

Trends in computational failure mechanics: multiple scales, multi-physics and discontinuities

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Introduction

Underlying trends:

- Improved experimental techniques (AFM, ESEM,)
- More powerful computational methods
 - Hardware: parallel processing
 - Computational mechanics/mathematics: new concepts
- Quantification of material *parameters* at lower scales
- *Multiscale concepts* aim at explaining/predicting properties at level of visible observation from lower scales

Introduction

- Scaling down of analysis is accompanied by necessity to model (evolving) *discontinuities*:
 - Static instabilities: cracks and shear bands
 - Propagative instabilities (PLC-bands, Lüders bands)
 - Grain boundaries in crystalline materials
 - Solid-solid phase boundaries (austenite-martensite)
 - Discrete dislocation dynamics

Introduction

- Traditional discretisation methods (finite elements, finite differences,.....) have been designed to solve *continuum* problems for one length and time scale
- They cannot directly handle (evolving) *discontinuities*
- They can become inaccurate when the *length* or *time* scales have different orders of magnitude

Introduction

- Time scales in coupled moisture/ion transport
- Synopsis of typical model for skin:
 - Diffusion-type relation for water:

$$n_f(\mathbf{v}_f - \mathbf{v}_s) = -\mathbf{K} \cdot \left(\nabla \mu_f + \frac{n_i}{n_f} \nabla \mu_i \right)$$

- Diffusion-type relation for ions:

$$n_i (\mathbf{v}_i - \mathbf{v}_f) = -\mathbf{D}_i \cdot \nabla \mu_i$$

Permeability coefficients in \mathbf{K} and diffusion coefficients in \mathbf{D}_i typically have a very different order of magnitude

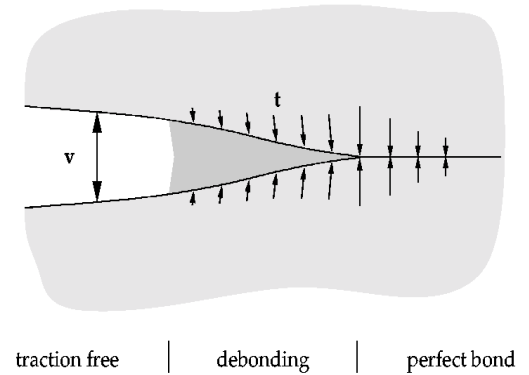
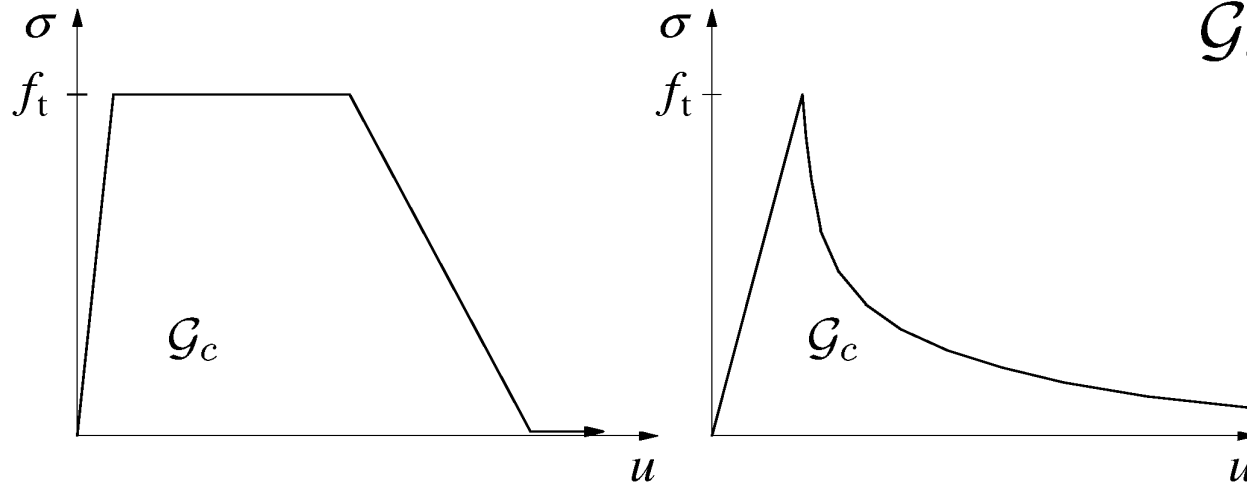
Cohesive-zone models

Discrete traction separation law:

$$\mathbf{t}_i = \mathbf{t}_i(\mathbf{v}, \kappa)$$

with tangential stiffness:

$$\mathbf{T} = \frac{\partial \mathbf{t}_i}{\partial \mathbf{v}} + \frac{\partial \mathbf{t}_i}{\partial \kappa} \frac{\partial \kappa}{\partial \mathbf{v}}$$



Work of separation:

$$\mathcal{G}_c = \int \sigma \, dv$$

Length scale:

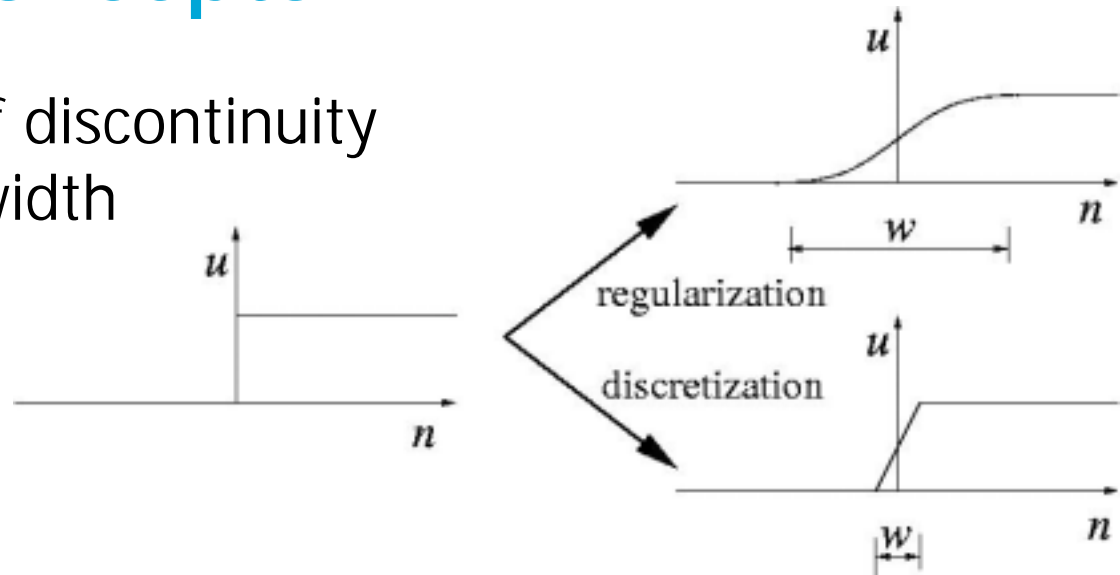
$$\ell \sim \mathcal{G}_c / E$$

Strategies for capturing discontinuities

- Distributing the discontinuity over a finite width:
 - Smeared concepts
 - Embedded discontinuity concepts
- Capturing the discontinuity in a direct manner:
 - Conventional interface elements
 - Meshfree methods
 - Partition-of-unity based methods
 - Discontinuous Galerkin methods

Smearred concepts

- Distribution of discontinuity over a finite width



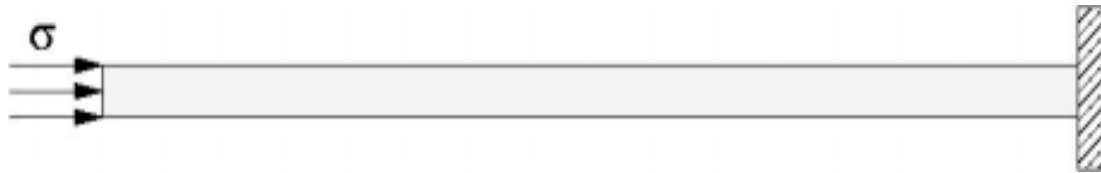
- Example:

Cohesive Zone Models: $\mathcal{G}_c = \iint \sigma \, d\epsilon(n) \, dn$

- Consequence: grid-size dependent softening modulus
- Mathematically: ill-posedness persists
- Numerically: some form of mesh dependence remains

Smearred concepts

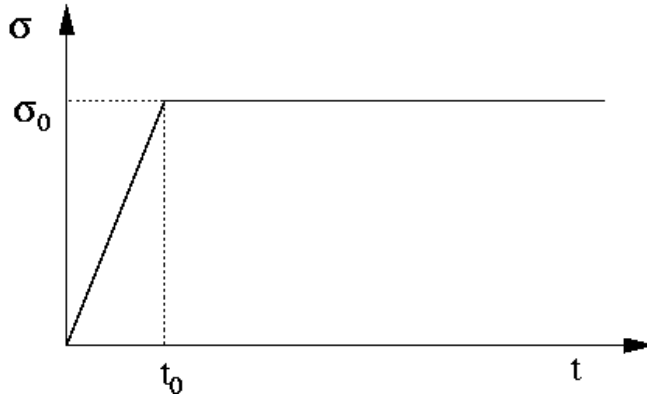
1D example: wave propagation in *fluid-saturated* medium



