Computational modeling of material failure

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in collaboration with

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Outline

- Computational models for fracture
  - Continuum mechanics: LEFM, Cohesive zone models
  - Peridynamics
  - Continuous/discontinuous description of failure (Damage models, XFEM, interface elements)

- Multiscale modeling of fracture
  - Hierarchical, semi-concurrent and concurrent methods
  - Computational homogenization models for fracture

- Image-based modeling
  - Conforming mesh methods
  - Level Set/XFEM, Finite Cell Method (non-conforming)
  - Voxel based methods

Continuum mechanics theories

Cauchy, Euler, Lagrange...

$$\sigma_{ij,j} + \rho b_i = \rho \ddot{u}_i$$

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

+

Fracture Mechanics

Damage Mechanics

PDE

spatial derivatives of displacements:
do not exist at discontinuities (cracks)

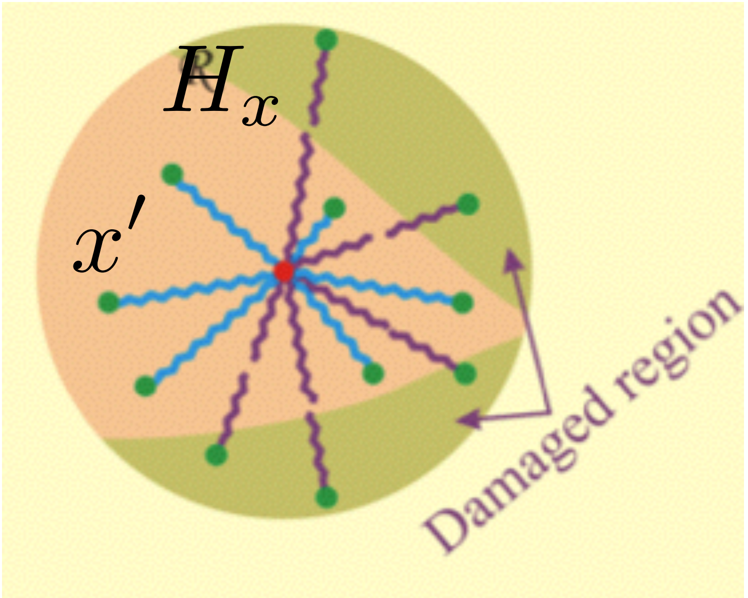
S. Silling 2000

Peridynamics

Peridynamics is a formulation of continuum mechanics that is oriented toward deformations with discontinuities, especially fractures.

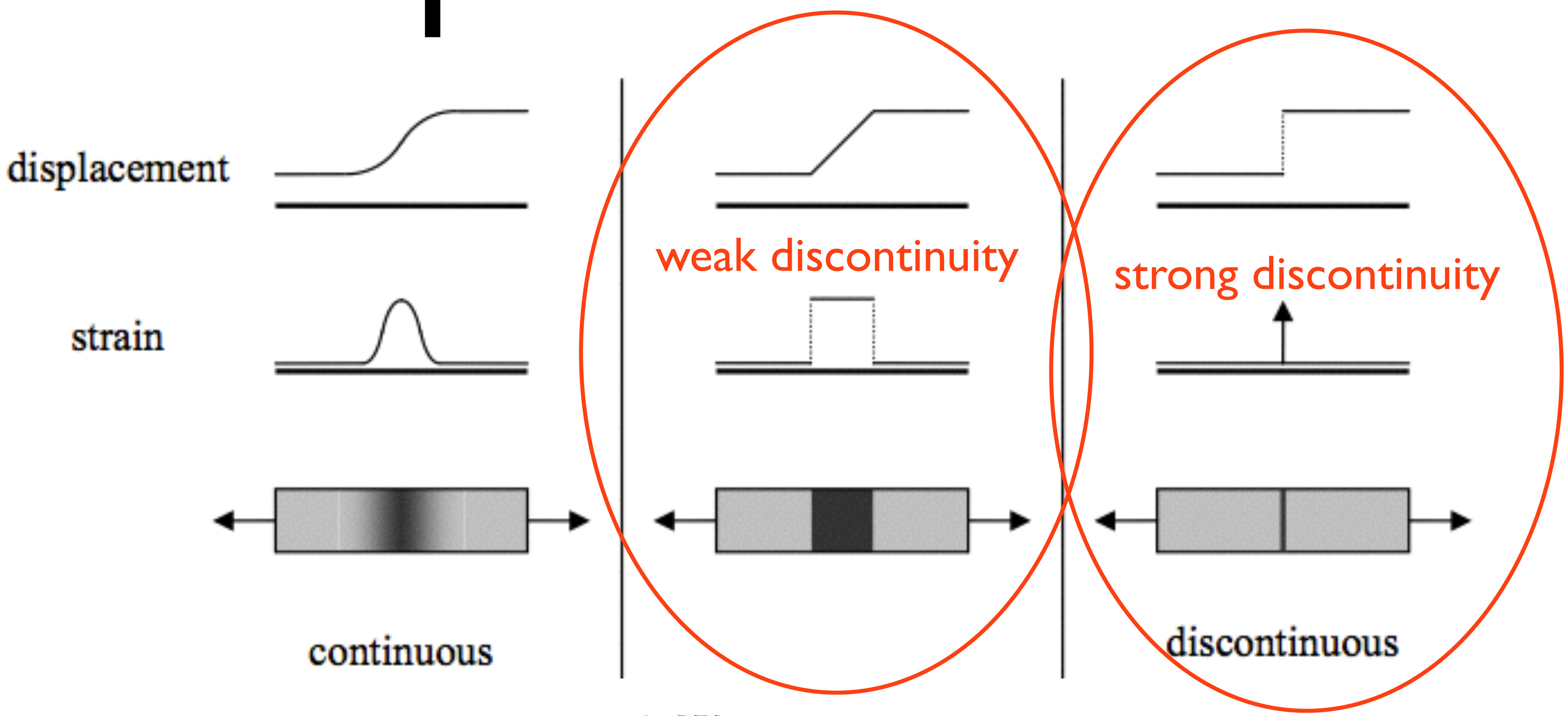
Integral equation

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H_\mathbf{x}} \mathbf{f}(\mathbf{u}(\mathbf{x}',t) - \mathbf{u}(\mathbf{x},t), \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} - \mathbf{b}(\mathbf{x},t)$$



No spatial derivatives of displacements

Continuous/discontinuous description of fracture



Damage Mechanics

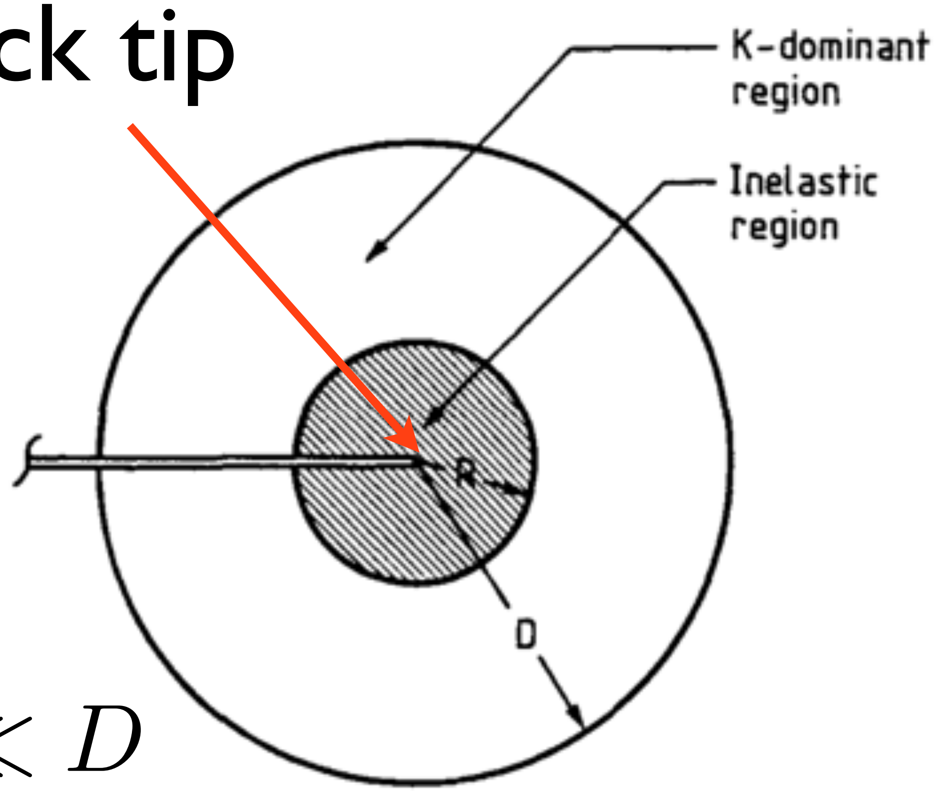
Isotropic damage models
Softening plasticity models
Damage-plastic models

Fracture Mechanics

LEFM, EPFM, CZM

Fracture mechanics models

crack tip



$R \ll D$

Linear Elastic Fracture Mechanics (LEFM):
- brittle materials
- ductile materials under Small Scale Yielding (SSY) condition
- an existing crack is required

