theta \right\}
\end{align*}
\]

was substituted by

\[
\begin{align*}
\mathbf{u}_x &= (\psi_1) \sqrt{r} \sin \frac{\theta}{2} + (\psi_2) \sqrt{r} \cos \frac{\theta}{2} + (\psi_3) \sqrt{r} \sin \frac{\theta}{2} \sin \theta + (\psi_4) \sqrt{r} \cos \frac{\theta}{2} \sin \theta
\end{align*}
\]
• **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
        » 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)
          $I^s = J^s - J - J^{aux} = \frac{2}{E'} (K_I K_I^{aux} + K_{II} K_{II}^{aux}) + \frac{1}{\mu} K_{III} K_{III}^{aux}$
          » 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
      \[
      \left( \sqrt{2\pi r} \sigma_{\theta\theta} (r, \theta^*) \right) \geq K_C \quad \text{with} \quad \partial_\theta \sigma_{\theta\theta} |_{\theta^*} = 0 \quad \& \quad \partial^2_{\theta\theta} \sigma_{\theta\theta} |_{\theta^*} < 0
      \]
eXtended Finite Element Method

• 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
Ductile materials

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

- **Introduction to damage (1D)**
  - As there are voids in the material, only a reduced surface is balancing the traction
    - Virgin section $S \rightarrow \sigma_{xx}^{\text{virgin}} = \frac{F}{S} = \sigma_{xx}$
    - 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 $\hat{\sigma}_{xx} = \frac{F}{S (1 - D)} = \frac{\sigma_{xx}}{1 - D}$
  - Resulting deformation
    - Hooke’s law is still valid if it uses the effective stress $\varepsilon_{xx} = \frac{\hat{\sigma}}{E} = \frac{\sigma_{xx}}{E (1 - D)}$
    - So everything is happening as if Hooke’s law was multiplied by $(1-D)$
  - Isotropic 3D linear elasticity $\sigma = (1 - D) \mathcal{H} : \varepsilon$
  - Failure criterion: $D = D_C$, with $0 < D_C < 1$

- But how to evaluate $D$, and how does it evolve?
Ductile materials

- Evolution of damage $D$ for isotropic elasticity
  - Equations
    - Stresses $\sigma = (1 - D) \mathcal{H} : \varepsilon$
    - Example of damage criterion $f(\varepsilon, D) = (1 - D) \frac{\varepsilon : \mathcal{H} : \varepsilon}{2} - Y_C \leq 0$
      - $Y_C$ 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
Ductile materials

- **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:
        \[
        f_V = \frac{V_{\text{void}}}{V} = 1 - \hat{V}
        \]
        with $\hat{V}$ the material part of the volume
      - Material rigid-perfectly plastic $\rightarrow$ elastic deformations negligible
  - **Define**
    - Macroscopic strains and stresses: $\varepsilon$ & $\sigma$
    - Microscopic strains and stresses: $\hat{\varepsilon}$ & $\hat{\sigma}$
    - The Macroscopic strains are defined by
      \[
      \dot{\varepsilon} = \frac{1}{V} \int_V \hat{\varepsilon} dV = \frac{1}{V} \int_V \hat{\varepsilon} dV + \frac{1}{V} \int_{V_{\text{void}}} \hat{\varepsilon} dV
      \]
Ductile materials

- **Gurson’s model, 1977 (2)**

  - Macroscopic strains
    \[ \dot{\varepsilon} = \frac{1}{V} \int_V \dot{\varepsilon} \, dV = \frac{1}{V} \int_V \dot{\varepsilon} \, dV + \frac{1}{V} \int_{V_{\text{void}}} \dot{\varepsilon} \, dV \]

  - Gauss theorem
    \[ \dot{\varepsilon} = \frac{1}{V} \int_V \dot{\varepsilon} \, dV + \frac{1}{2V} \int_{S_{\text{void}}} \dot{\mathbf{u}} \otimes \mathbf{n} + \mathbf{n} \otimes \dot{\mathbf{u}} \, dV \]