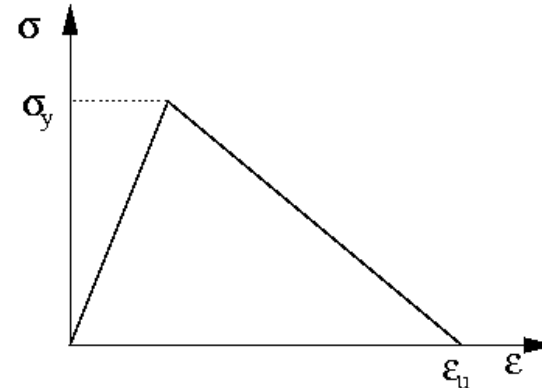
Finite differences in space
Fully explicit time integration



to avoid numerical
regularization

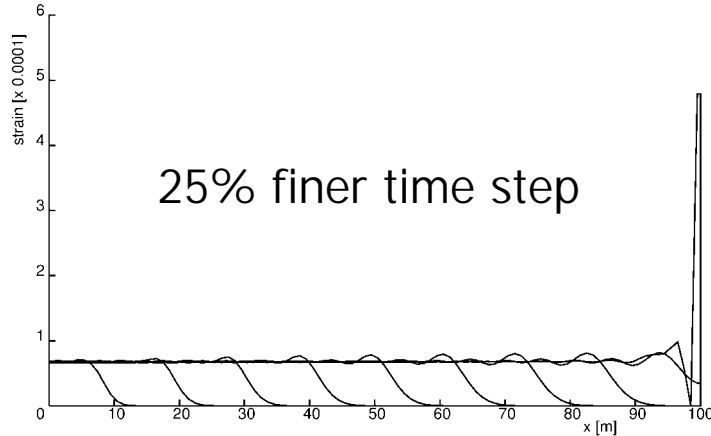
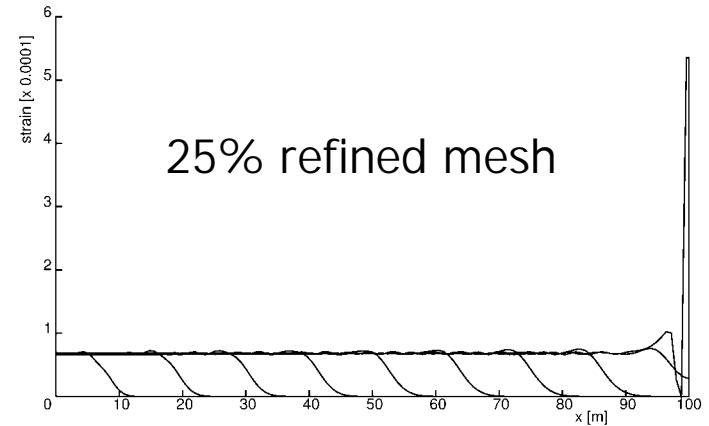
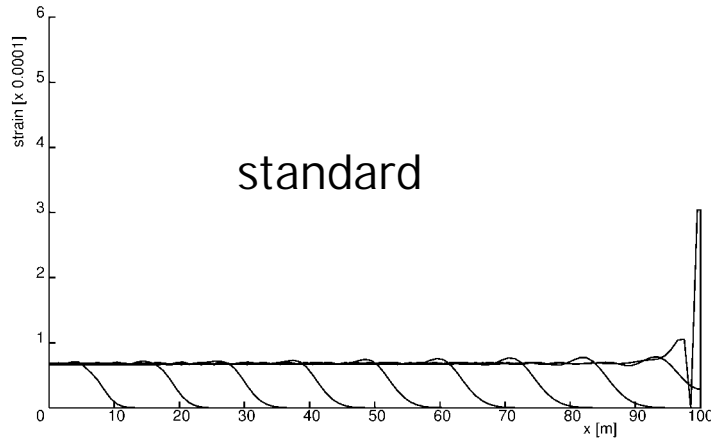


loading scheme



softening relation

Smeared concepts



As in single-phase medium, solution depends on:

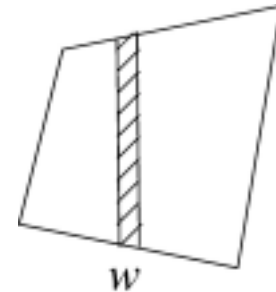
- Grid spacing
- Time step

Embedded discontinuities

- Refinement: Incorporate \mathcal{G}_c in discontinuity kinematics

$$\epsilon^- = \bar{\epsilon} + \frac{\alpha^-}{2}(\mathbf{n} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{n})$$

$$\epsilon^+ = \bar{\epsilon} + \frac{\alpha^+}{2}(\mathbf{n} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{n})$$



- Two possibilities:
 - Strain discontinuity (weak form)
 - Displacement discontinuity (strong form)
- Remarks:
 - Strong form limiting case of weak form ($w \rightarrow 0$)
 - Improved deformation capability (Petrov-Galerkin form)
 - Condensation at element level: *no* real discontinuity

Embedded discontinuities

For constant strain triangles [Borja]:

$$\mathbf{K}_{\text{con}} = V_{\text{elem}} \mathbf{B}^T \left(\mathbf{D} - \frac{\mathbf{D}(\mathbf{G}\mathbf{m})(\mathbf{G}^*\mathbf{m})^T \mathbf{D}}{\underbrace{-\mathbf{m}^T \mathbf{T} \mathbf{m}}_h + (\mathbf{G}^*\mathbf{m})^T \mathbf{D}(\mathbf{G}\mathbf{m})} \right) \mathbf{B}$$

- Non-symmetry for $\mathbf{G}^* \neq \mathbf{G}$
- Stiffness matrix similar to non-associated plasticity
- Under certain assumptions, embedded discontinuity models become identical to standard FEM

Interface elements

Relative displacements:

$$\mathbf{v} = \mathbf{L}\mathbf{u}$$

with standard interpolation

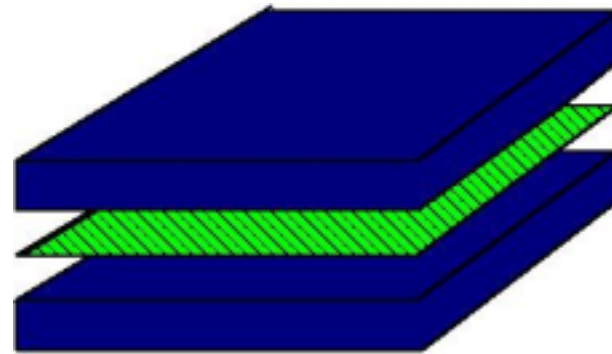
$$\mathbf{u} = \mathbf{H}\mathbf{a}$$

Relative displacements vs nodal displacements

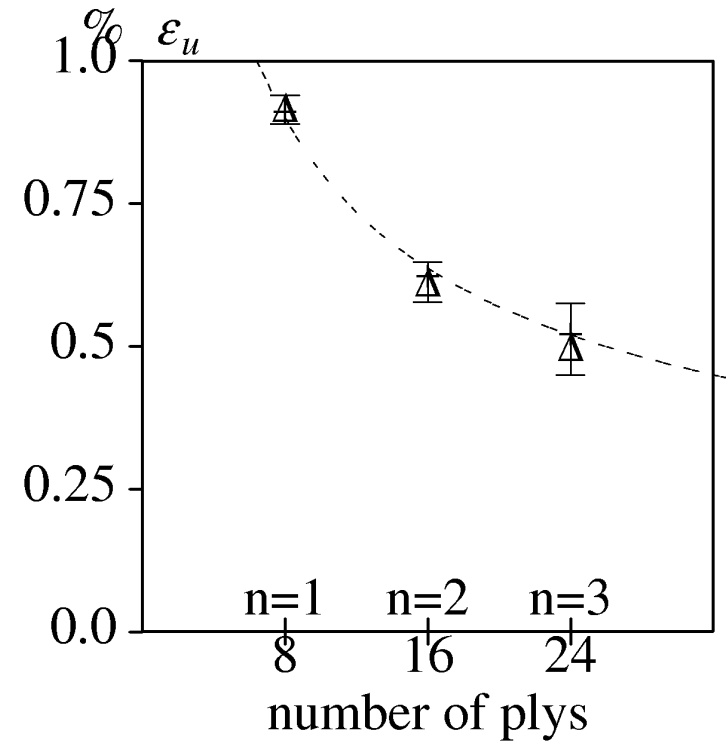
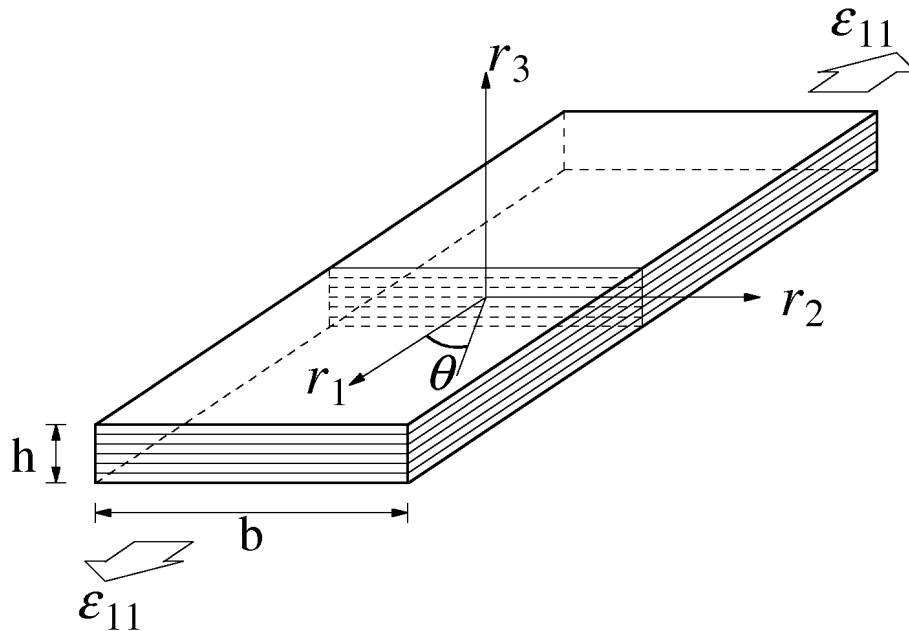
$$\mathbf{v} = \mathbf{LH}\mathbf{a} = \mathbf{B}_i\mathbf{a}$$