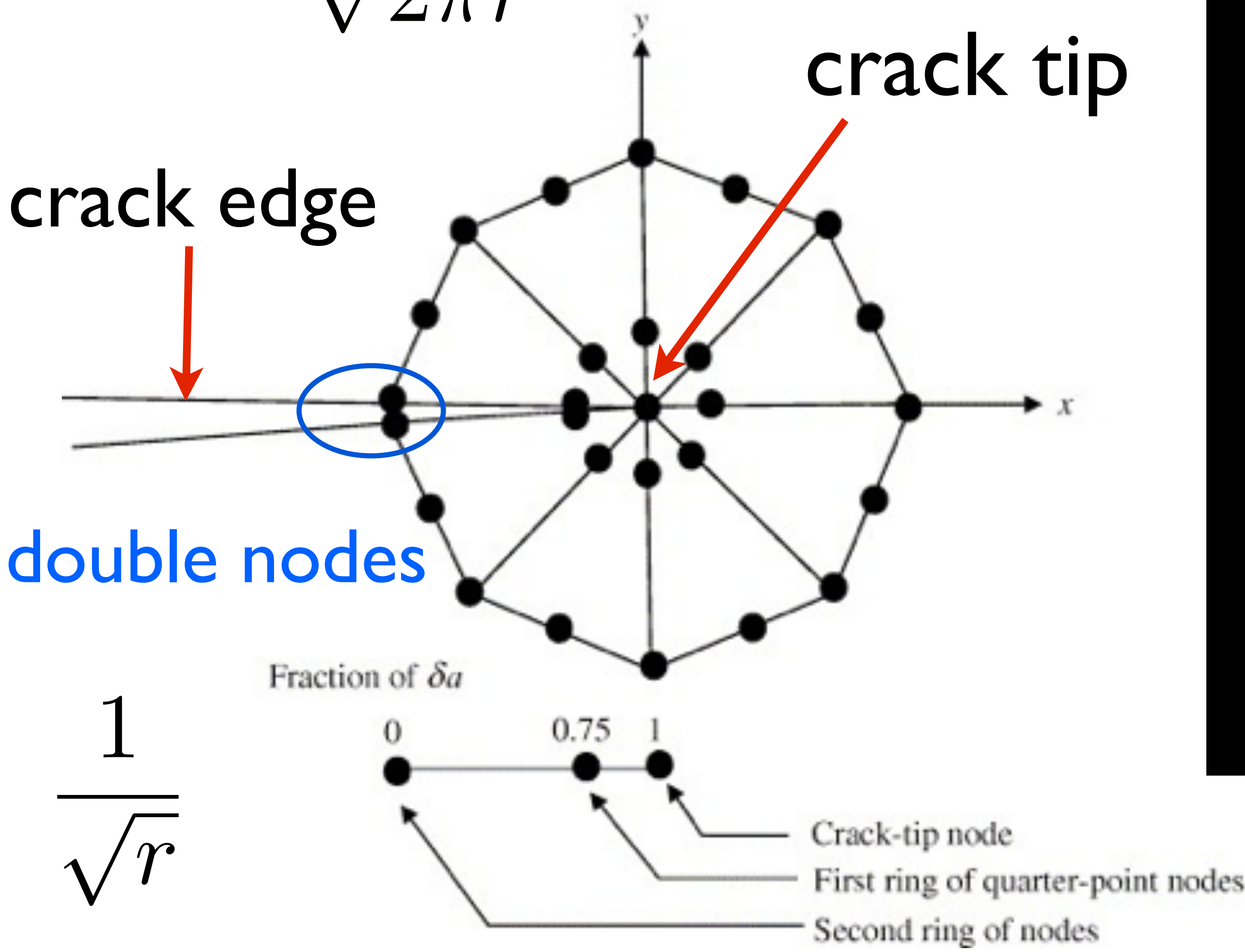
Elastic Plastic Fracture Mechanics (EPFM):
- ductile materials
- an existing crack is required

Cohesive Zone Models (CZMs):
- quasi-brittle materials (concrete)
- ductile materials
- no existing crack is needed

Linear Elastic Fracture Mechanics (LEFM)

SIF

$$\sigma_{ij} = \frac{K}{\sqrt{2\pi r}} f_{ij}(\theta) + \mathrm{H.O.T}$$



$$\frac{1}{\sqrt{r}}$$

crack must locate on element edges

Barsoum element [1970s]

Remeshing is a key point.

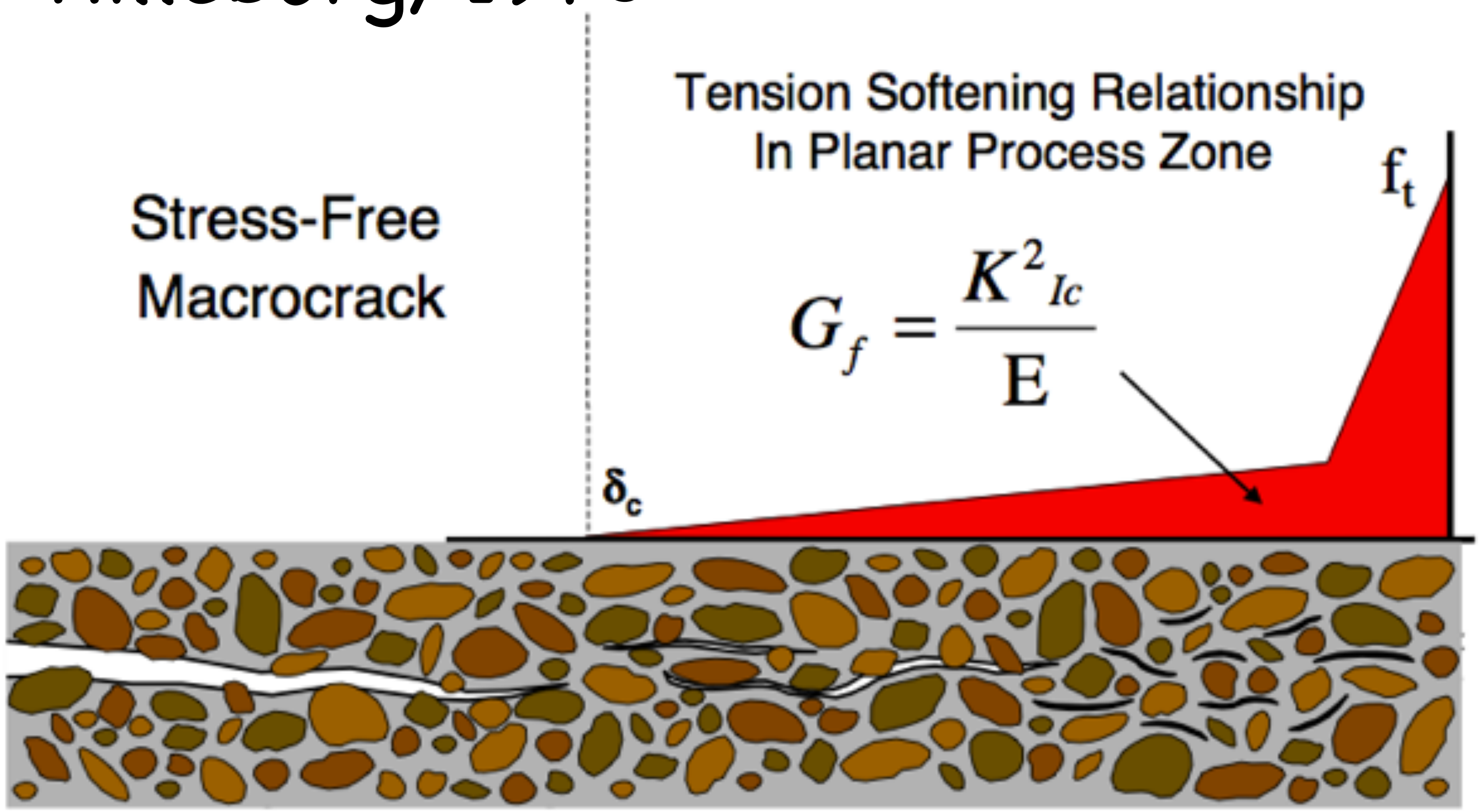
Very useful for fatigue life estimation $\frac{da}{dN} = C(\Delta K)^m$

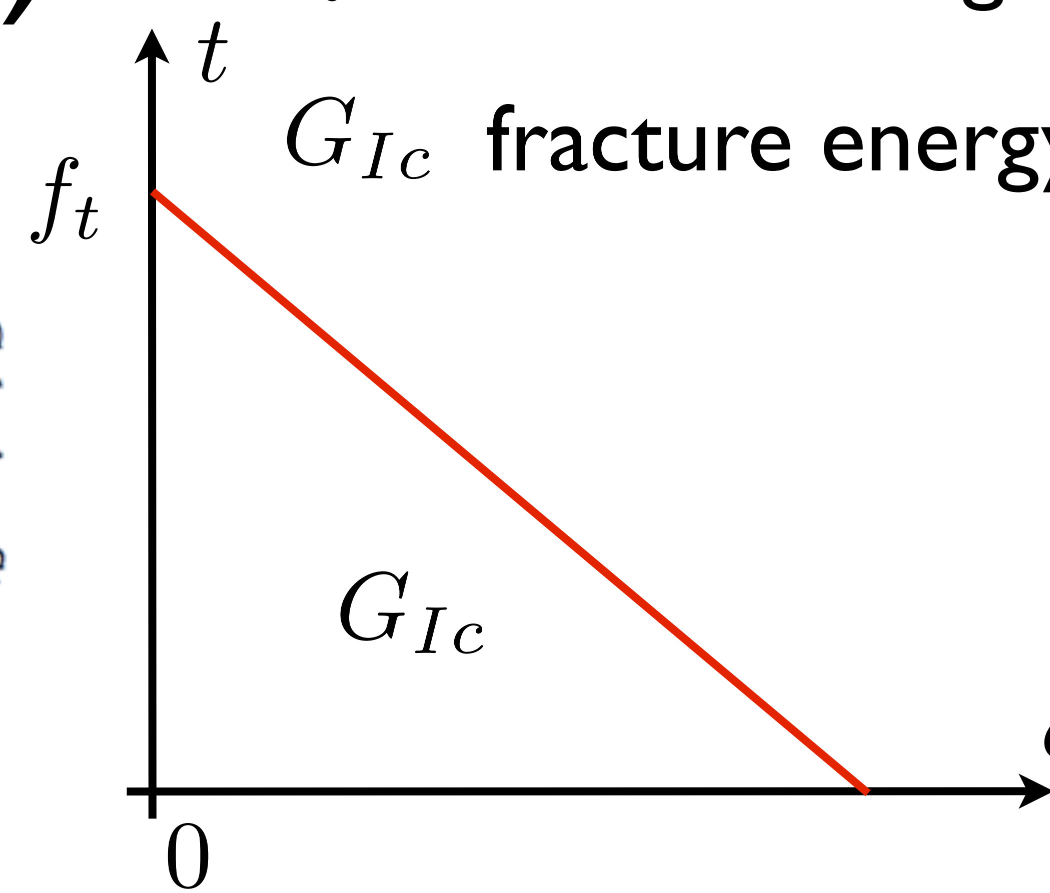
Cohesive Zone Models (CZMs)