  - Stresses
    - In microscopic stresses \( \hat{\varepsilon} \) are related to the microscopic deformations \( \dot{\varepsilon} \)
      - In terms of an energy rate
        \[ \hat{\sigma} = \frac{\partial \dot{W}}{\partial \dot{\varepsilon}} \]
    - As the energy rate has to be conserved
      \[ \dot{W} (\dot{\varepsilon}) = \frac{1}{V} \int_V \dot{W} \left( \dot{\varepsilon} \right) \, dV \]
    - \( \sigma = \frac{\partial \dot{W}}{\partial \dot{\varepsilon}} = \frac{1}{V} \int_V \frac{\partial \dot{W}}{\partial \dot{\varepsilon}} : \frac{\partial \dot{\varepsilon}}{\partial \dot{\varepsilon}} \, dV = \frac{1}{V} \int_V \sigma : \frac{\partial \dot{\varepsilon}}{\partial \dot{\varepsilon}} \, dV \)
    - Gurson solved these equations
      - For a rigid-perfectly-plastic microscopic behavior
      - Which leads to a new macroscopic yield function depending on the porosity

\[ f (\sigma) = \left( \frac{\sigma_0}{\sigma_p} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_0} - f_V^2 - 1 \leq 0 \]
Ductile materials

- **Gurson’s model, 1977 (3)**
  - Gurson deduced the yield surface accounting for the voids

\[ f(\sigma) = \left( \frac{\sigma_e}{\sigma_0} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_0} - f_V^2 - 1 \leq 0 \text{ with } \sigma_e = \sqrt{\frac{3}{2}} \mathbf{s} : \mathbf{s} \]

- If \( f_V = 0 \), it corresponds to J2 plasticity
- When voids are present, a hydrostatic stress state can induce plasticity
  - If \( f_V^2 - 2f_V \cosh \frac{3p}{2\sigma_0} + 1 = 0 \quad \Rightarrow \quad f_V = \cosh \frac{3p}{2\sigma_0} \pm \sinh \frac{3p}{2\sigma_0} \)
  - Or \( f_V = \frac{\exp \frac{3p}{2\sigma_0} + \exp -\frac{3p}{2\sigma_0}}{2} \pm \exp \frac{3p}{2\sigma_0} + \exp -\frac{3p}{2\sigma_0} = \exp \pm \frac{3p}{2\sigma_0} \)
  - Eventually \( \frac{3p}{2\sigma_p} = \pm \ln f_V \)
  - Sign – to be selected as for \( f_V = 0 \), \( p \) cannot induce plasticity
Ductile materials

- **Gurson’s model, 1977 (4)**
  - Shape of the new yield surface
    \[ f(\sigma) = \left( \frac{\sigma_e}{\sigma_p^0} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_p^0} - f_V^2 - 1 \leq 0 \]
  - Normal flow
    \[ \dot{\varepsilon}_p = \dot{\lambda} \frac{\partial f}{\partial \sigma} \]
  - What remains to be defined is the evolution of the porosity \( f_V \)
Ductile materials

- **Gurson’s model, 1977 (5)**
  - Evolution of the porosity \( f_V \)
    - Volume of material \( \hat{V} = (1 - f_V) V \) is constant as
      - Elastic deformations are neglected
      - Plastic deformations are isochoric

  \[
  \frac{dV}{V} = \text{tr} (d\varepsilon) = \text{tr} (d\varepsilon^p) \quad \text{as elastic deformations are neglected}
  \]

  \[
  \hat{f}_V = (1 - f_V) \frac{\dot{V}}{V}
  \]
Ductile materials

• Gurson’s model, 1977 (6)
  – Eventually
    • The porosity is actually not an independent internal variable
    • Yield surface \[ f(\sigma) = \left( \frac{\sigma_c}{\sigma_p^0} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_p^0} - f_V^2 - 1 \leq 0 \]
    • Normal flow \[ \dot{\varepsilon}_V = \lambda \frac{\partial f}{\partial \sigma} \quad \text{with} \quad \dot{f}_V = (1 - f_V) \text{tr} (\dot{\varepsilon}_p) \]
  – Assumptions were
    • Rigid perfectly-plastic material
    • Initial porosity (no void nucleation)
    • No voids interaction
    • No voids coalescence
  – More evolved models have been developed to account for
    • Hardening
    • Voids nucleation, interactions and coalescences
Ductile materials