Element stiffness matrix:

$$\mathbf{K} = \int \mathbf{B}_i^T \mathbf{T} \mathbf{B}_i d\Gamma$$

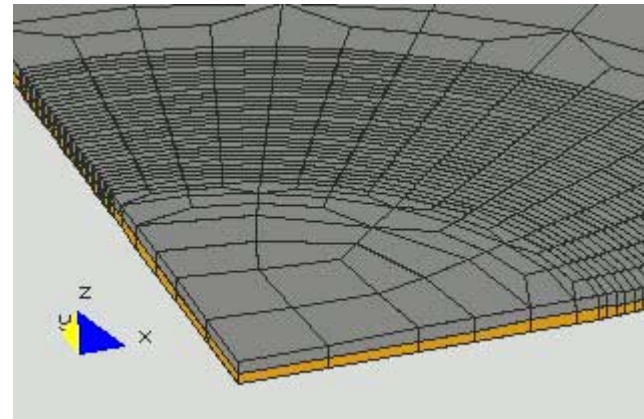
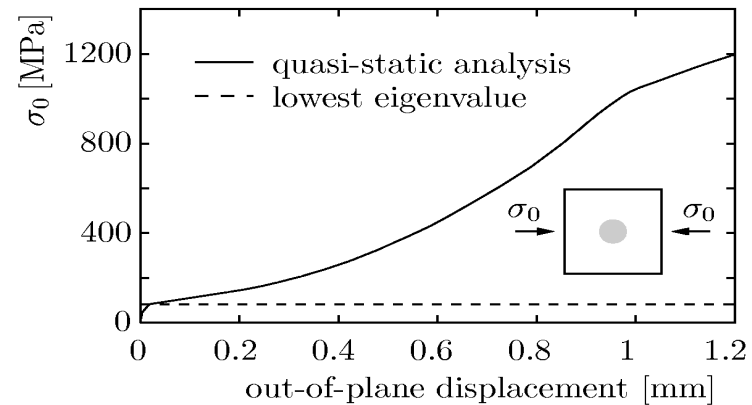
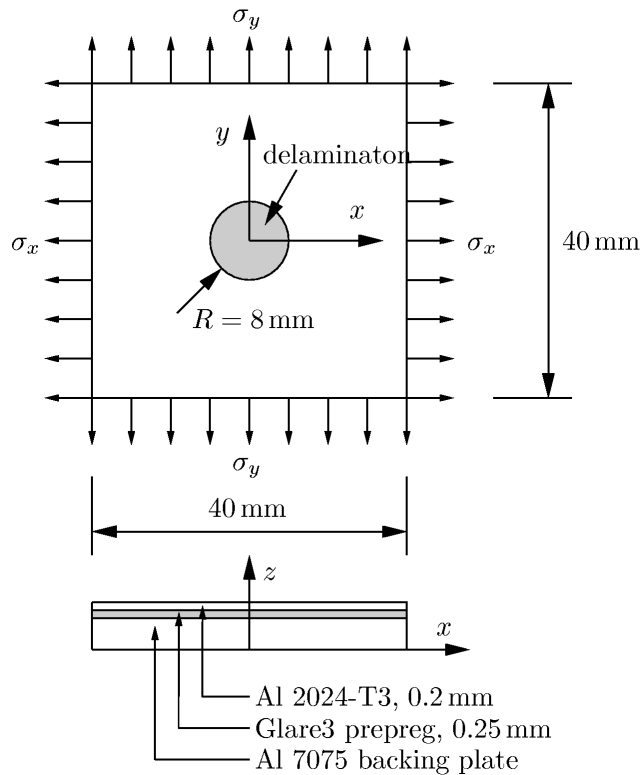


Interface elements



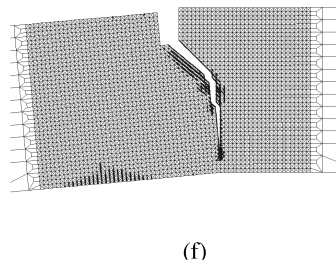
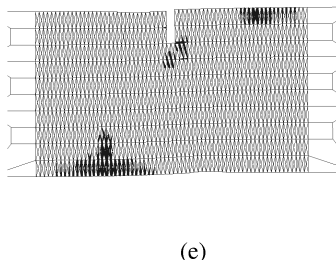
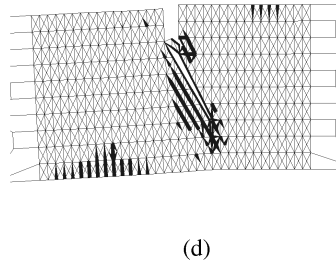
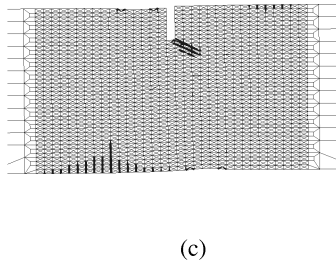
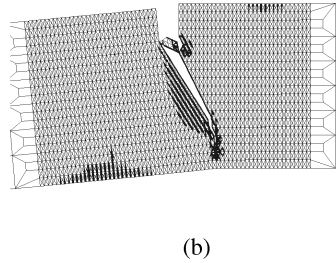
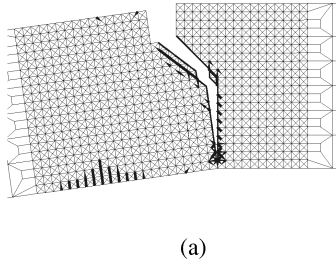
Delamination and thickness effect in a composite panel

Interface elements



Glare3: Example with buckling-delamination

Interface elements



Xu/Needleman approach:

Interface elements between
all continuum elements

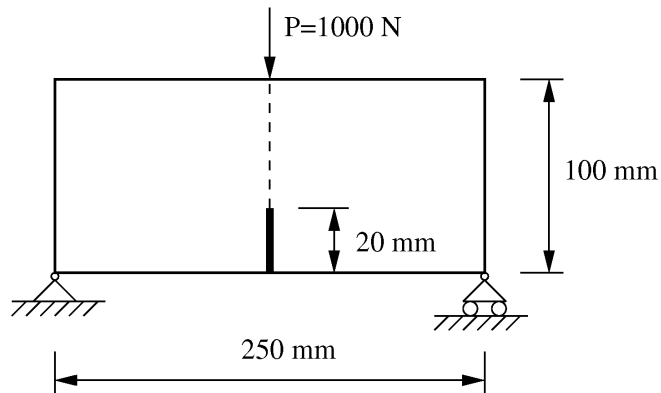
Results for various:

- discretizations
- integration schemes

Conclusion:

- mesh dependency!

Interface elements



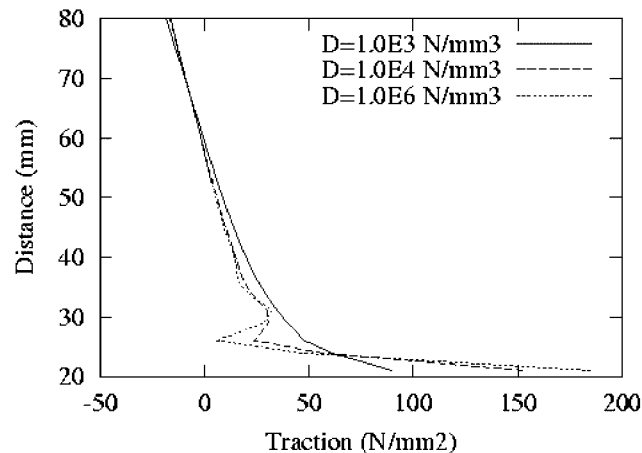
Prior to separation:

$$\mathbf{T} = \begin{bmatrix} d_n & 0 & 0 \\ 0 & d_s & 0 \\ 0 & 0 & d_t \end{bmatrix}$$

$$\mathbf{K} = \begin{bmatrix} d_n \mathbf{h}^\top \mathbf{h} & 0 & 0 \\ 0 & d_s \mathbf{h}^\top \mathbf{h} & 0 \\ 0 & 0 & d_t \mathbf{h}^\top \mathbf{h} \end{bmatrix}$$

Disadvantages:

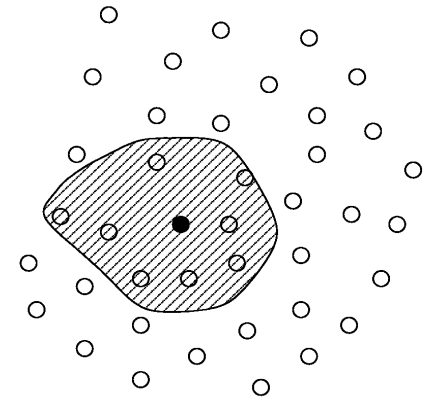
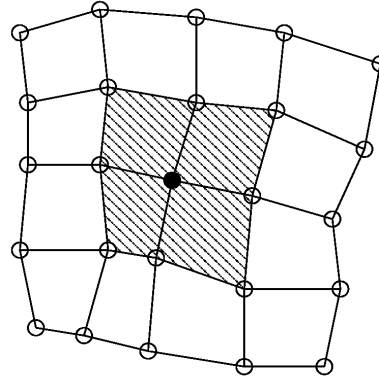
- Traction oscillations
- Spurious reflections



Meshfree methods

Meshfree methods aim at:

- Avoiding connectivity
- Obviating remeshing
- High resolution at singularities



Interpolation: $u^h(\mathbf{x}) = \mathbf{p}^\top(\mathbf{x})\mathbf{a}(\mathbf{x})$

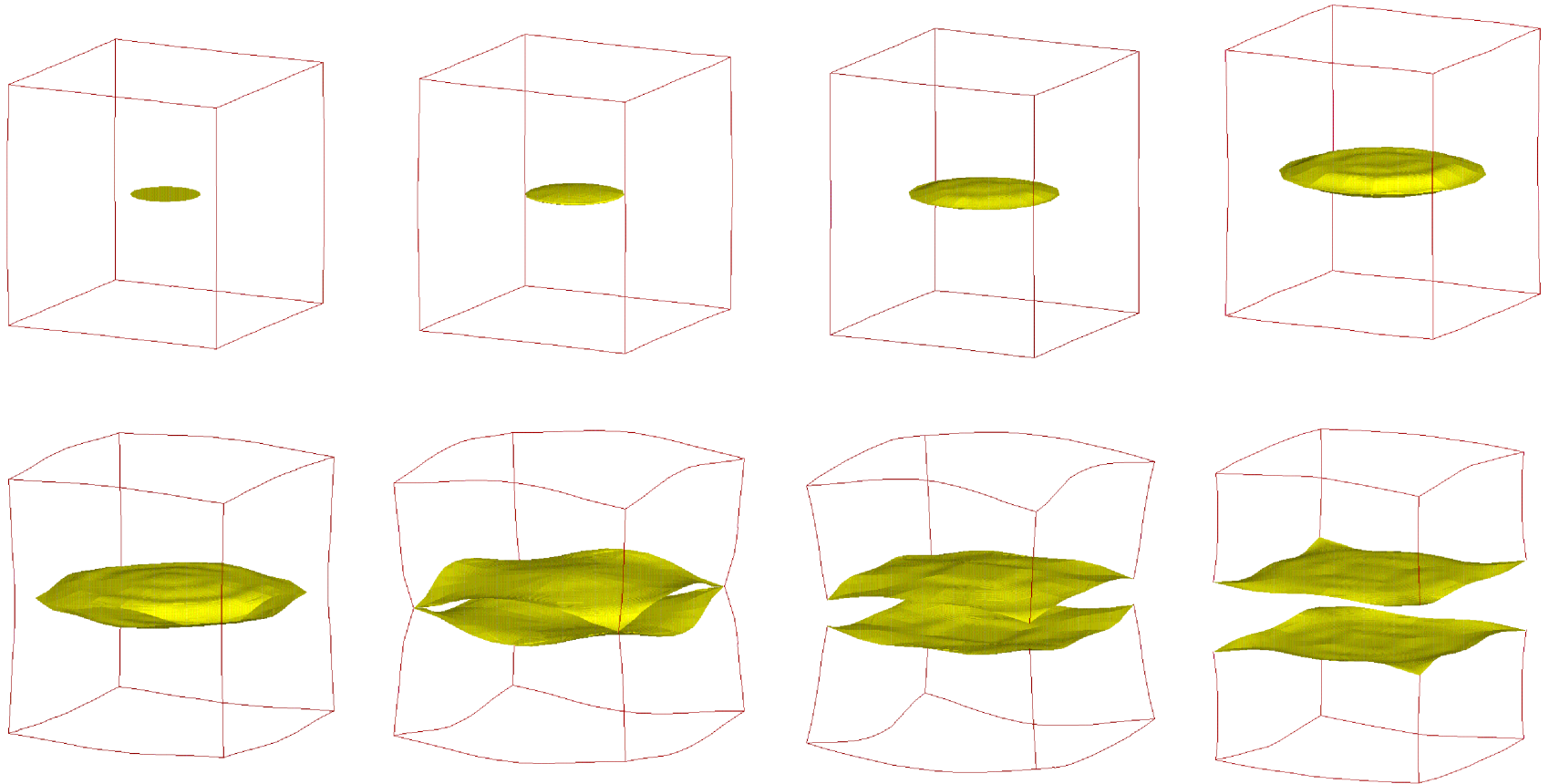
Meshfree methods

Minimization of Moving Least Squares sum:

$$\frac{\partial J^{\text{mls}}}{\partial \mathbf{a}(\mathbf{x})} = \mathbf{0} \quad \text{with} \quad J^{\text{mls}} = \sum_{i=1}^n w_i(\mathbf{x}) \left(\mathbf{p}^{\top}(\mathbf{x}_i) \mathbf{a}(\mathbf{x}) - u_i \right)^2$$

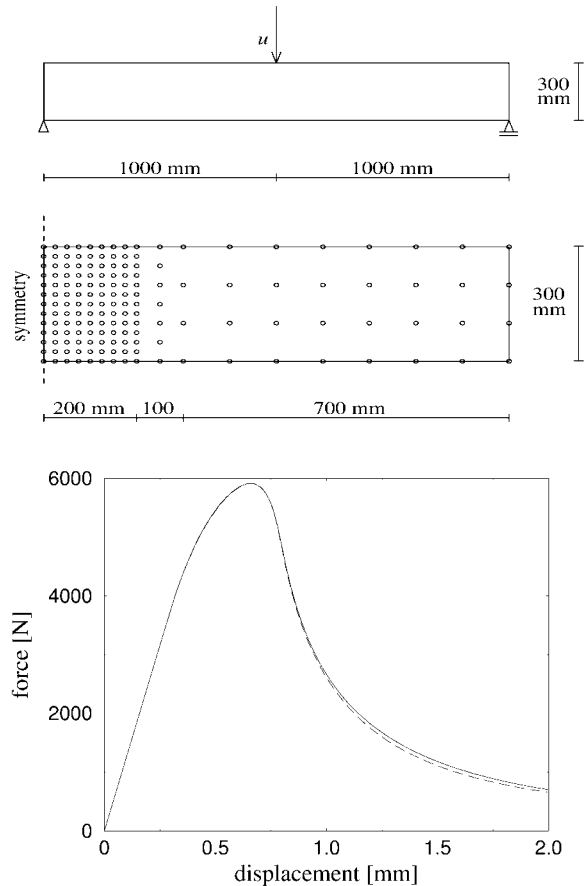
$$\text{Interpolation functions: } u^h(\mathbf{x}) = \underbrace{\mathbf{p}^{\top}(\mathbf{x}) \mathbf{A}^{-1}(\mathbf{x}) \mathbf{C}(\mathbf{x})}_{\mathbf{H}(\mathbf{x})} \mathbf{u}$$

Meshfree methods



Example for linear elastic fracture mechanics [Krysl & Belytschko]

Meshfree methods



Gradient damage mechanics:

$$\boldsymbol{\sigma} = (1 - \omega) \mathbf{D}^e : \boldsymbol{\epsilon}$$

$$\omega = \omega(\kappa)$$

$$f = \bar{\epsilon} - \kappa$$

$$\bar{\epsilon} - c_1 \nabla^2 \bar{\epsilon} - c_2 \nabla^4 \bar{\epsilon} = \tilde{\epsilon}$$

$$\tilde{\epsilon} = \tilde{\epsilon}(\boldsymbol{\epsilon}) \quad , \quad c_1 \sim \ell^2 \quad , \quad c_2 \sim \ell^4$$

Example for damage evolution

Partition-of-unity method

Enhanced interpolation:

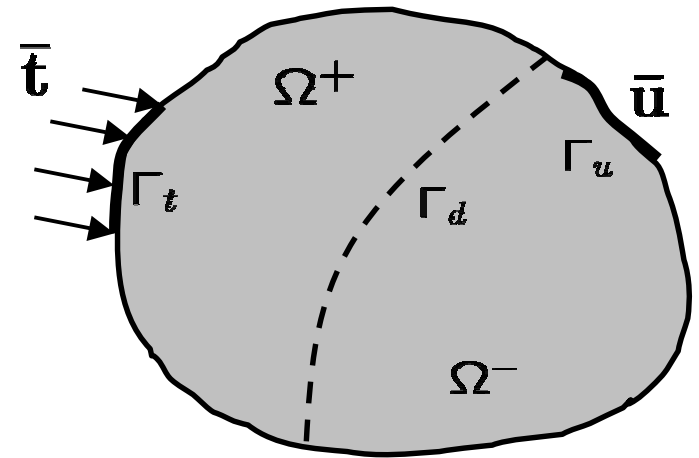
$$u(\mathbf{x}) = \sum_{i=1}^n \phi_i(\mathbf{x}) \left(\bar{a}_i + \sum_{j=1}^m \psi_j(\mathbf{x}) \tilde{a}_{ij} \right)$$

Conventional FE notation:

$$\mathbf{u} = \mathbf{H}(\bar{\mathbf{a}} + \boldsymbol{\Psi} \tilde{\mathbf{a}})$$

Discontinuity as enhanced field: $\boldsymbol{\Psi} = \mathcal{H}_{\Gamma_d} \mathbf{I}$

Resulting interpolation: $\mathbf{u} = \underbrace{\mathbf{H}\bar{\mathbf{a}}}_{\bar{\mathbf{u}}} + \mathcal{H}_{\Gamma_d} \underbrace{\mathbf{H}\tilde{\mathbf{a}}}_{\tilde{\mathbf{u}}}$



➤ Special case of *Variational Multiscale Method*

Partition-of-unity method

Balance of momentum:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} = \mathbf{0}$$