Barrenblatt 1962
Dugdale 1960
Hilleborg, 1976

f_t tensile strength

G_{Ic} fracture energy





[Extrinsic] Cohesive law
[Initially rigid] TSL
(Traction Separation Law)

Constitutive equations

$\dot{\boldsymbol{\sigma}} = \mathbf{D}\dot{\boldsymbol{\epsilon}} \longrightarrow$ deformation

$\dot{\mathbf{t}}^c = \mathbf{T}[\![\dot{\mathbf{u}}]\!] \longrightarrow$ separation

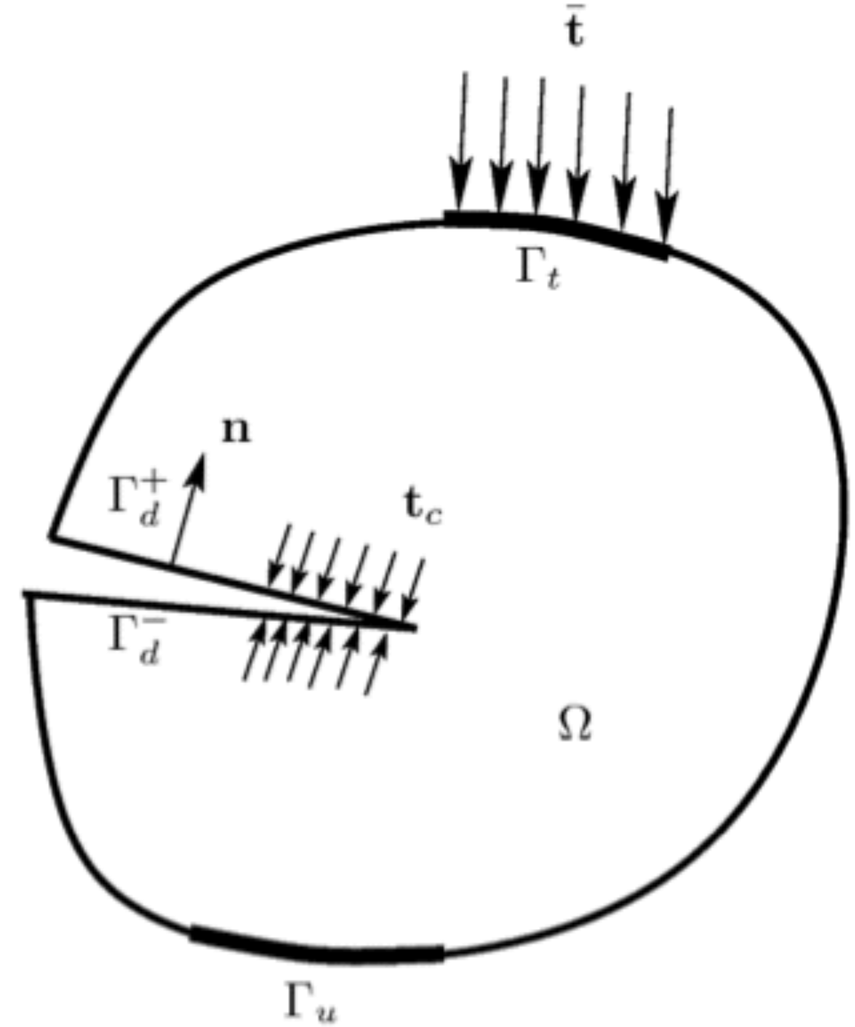
crack initiation
$\sigma_1^{\max} \geq f_t$

crack direction criterion

Cohesive crack model

Governing equations (strong form)

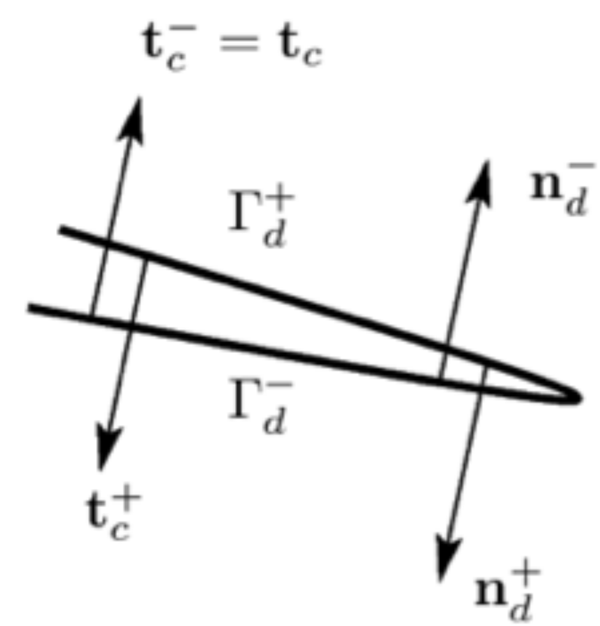
$$
\begin{aligned}
\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} - \rho \ddot{\mathbf{u}} &= 0 \quad \mathbf{x} \in \Omega \\
\mathbf{n} \cdot \boldsymbol{\sigma} &= \bar{\mathbf{t}} \quad \mathbf{x} \in \Gamma_t \\
\mathbf{u} &= \bar{\mathbf{u}} \quad \mathbf{x} \in \Gamma_u \\
\mathbf{n}_d^+ \cdot \boldsymbol{\sigma} = \mathbf{t}_c^+; \quad \mathbf{n}_d^- \cdot \boldsymbol{\sigma} &= \mathbf{t}_c^-; \quad \mathbf{t}_c^+ = -\mathbf{t}_c = -\mathbf{t}_c^- \quad \mathbf{x} \in \Gamma_d
\end{aligned}
$$



Constitutional equations

$\dot{\boldsymbol{\sigma}} = \mathbf{D}\dot{\boldsymbol{\epsilon}}$ ⟶ deformation

$\dot{\mathbf{t}}^c = \mathbf{T}[\![\dot{\mathbf{u}}]\!]$ ⟶ separation



Cohesive crack model

Weak form

$$\delta W^{\text{kin}} = \delta W^{\text{ext}} - \delta W^{\text{int}} - \delta W^{\text{coh}}$$

new term

where

$$\delta W^{\text{kin}} = \int_{\Omega} \delta \mathbf{u} \cdot \rho \ddot{\mathbf{u}} \mathrm{d}\Omega$$

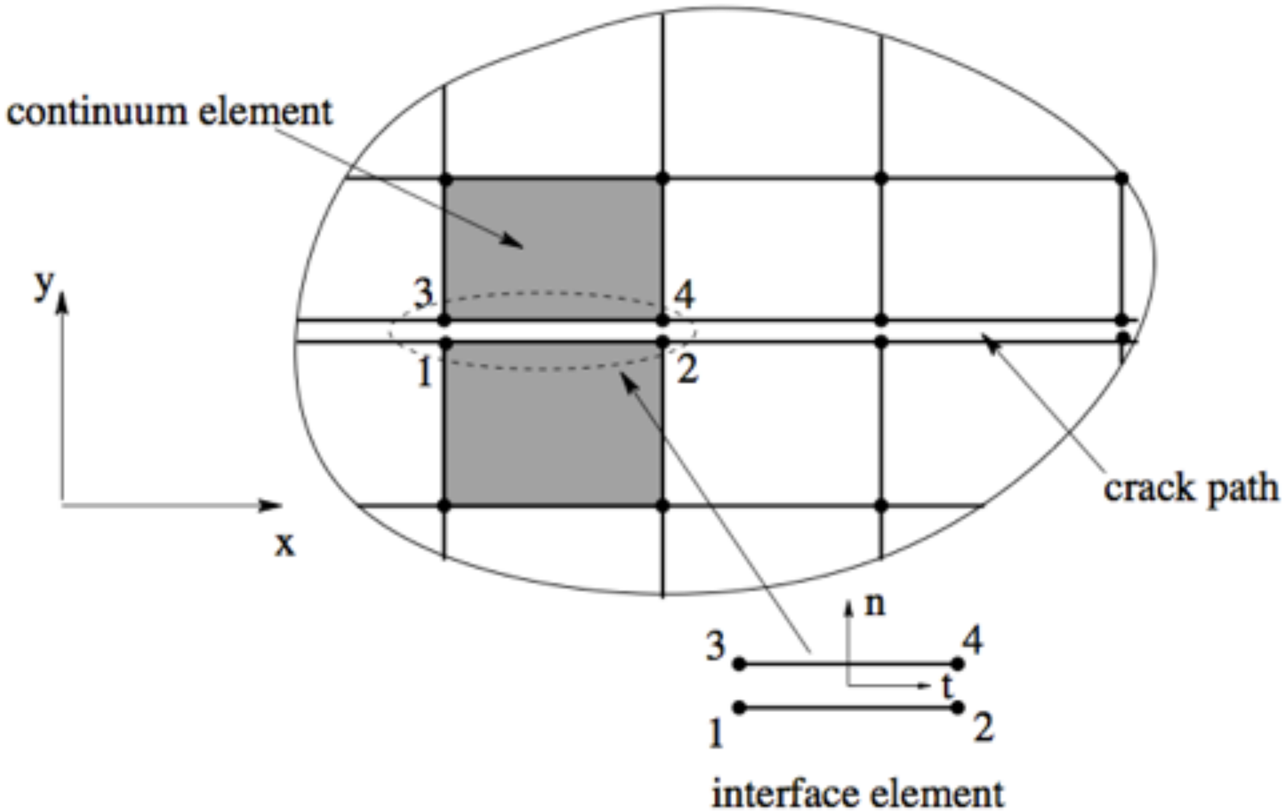
$$\delta W^{\text{int}} = \int_{\Omega} \nabla^s \delta \mathbf{u} : \boldsymbol{\sigma} \mathrm{d}\Omega$$