- **Hardening**
  - Yield criterion $f(\sigma) = \left(\frac{\sigma_c}{\sigma^0_p}\right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma^0_p} - f^2_V - 1 \leq 0$ remains valid but one has to account for the hardening of the matrix $\sigma^0_p \rightarrow \sigma_p (\hat{\varepsilon}^p)$
  - In this expression, the equivalent plastic strain of the matrix $\hat{\varepsilon}^p$ is used instead of the macroscopic one $\bar{\varepsilon}^p$
  - Values related to the matrix and the macroscopic volume are dependant as the dissipated energies have to match $\Rightarrow (1 - f_V) \sigma_p (\hat{\varepsilon}^p) \dot{\hat{\varepsilon}}^p = \sigma : \dot{\varepsilon}$

- **Voids nucleation**
  - Increase rate of porosity results from
    - Matrix incompressibility
    - Creation of new voids
      - The nucleation rate can be modeled as strain controlled $\Rightarrow \dot{f}_V = (1 - f_V) \text{tr}(\dot{\varepsilon}^p) + \dot{f}_{\text{nucl}}$
      - Represented by 1 void $\Rightarrow \dot{f}_{\text{nucl}} = A (\hat{\varepsilon}^p) \dot{\hat{\varepsilon}}^p$
Ductile materials

- Voids interaction
  - 1981, Tvergaard
    - In Gurson model a void is considered isolated
    - The presence of neighboring voids decreases the maximal loading as the stress distribution changes

\[
f(\sigma) = \left( \frac{\sigma_e}{\sigma_p(\hat{\varepsilon})} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_p(\hat{\varepsilon})} - f_V^2 - 1 \leq 0
\]

- With \( 1 < q < 2 \) depending on the hardening exponent
**Ductile materials**

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

\[
 f(\sigma) = \left( \frac{\sigma_e}{\sigma_p (\hat{\epsilon}p)} \right)^2 + 2f_V \cosh \frac{\text{tr}(\sigma)}{2\sigma_p (\hat{\epsilon}p)} - f_V^2 - 1 \leq 0
\]

\[
 f(\sigma) = \left( \frac{\sigma_e}{\sigma_p (\hat{\epsilon}p)} \right)^2 + 2q f_V^* \cosh \frac{\text{tr}(\sigma)}{2\sigma_p (\hat{\epsilon}p)} - q^2 f_V^{*2} - 1 \leq 0
\]

- with
  \[
  f_V^* = \begin{cases} 
  f_V & \text{if } f_V < f_C \\
  f_C + \frac{1}{q-f_C} (f_V - f_C) & \text{if } f_V > f_C 
  \end{cases}
  \]
• **Softening response**
  – Loss of solution uniqueness \( \rightarrow \) mesh dependency

\[
\begin{align*}
F, d \\
\Delta d \\
F, d \\
\Delta d \\
F, d \\
\Delta d
\end{align*}
\]
Ductile materials

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

Dr.-Ing. Frederik Reusch, University of Dortmund, Department of Mechanical Engineering Mechanics, http://www.mech.mb.uni-dortmund.de/lsm/contents/research/topics/mm(nonlocaldamage).html
Why multiscale?

- Previous methods are models based on macroscopic results
- The idea is to simulate what is happening at small scale with correct physical models and to extract responses that can be used at macroscopic scale
  - Gurson’s model is actually a multiscale model
Principle

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
• **Example: Failure of composite laminates**
  - Heterogeneous materials: failure involves complex mechanisms

– **Use**
  - Multi-scale model with non-local continuum damage within each ply
  - Cohesive elements for delamination
- Failure of composite $[90^\circ / 45^\circ / -45^\circ / 90^\circ / 0^\circ]_S$- open hole laminate
• 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: 3.28 nm
Grain size: 6.56 nm
• **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
References

• Lecture notes

• Other references
  – « on-line »
  – Book