Interpolation of test functions in same space:

$$\mathbf{w} = \bar{\mathbf{w}} + \mathcal{H}_{\Gamma_d} \tilde{\mathbf{w}}$$

Resulting set of coupled equations:

$$\int_{\Omega} \nabla^{\text{sym}} \bar{\mathbf{w}} : \boldsymbol{\sigma} d\Omega = \int_{\Omega} \bar{\mathbf{w}} \cdot \rho \mathbf{g} d\Omega + \int_{\Gamma} \bar{\mathbf{w}} \cdot \mathbf{t} d\Gamma$$

$$\int_{\Omega^+} \nabla^{\text{sym}} \tilde{\mathbf{w}} : \boldsymbol{\sigma} d\Omega + \int_{\Gamma_d} \tilde{\mathbf{w}} \cdot \mathbf{t}_d d\Gamma = \int_{\Omega^+} \tilde{\mathbf{w}} \cdot \rho \mathbf{g} d\Omega + \int_{\Gamma} \mathcal{H}_{\Gamma_d} \tilde{\mathbf{w}} \cdot \mathbf{t} d\Gamma$$

Partition-of-unity method

Discretization and linearization of interface term:

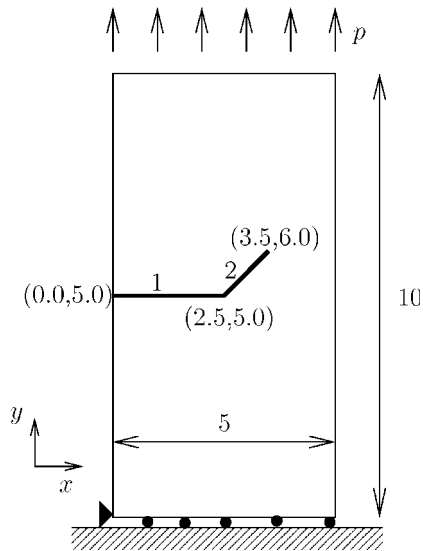
$$\int_{\Gamma_d} \tilde{\mathbf{w}} \cdot \mathbf{t}_d d\Gamma \rightarrow \int_{\Gamma_d} \mathbf{H}^\top \mathbf{T} \mathbf{H} d\Gamma$$

Limiting case: discontinuity at the edge

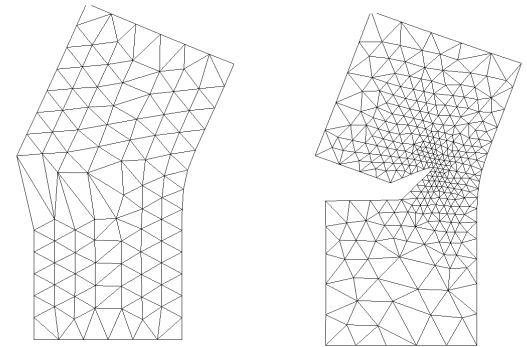
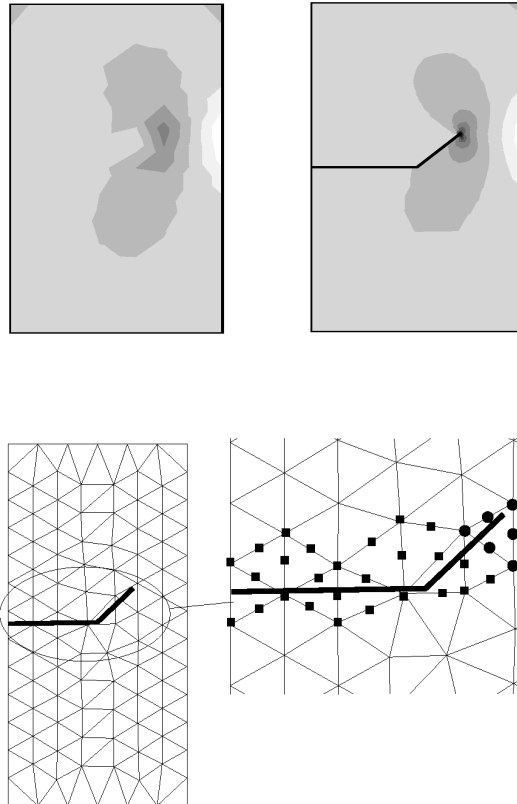
$$\int_{\Gamma_d} \mathbf{H}^\top \mathbf{T} \mathbf{H} d\Gamma = \begin{bmatrix} d_n \mathbf{h}^\top \mathbf{h} & 0 & 0 \\ 0 & d_s \mathbf{h}^\top \mathbf{h} & 0 \\ 0 & 0 & d_t \mathbf{h}^\top \mathbf{h} \end{bmatrix}$$

- Equivalence with interface formulation
- But: no traction oscillations because integral only exists after onset of cracking

Partition-of-unity method



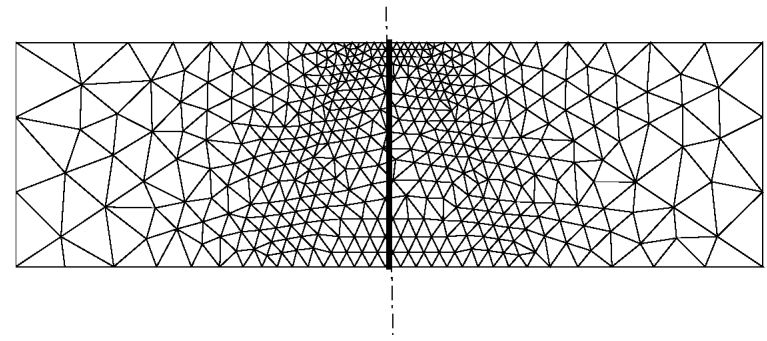
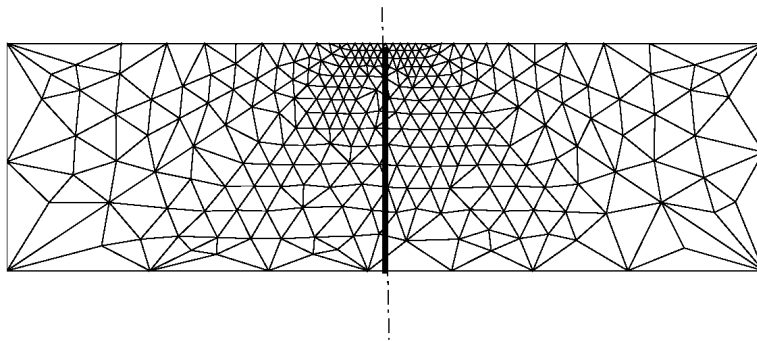
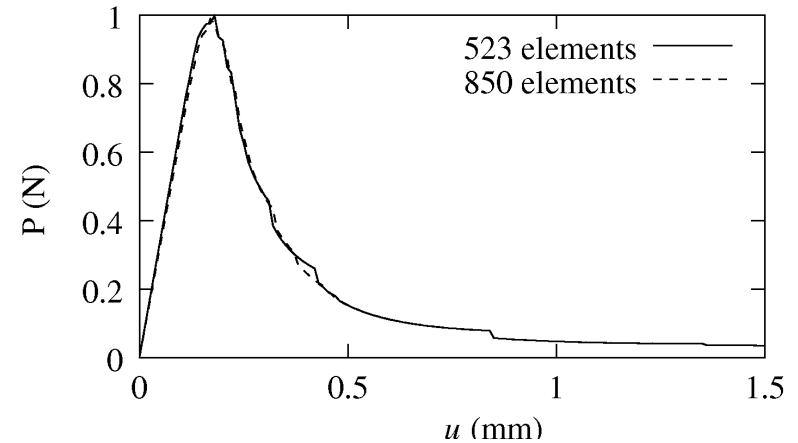
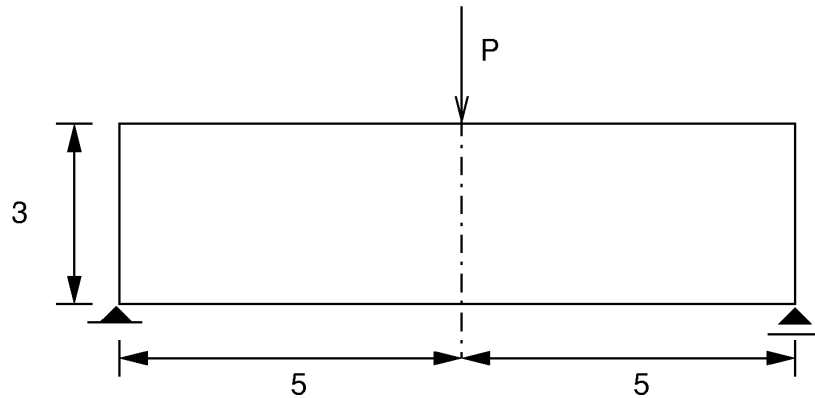
Kinked crack



- Squares: nodes enriched by stepfunction
- Circles: nodes enriched by singularity functions

Example for Linear Elastic Fracture Mechanics

Partition-of-unity method

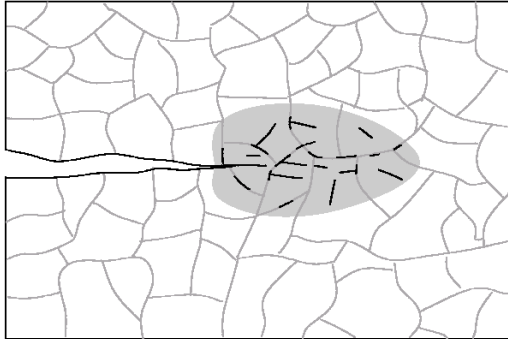


Example with cohesive-zone model

Cohesive-segments method

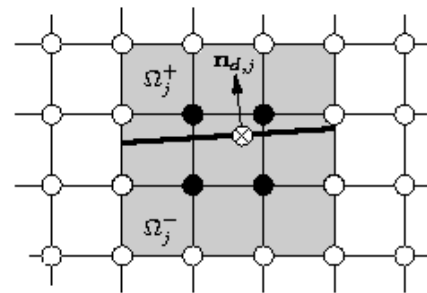
Heterogeneous materials:

- nucleation of multiple cracks
- coalescence
- branching

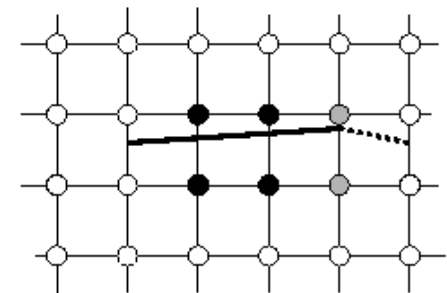


Define *cohesive segments*:

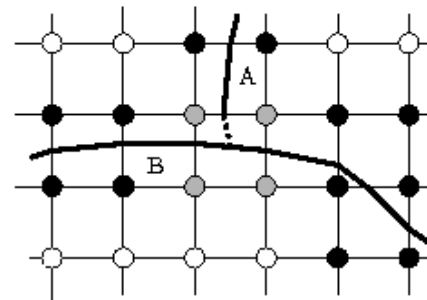
- nucleation in Gauss point
- extend over a patch
- can extend and join



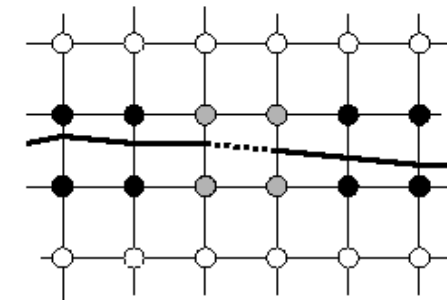
(a)



(b)

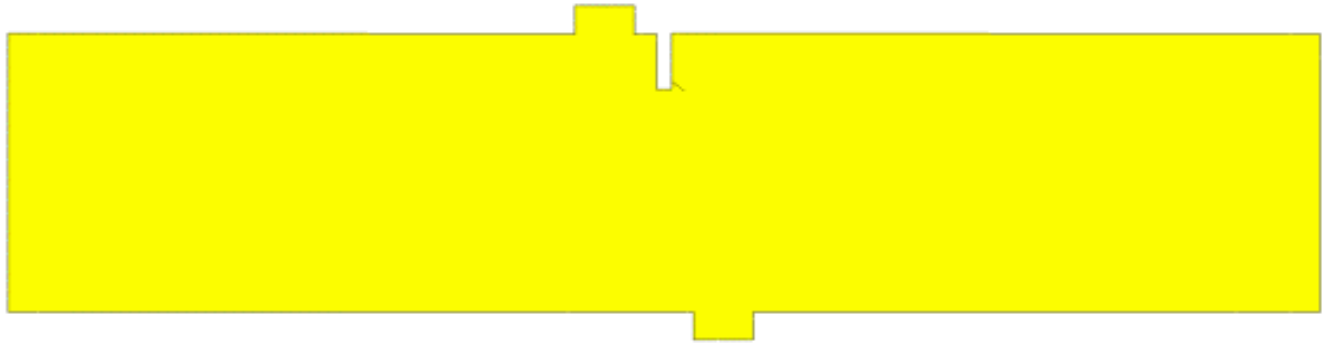


(a)



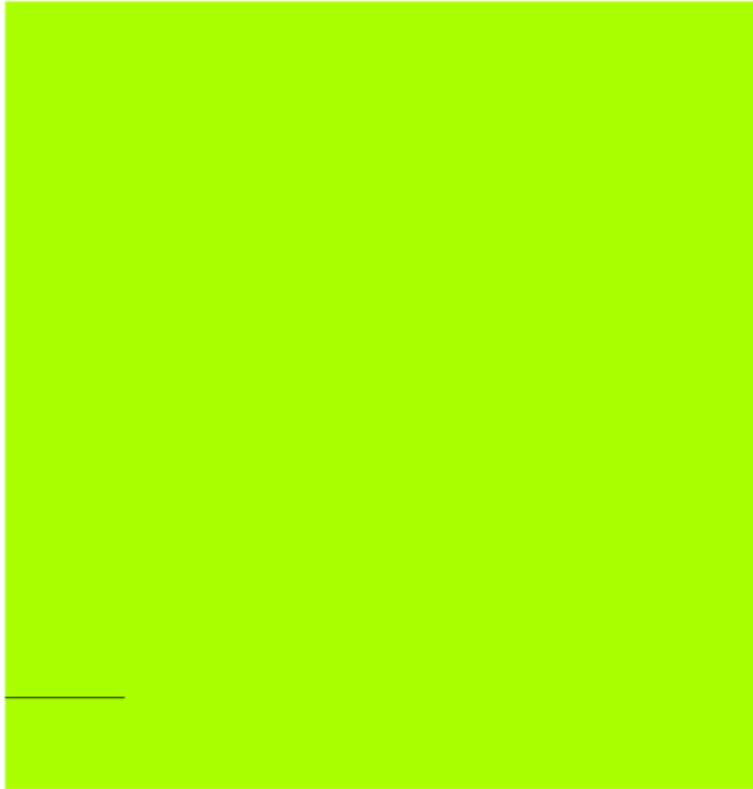
(b)