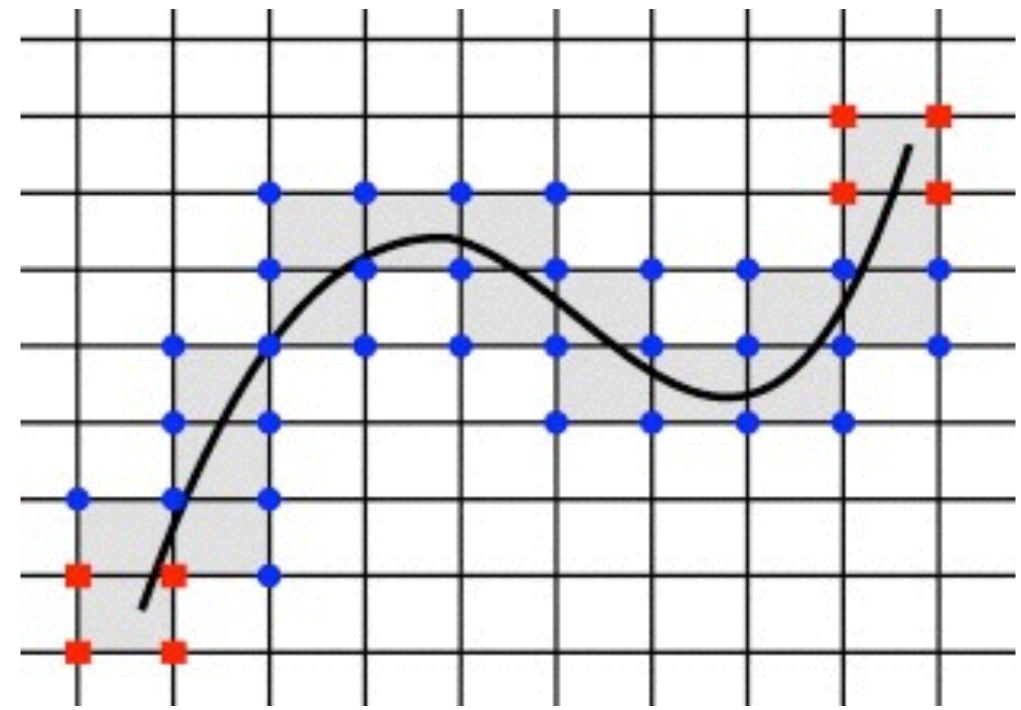
$$\delta W^{\text{ext}} = \int_{\Omega} \delta \mathbf{u} \cdot \rho \mathbf{b} \mathrm{d}\Omega + \int_{\Gamma_t} \delta \mathbf{u} \cdot \bar{\mathbf{t}} \mathrm{d}\Gamma_t$$

$$\delta W^{\text{coh}} = \int_{\Gamma_d} \delta [\![\mathbf{u}]\!] \cdot \mathbf{t}^{\text{c}} \mathrm{d}\Gamma_d$$

different techniques

Crack discretization techniques

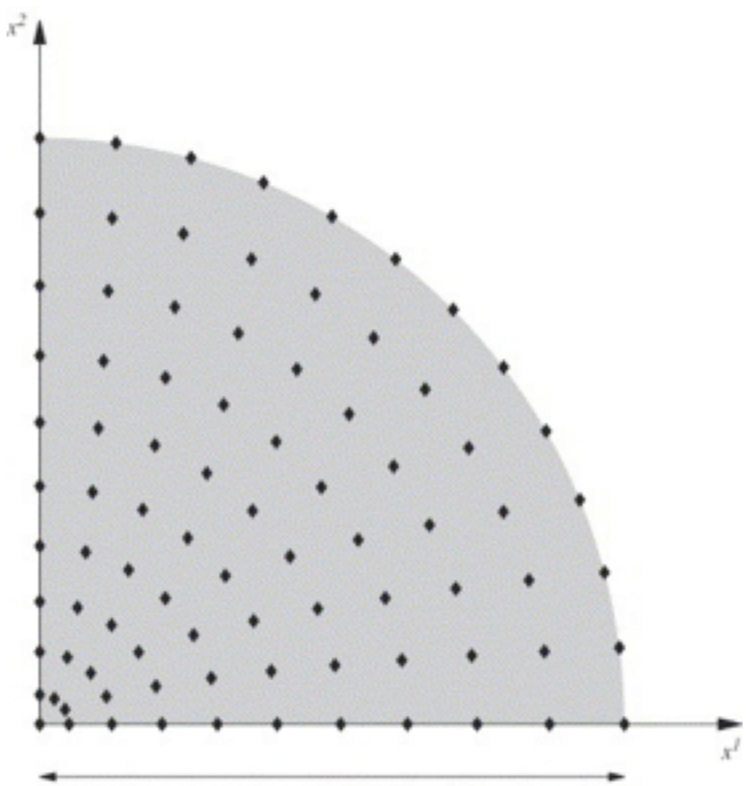


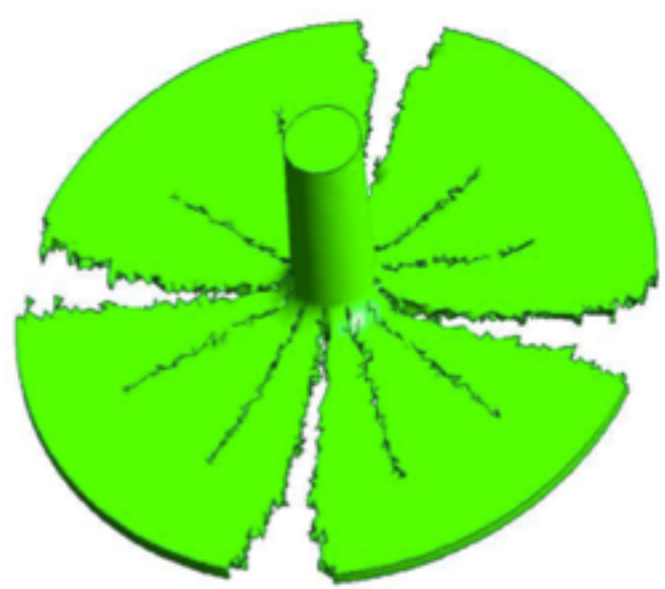


Zero-thickness interface elements, 1968

PUM FEM, 1999

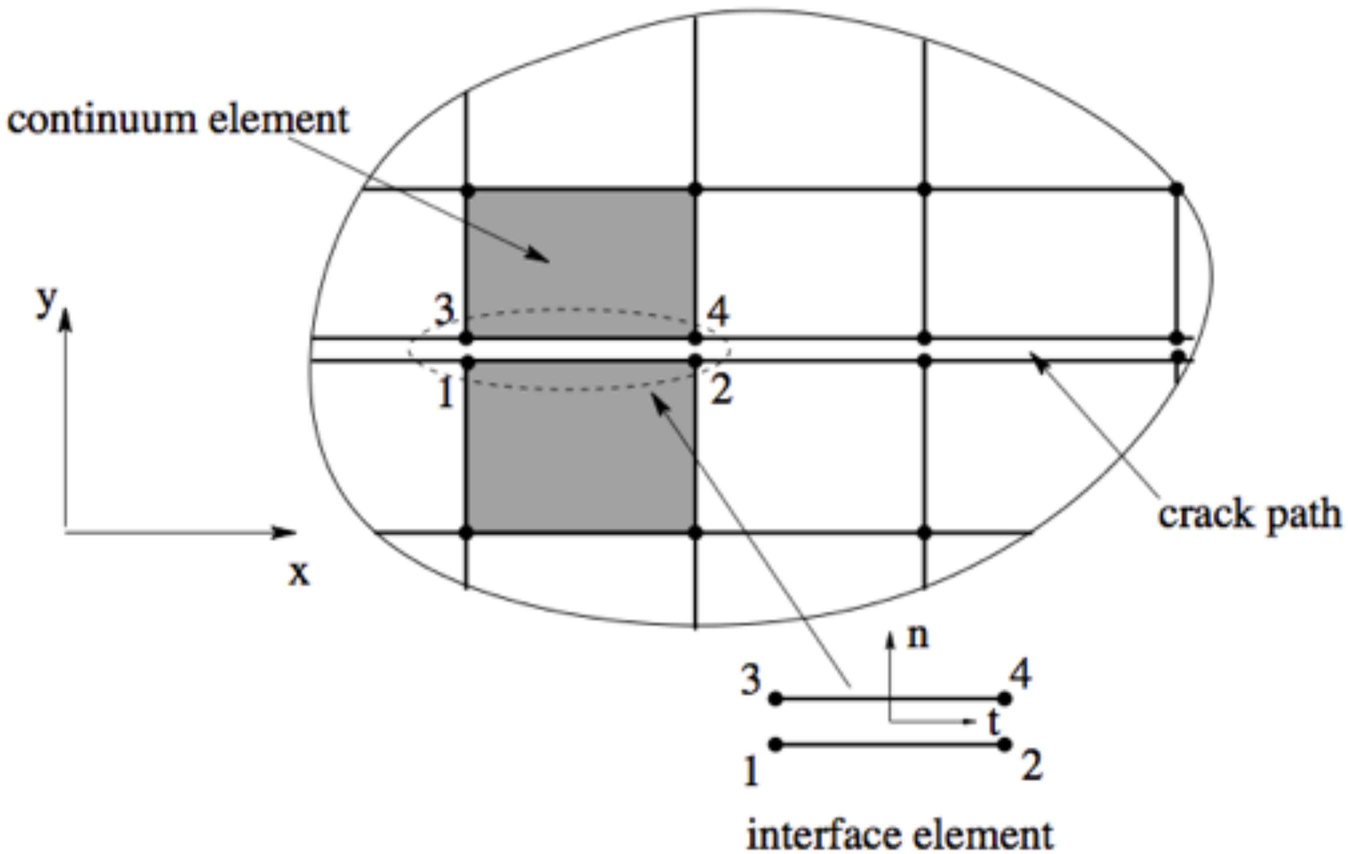
Embedded strong discontinuity, 1987

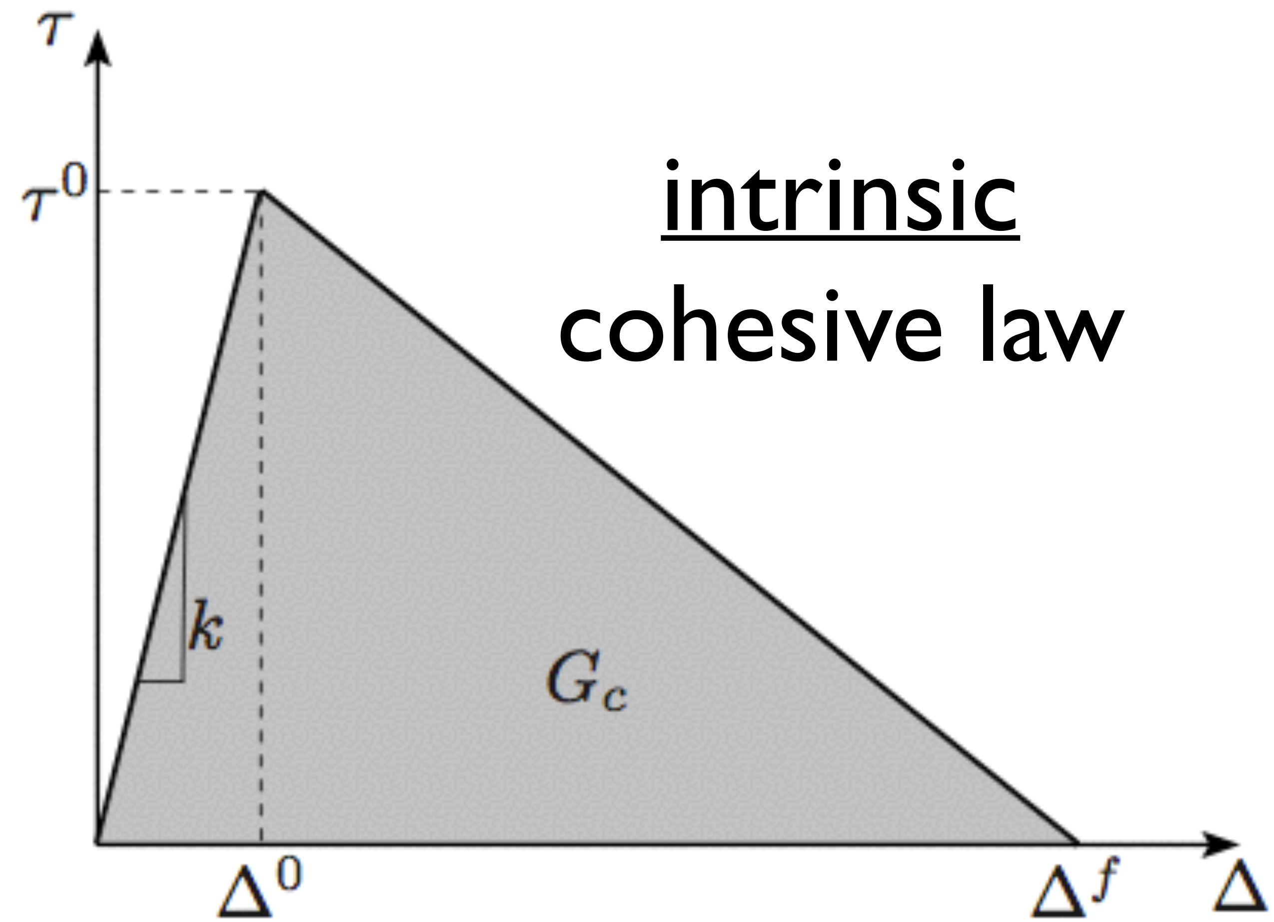




Meshless/Meshfree methods, 1994

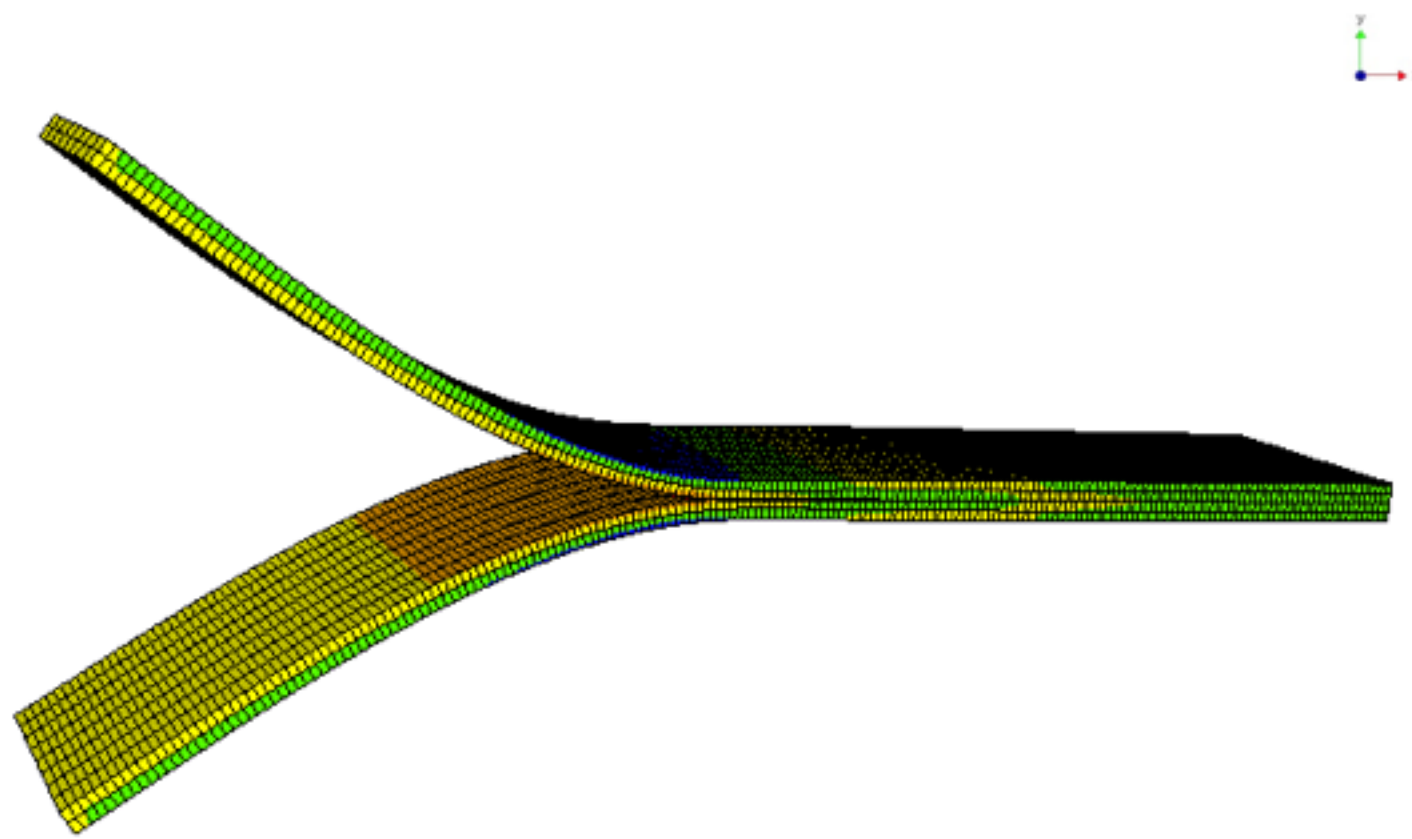
Interface elements





<u>intrinsic</u>
cohesive law

$$\mathbf{u}^+, \mathbf{u}^- \longrightarrow [\![\mathbf{u}]\!] \longrightarrow \Delta \longrightarrow \tau$$