Example with cohesive segments



Crack propagation with cohesive segments in SEN-beam

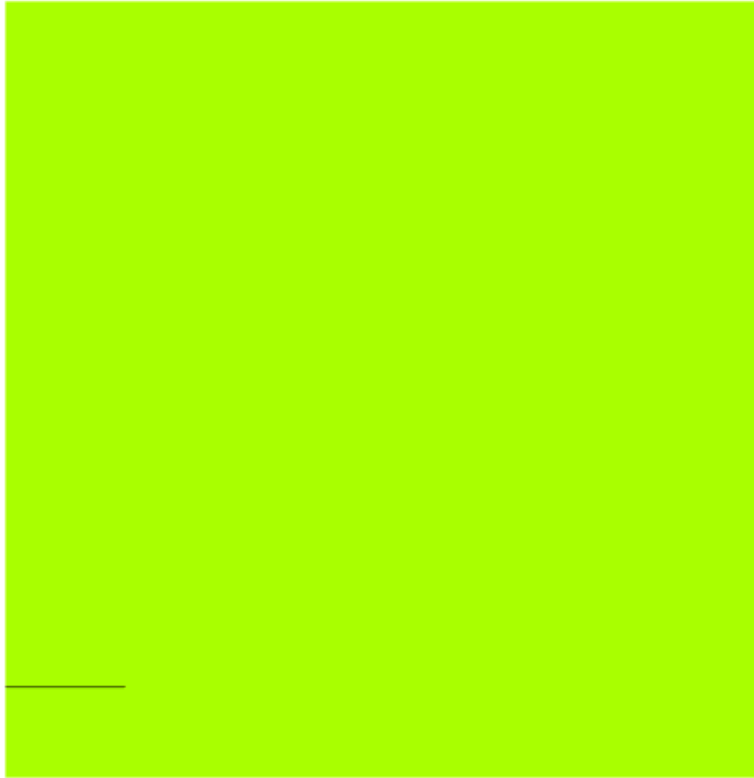
Example with cohesive segments



Dynamic crack propagation

Kalthoff experiment:
Low speed of impactor

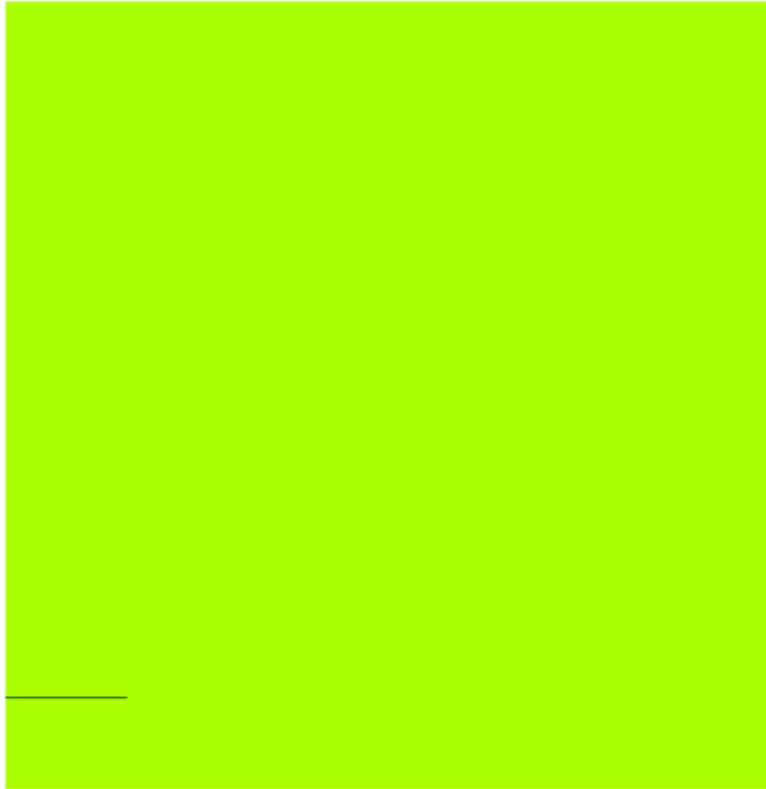
Example with cohesive segments



Dynamic crack propagation

Kalthoff experiment:
Medium speed of impactor

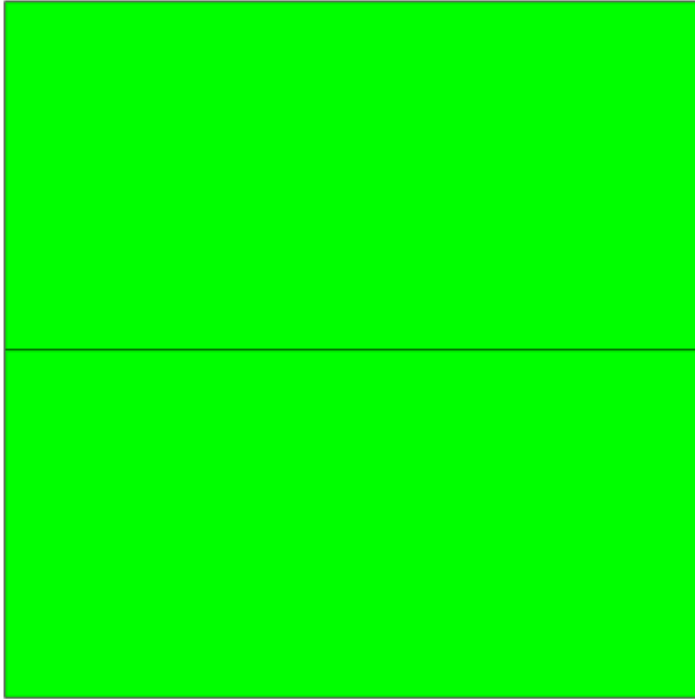
Example with cohesive segments



Dynamic crack propagation

Kalthoff experiment:
High speed of impactor

Example with cohesive segments



Dynamic crack propagation

Crack branching

Two-phase medium

- Durability problems involve coupling of fracture to diffusion-type problems

Momentum and mass balances:

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$$

$$\nabla \cdot \dot{\mathbf{u}} + \nabla \cdot (n_f \mathbf{w}_f) + Q^{-1} \dot{p} = 0$$

Boundary conditions:

$$\mathbf{n}_\Gamma \cdot \boldsymbol{\sigma} = \mathbf{t}_p, \quad \mathbf{u} = \mathbf{u}_p$$

$$n_f \mathbf{w}_f = \mathbf{q}_p, \quad p = p_p$$

Two-phase medium

- Assumptions for discontinuity:
 - For solid: $\mathbf{u} = \bar{\mathbf{u}} + \mathcal{H}_{\Gamma_d} \tilde{\mathbf{u}}$
 - For fluid: $p = \bar{p} + \mathcal{H}_{\Gamma_d} \tilde{p}$
- Assumption for pressure field different from:
 - Runesson/Larsson: regularized Dirac function
 - Armero/Callari: continuous pressure
- \tilde{p} is *not* necessarily spatially constant
- Derivation of discretized equations via standard Bubnov-Galerkin procedure

Two-phase medium

- Standard constitutive assumptions for the solid
- Assumptions for the fluid:

- In the bulk (Darcy): $n_f \mathbf{w}_f = -k_f \nabla p$
- At the interface:
 - Diaphragm of permeability k_d

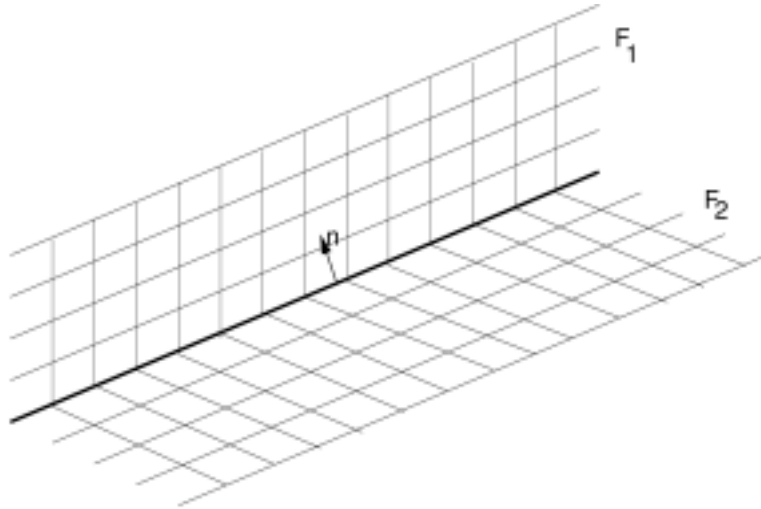
$$\mathbf{n}_{\Gamma_d} \cdot \mathbf{q}_d = -k_d(p^+ - p^-) = -k_d \tilde{p} \mid_{\mathbf{x} \in \Gamma_d}$$

- Drain or line source

$$\mathbf{n}_{\Gamma_d} \cdot \mathbf{q}_d = q_d \mid_{\mathbf{x} \in \Gamma_d}$$

Solid-solid phase boundaries

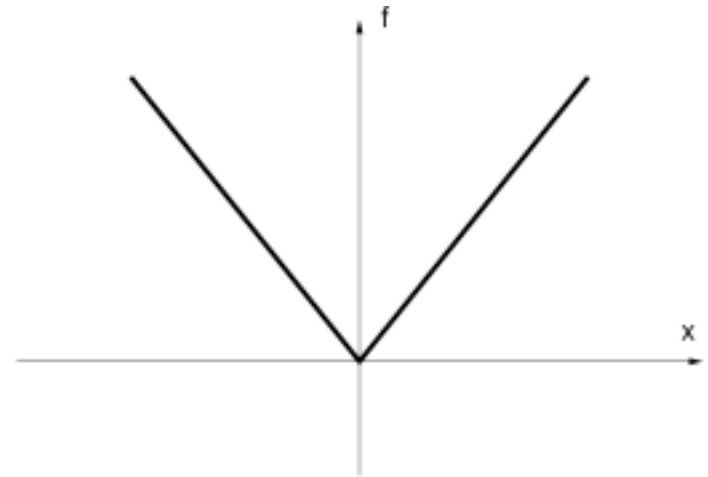
- Example: twinning of martensite



Weak discontinuity:

$$[[u]] = 0, \quad [[\nabla u]] \neq 0$$

- Trace weak discontinuity by level set function



Enrichment function:

$$\psi = |f(\mathbf{x})|$$

Solid-solid phase boundaries

- Enhanced interpolation weak discontinuity:

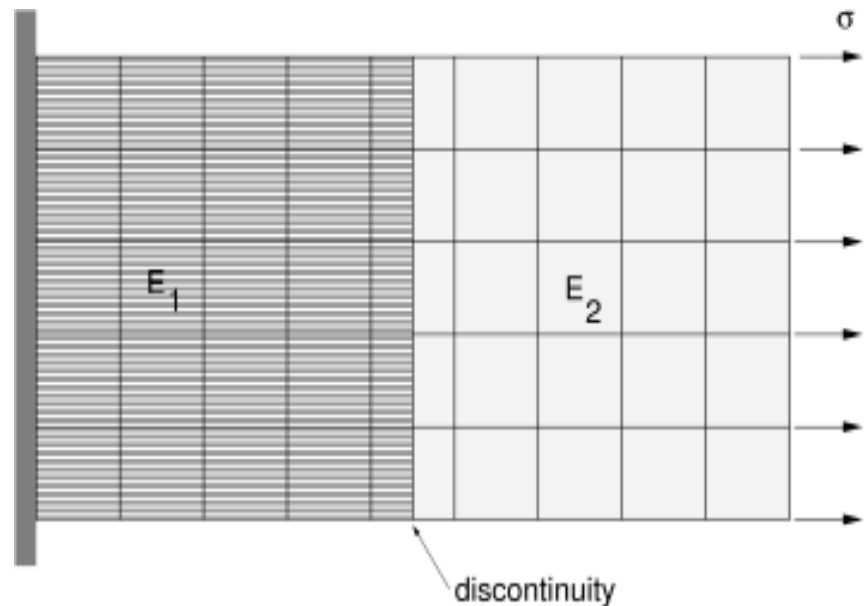
$$\Psi = \psi \mathbf{I} \rightarrow$$

$$\mathbf{u} = \mathbf{H}\mathbf{a} + \psi \mathbf{H}\mathbf{b}$$

Enhanced strain field:

$$\epsilon = \underbrace{\nabla \mathbf{H}}_{\mathbf{B}} \mathbf{a} + \underbrace{\nabla(\psi \mathbf{H})}_{\mathbf{B}_\psi} \mathbf{b}$$

- Example of weak discontinuity: plate with two stiffness moduli



Solid-solid phase boundaries

- Propagation of phase boundary governed by evolution equation for level set function:

$$\dot{\psi} + V_n |\nabla \psi| = 0$$

- Propagation speed: $V_n = g(f, \mathbf{n})$

f driving force , \mathbf{n} normal to phase boundary

- Solution of mechano-metallurgy problem via staggered scheme (Picard type iteration):
 - update of phase boundary by solving level set function
 - solution of mechanical problem by finite elements, *etc.*

Discontinuous Galerkin methods

Divide domain Ω into subdomains Ω^- , Ω^+ :

$$\int_{\Omega} \nabla^{\text{sym}} \mathbf{w} : \boldsymbol{\sigma} d\Omega - \int_{\Gamma_d} \mathbf{w}^+ \cdot \mathbf{t}_d^+ d\Gamma - \int_{\Gamma_d} \mathbf{w}^- \cdot \mathbf{t}_d^- d\Gamma = \text{r.h.s.}$$

Displacement and traction continuity at Γ_d :

$$\mathbf{u}^+ = \mathbf{u}^-$$

$$\mathbf{t}_d^+ = \mathbf{n}_{\Gamma_d} \cdot \boldsymbol{\sigma}^+ = -\mathbf{n}_{\Gamma_d} \cdot \boldsymbol{\sigma}^- = -\mathbf{t}_d^-$$

Discontinuous Galerkin methods

- Lagrange multipliers: $\lambda = \mathbf{t}_d^+ = -\mathbf{t}_d^-$

$$\int_{\Omega} \nabla^{\text{sym}} \mathbf{w} : \boldsymbol{\sigma} d\Omega - \int_{\Gamma_d} (\mathbf{w}^+ - \mathbf{w}^-) \cdot \boldsymbol{\lambda} d\Gamma = \text{r.h.s.}$$

$$\int_{\Gamma_d} \mathbf{z} \cdot (\mathbf{u}^+ - \mathbf{u}^-) d\Gamma = 0$$

Disadvantage: mixed format \rightarrow difficulties with solvers

Discontinuous Galerkin methods

- Pointwise enforcement of continuity: $\boldsymbol{\lambda} = -\mathbf{t}_d$

$$\int_{\Omega} \nabla^{\text{sym}} \mathbf{w} : \boldsymbol{\sigma} d\Omega - \int_{\Gamma_d} (\mathbf{w}^+ - \mathbf{w}^-) \cdot \mathbf{t}_d d\Gamma = \text{r.h.s.}$$

Discrete format:

$$\int_{\Gamma_d} (\mathbf{w}^+ - \mathbf{w}^-) \cdot \mathbf{t}_d d\Gamma = \mathbf{w}^T \left(\int_{\Gamma_d} \mathbf{B}_i^T \mathbf{T} \mathbf{B}_i d\Gamma \right) \mathbf{a}$$

→ same format as standard interface elements

Discontinuous Galerkin methods

- Average of tractions: $\lambda = \frac{1}{2} \mathbf{n}_{\Gamma_d} \cdot (\boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^-)$

Elaboration of surface integral:

$$\int_{\Gamma_d} (\mathbf{w}^+ - \mathbf{w}^-) \cdot \lambda d\Gamma = \int_{\Gamma_d} \frac{1}{2} (\mathbf{w}^+ - \mathbf{w}^-) \cdot \mathbf{n}_{\Gamma_d} \cdot (\boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^-) d\Gamma$$

For proper conditioning, add:

$$\alpha \int_{\Gamma_d} \frac{1}{2} (\nabla^{\text{sym}} \mathbf{w}^+ + \nabla^{\text{sym}} \mathbf{w}^-) : \mathbf{D} \cdot \mathbf{n}_{\Gamma_i} \cdot (\mathbf{u}^+ - \mathbf{u}^-) d\Gamma$$

For numerical stability, add: $\int_{\Gamma_d} \tau (\mathbf{w}^+ - \mathbf{w}^-) \cdot (\mathbf{u}^+ - \mathbf{u}^-) d\Gamma$

Discontinuous Galerkin methods

Linearized set of equations:

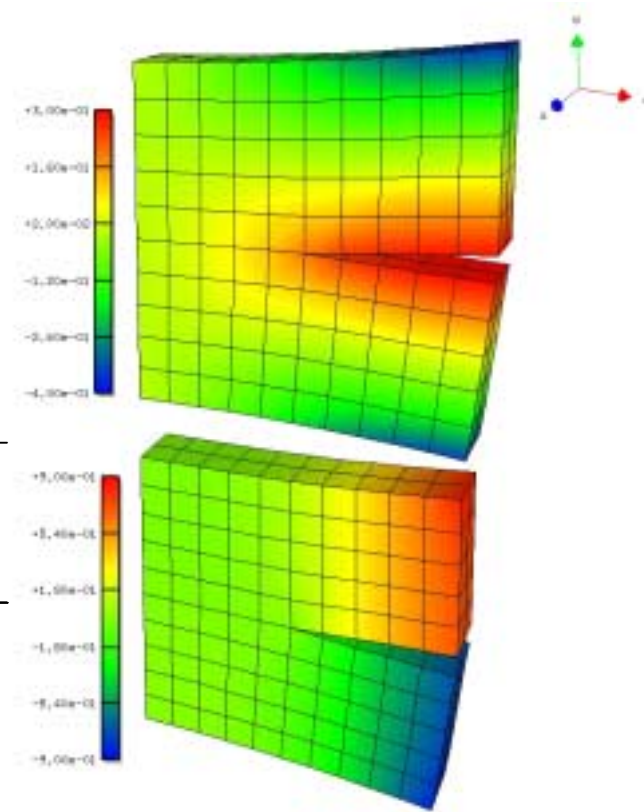
$$\begin{bmatrix} \mathbf{K}^{--} & \mathbf{K}^{-+} \\ \mathbf{K}^{+-} & \mathbf{K}^{++} \end{bmatrix} \begin{pmatrix} \mathbf{d}\mathbf{a}^- \\ \mathbf{d}\mathbf{a}^+ \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{\mathbf{a}^-}^{ext} - \mathbf{f}_{\mathbf{a}^-}^{int} \\ \mathbf{f}_{\mathbf{a}^+}^{ext} - \mathbf{f}_{\mathbf{a}^+}^{int} \end{pmatrix}$$

$$\mathbf{K}^{--} = \int_{\Omega^-} \mathbf{B}^T \mathbf{D} \mathbf{B} d\Omega + \frac{1}{2} \int_{\Gamma_d} \mathbf{N}^T \mathbf{n}_{\Gamma_i}^T \mathbf{D} \mathbf{B} d\Gamma + \frac{1}{2} \alpha \int_{\Gamma_d} \mathbf{B}^T \mathbf{D} \mathbf{n}_{\Gamma_i} \mathbf{N} d\Gamma$$

$$\mathbf{K}^{++} = \int_{\Omega^+} \mathbf{B}^T \mathbf{D} \mathbf{B} d\Omega - \frac{1}{2} \int_{\Gamma_d} \mathbf{N}^T \mathbf{n}_{\Gamma_d}^T \mathbf{D} \mathbf{B} d\Gamma - \frac{1}{2} \alpha \int_{\Gamma_d} \mathbf{B}^T \mathbf{D} \mathbf{n}_{\Gamma_d} \mathbf{N} d\Gamma$$

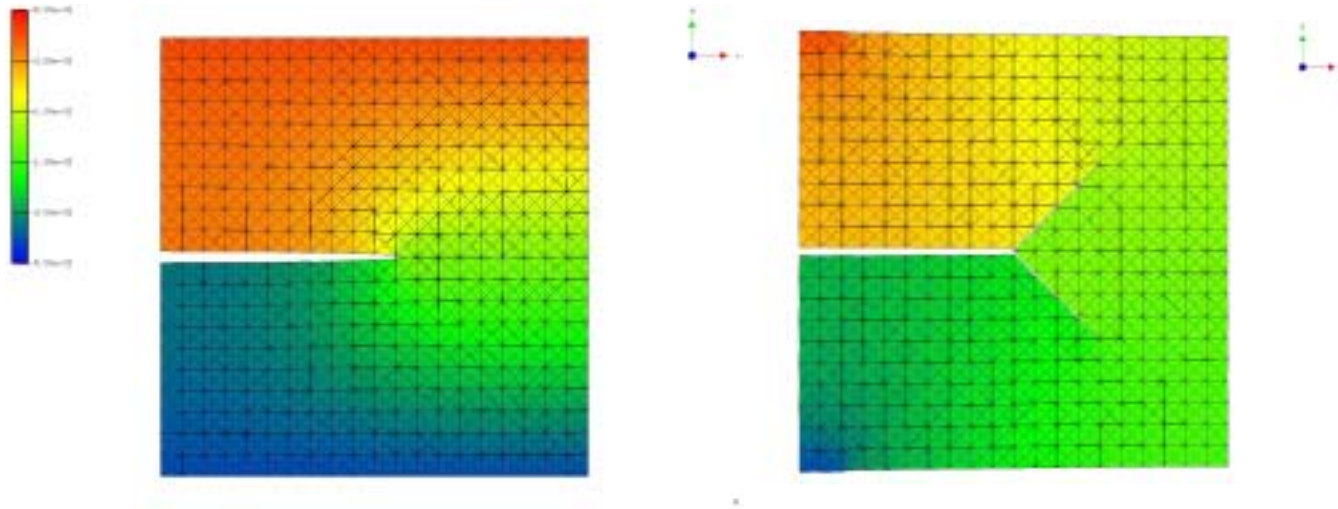
$$\mathbf{K}^{-+} = \frac{1}{2} \int_{\Gamma_d} \mathbf{N}^T \mathbf{n}_{\Gamma_d}^T \mathbf{D} \mathbf{B} d\Gamma - \frac{1}{2} \alpha \int_{\Gamma_d} \mathbf{B}^T \mathbf{D} \mathbf{n}_{\Gamma_d} \mathbf{N} d\Gamma$$

$$\mathbf{K}^{+-} = \frac{1}{2} \alpha \int_{\Gamma_d} \mathbf{B}^T \mathbf{D} \mathbf{n}_{\Gamma_d} \mathbf{N} d\Gamma - \frac{1}{2} \int_{\Gamma_d} \mathbf{N}^T \mathbf{n}_{\Gamma_d}^T \mathbf{D} \mathbf{B} d\Gamma$$



Example of 3D elasticity

Discontinuous Galerkin methods



Example with crack branching

- Disadvantage relative to PUM: no arbitrary crack direction
- Advantage relative to standard interfaces: no oscillations

Concluding remarks

- Modern experimental equipment and methods allow for quantification of parameters at lower scales
- To exploit this potential, new multiscale concepts are needed in computational mechanics
- Such concepts inevitably require capturing evolving discontinuities; they arise naturally at lower scales
- In many cases (durability, biomaterials,...) several physical phenomena have to be considered simultaneously
- This provides a formidable challenge for computational mechanics!