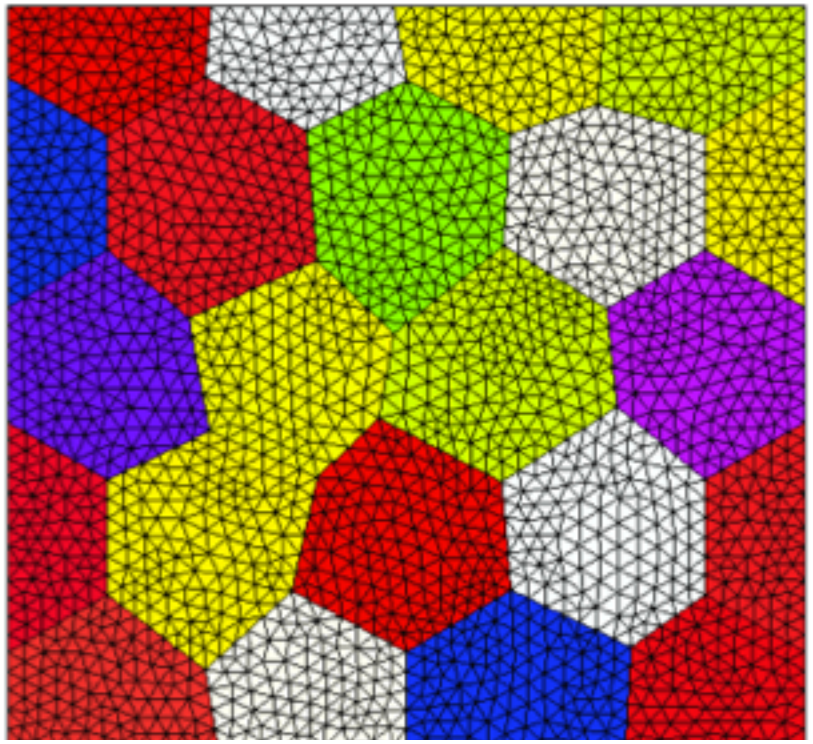


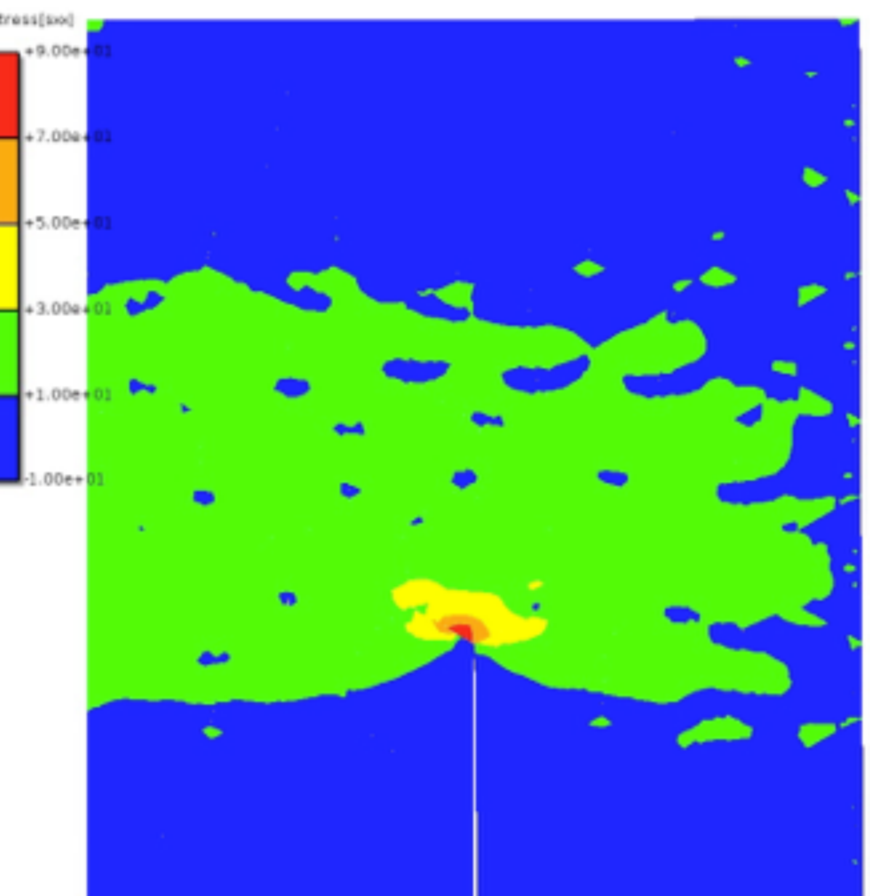
(+) easy to implement 2D/3D
(+) available in ABAQUS, LD-DYNA

- preprocessing: GMSH
- solver: jem/jive (C++)

Interface elements

inter-granular fracture of polycrystalline material





failure of a fiber reinforced composite

Interface elements with discontinuous Galerkin

Partition of Unity Methods

Melenk and Babuska 1996

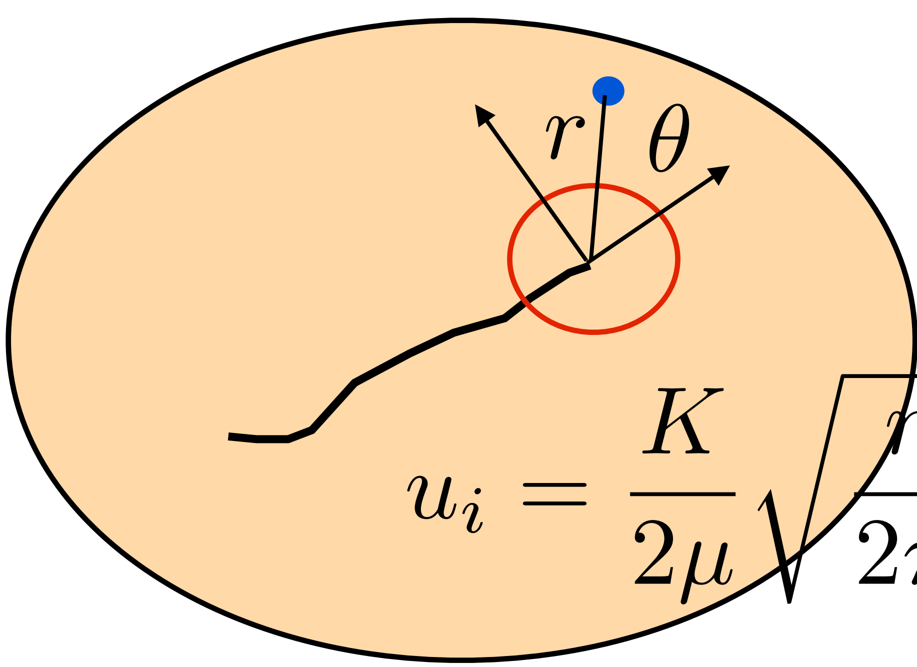
Approximation of the displacement field

Sum of shape functions is equal to one

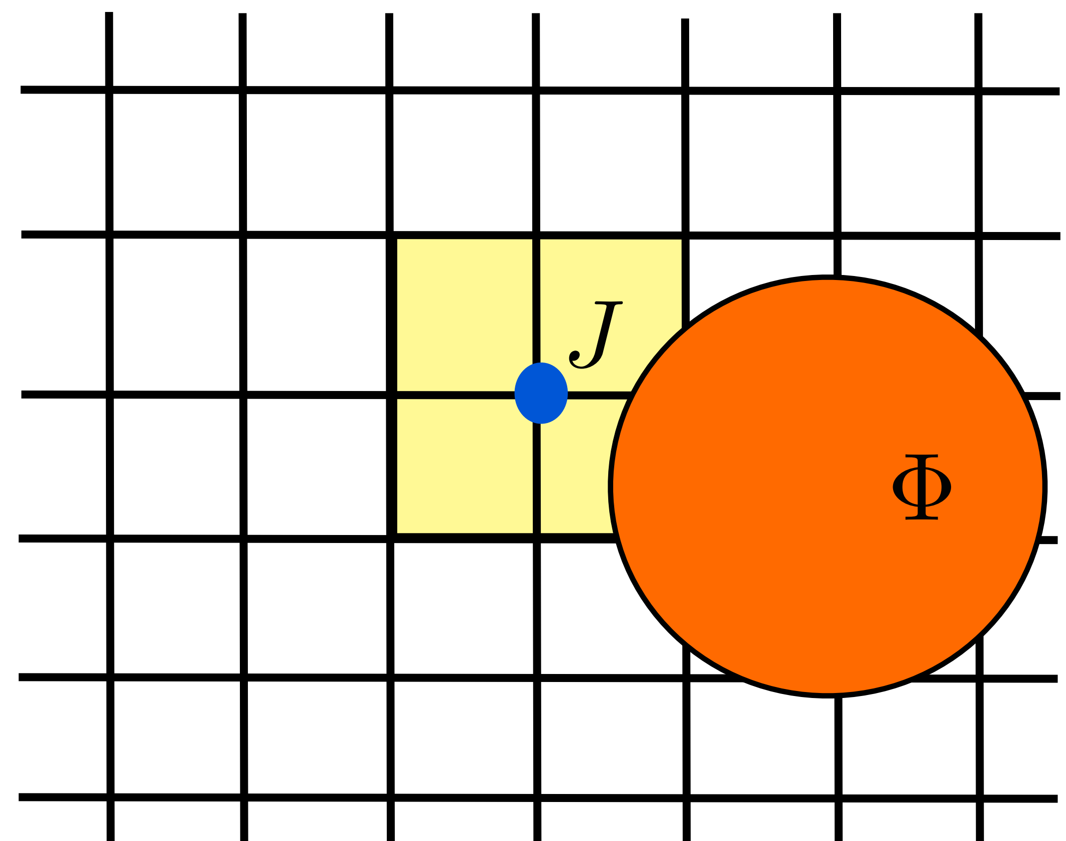
$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} N_I(\mathbf{x})\mathbf{u}_I + \sum_{J \in \mathcal{S}^c} N_J(\mathbf{x})\Phi(\mathbf{x})\mathbf{a}_J$$

$$\sum_J N_J(\mathbf{x}) = 1 \qquad \text{(PUM)}$$

$$\sum_J N_J(\mathbf{x})\Phi(\mathbf{x}) = \Phi(\mathbf{x})$$



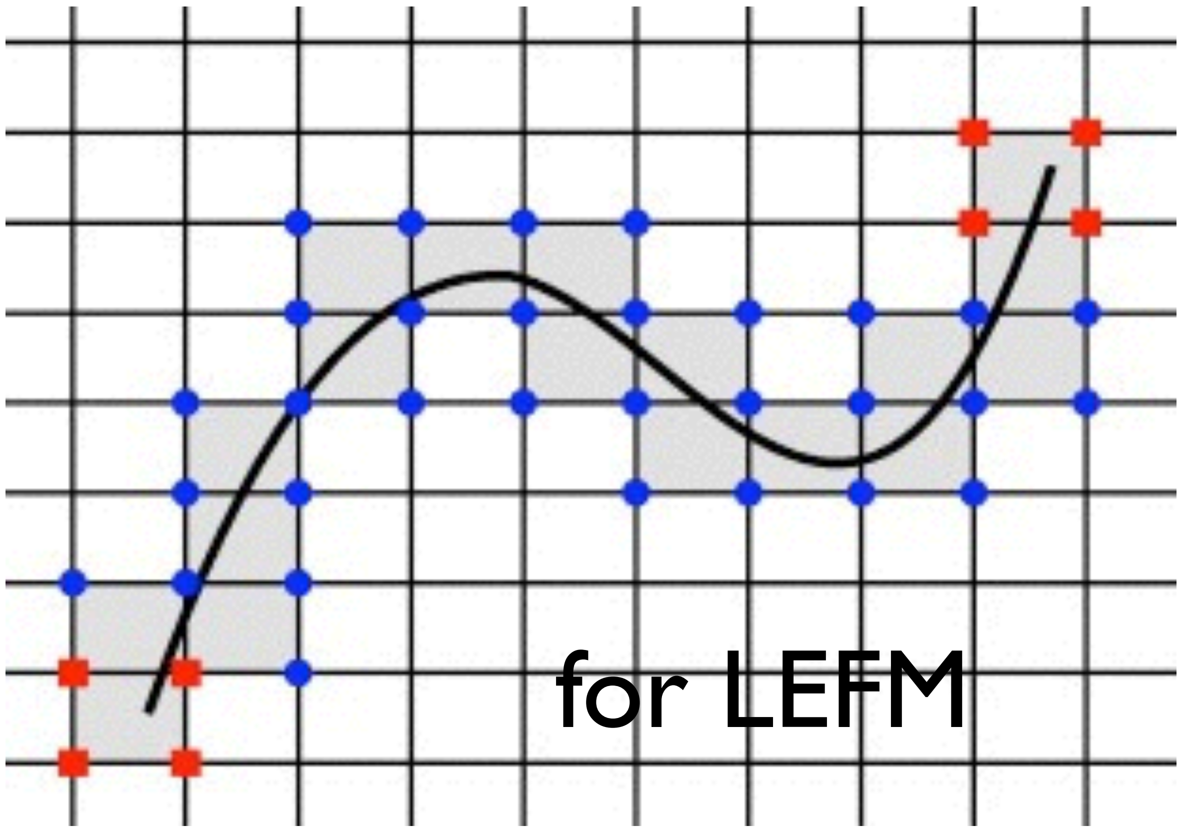
$$u_i = \frac{K}{2\mu}\sqrt{\frac{r}{2\pi}} f_{ij}(\theta)$$



Extended FEM (XFEM)

Belytschko et al., 1999

nothing but an instance of PUM for crack problems



$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} N_I(\mathbf{x})\mathbf{u}_I + \sum_{J \in \mathcal{S}^c} N_J(\mathbf{x}) H(\mathbf{x}) \mathbf{a}_J + \sum_{K \in \mathcal{S}^t} N_K(\mathbf{x}) \left(\sum_{\alpha=1}^{4} B_\alpha \mathbf{b}_K^\alpha \right)$$

$\mathcal{S}^c$ ● (blue circle)

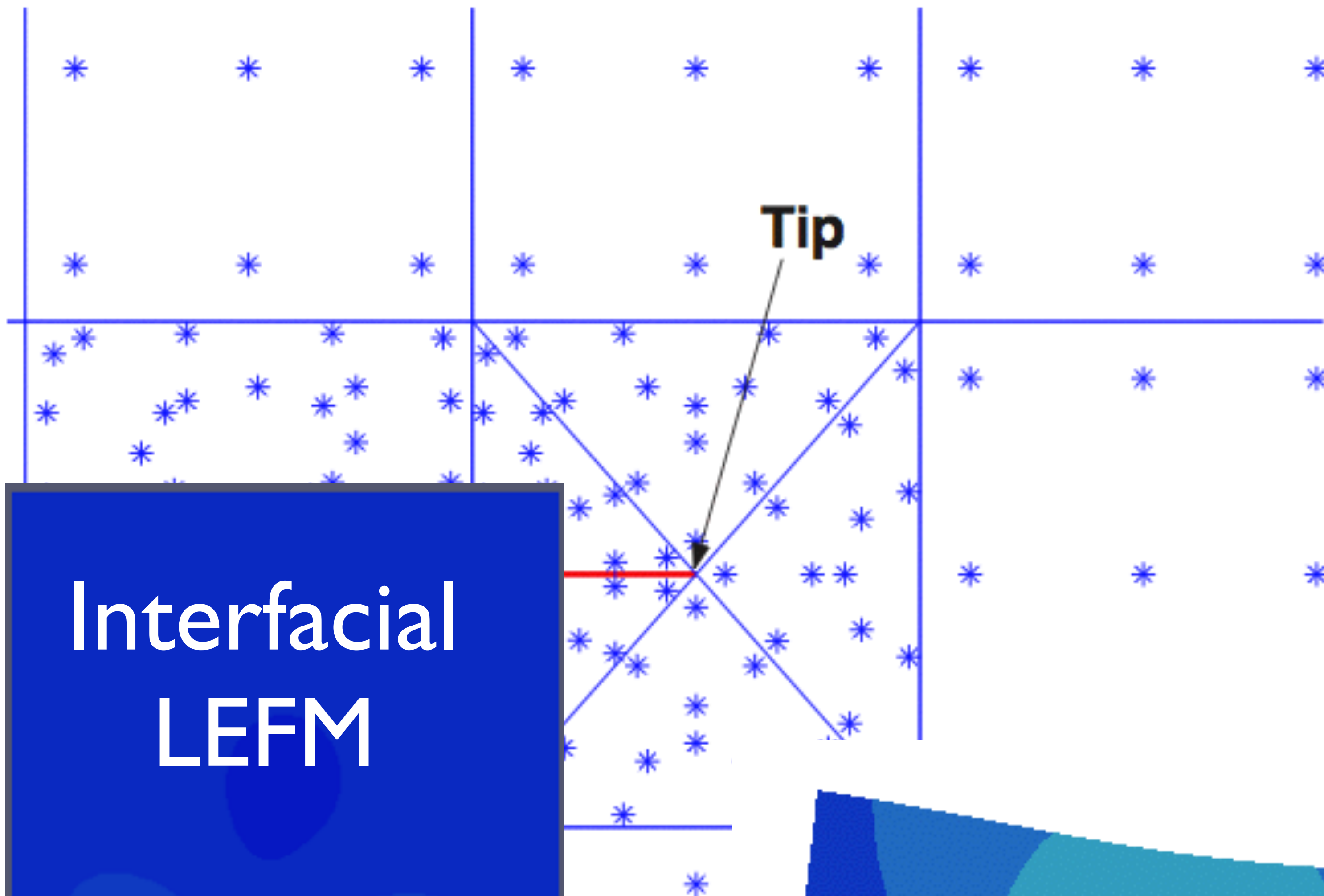
$\mathcal{S}^t$ ■ (red square)

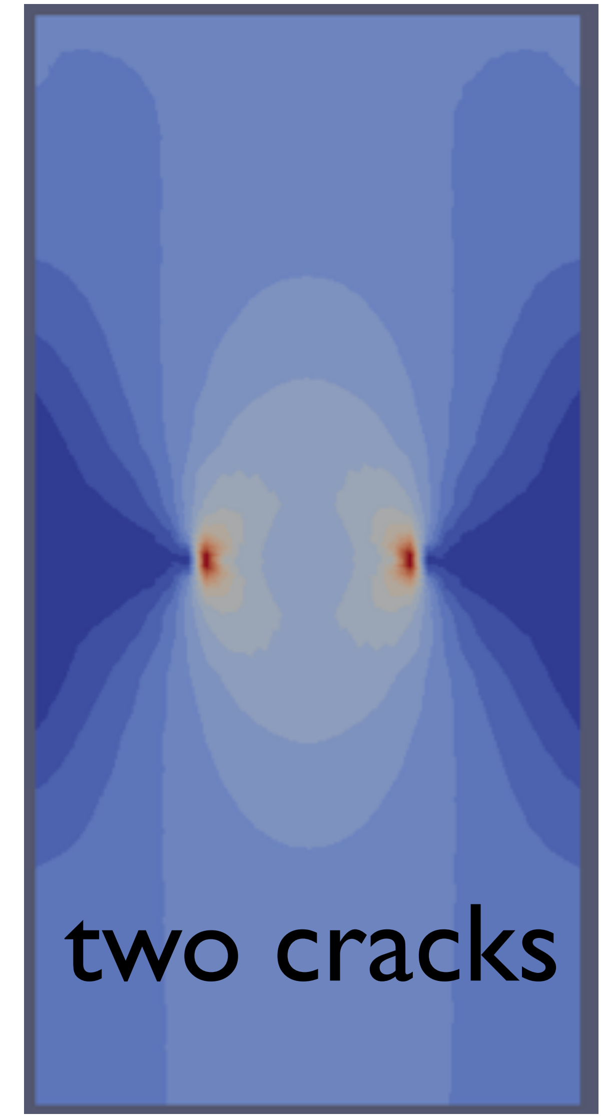
Enrichment functions

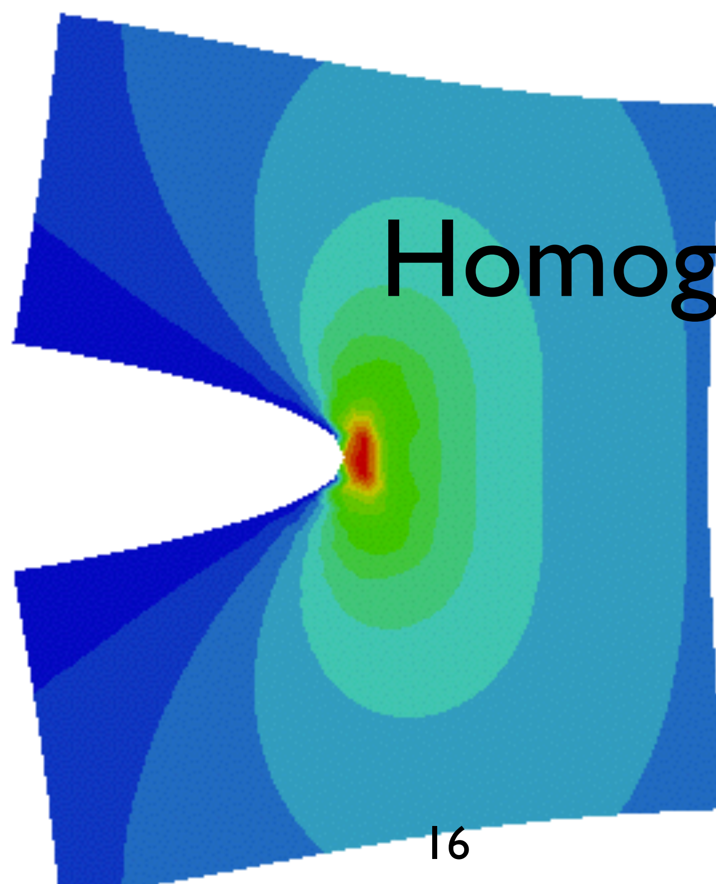
$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } (\mathbf{x} - \mathbf{x}^*) \cdot \mathbf{n} \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

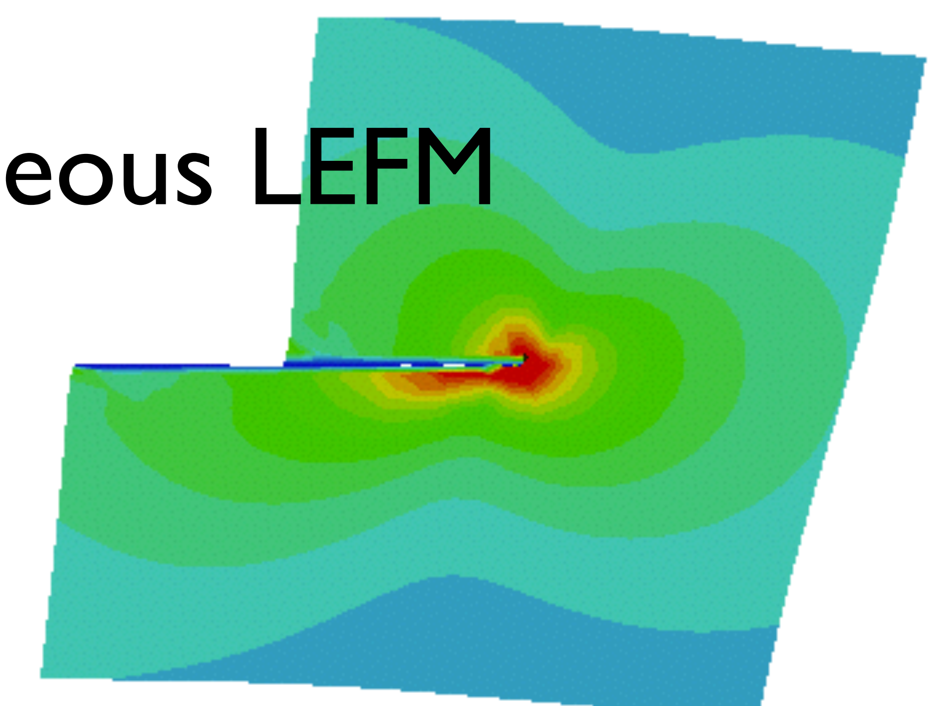
$$[B_\alpha] = \left[\sqrt{r} \sin\frac{\theta}{2}, \sqrt{r}\cos\frac{\theta}{2}, \sqrt{r}\sin\frac{\theta}{2}\sin\theta, \sqrt{r}\cos\frac{\theta}{2}\sin\theta \right]$$

Sub-triangulation for numerical integration









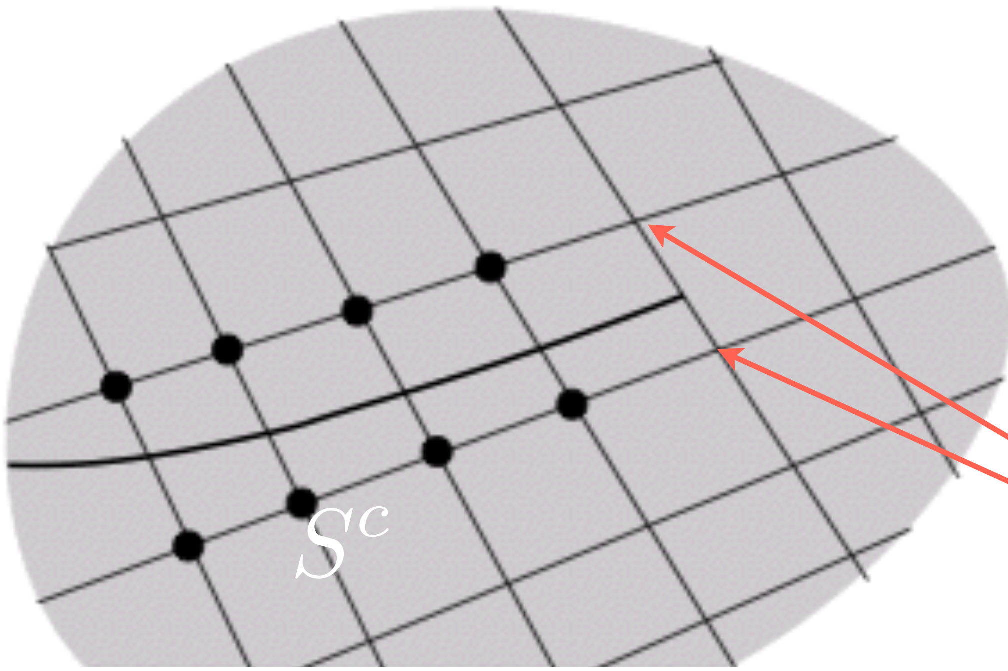
Homogeneous LEFM

Matlab code

XFEM for cohesive cracks

$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} N_I(\mathbf{x})\mathbf{u}_I + \sum_{J \in \mathcal{S}^c} N_J(\mathbf{x})H(\mathbf{x})\mathbf{a}_J$$

Wells, Sluys, 2001

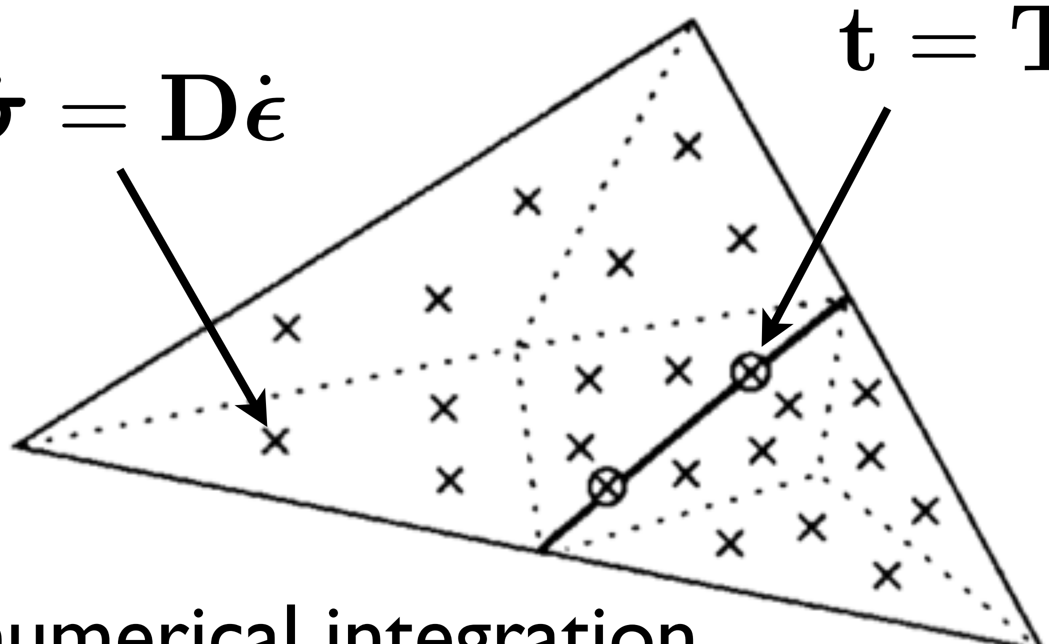


No good crack tip solution is known, no tip enrichment!!!

not enriched to ensure zero crack tip opening!!!

$\dot{\boldsymbol{\sigma}} = \mathbf{D}\dot{\boldsymbol{\epsilon}}$

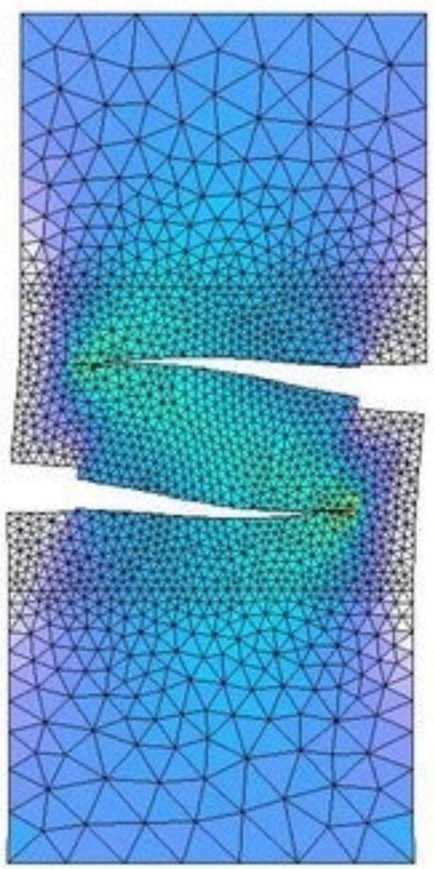
$\dot{\mathbf{t}} = \mathbf{T}[\![\dot{\mathbf{u}}]\!]$

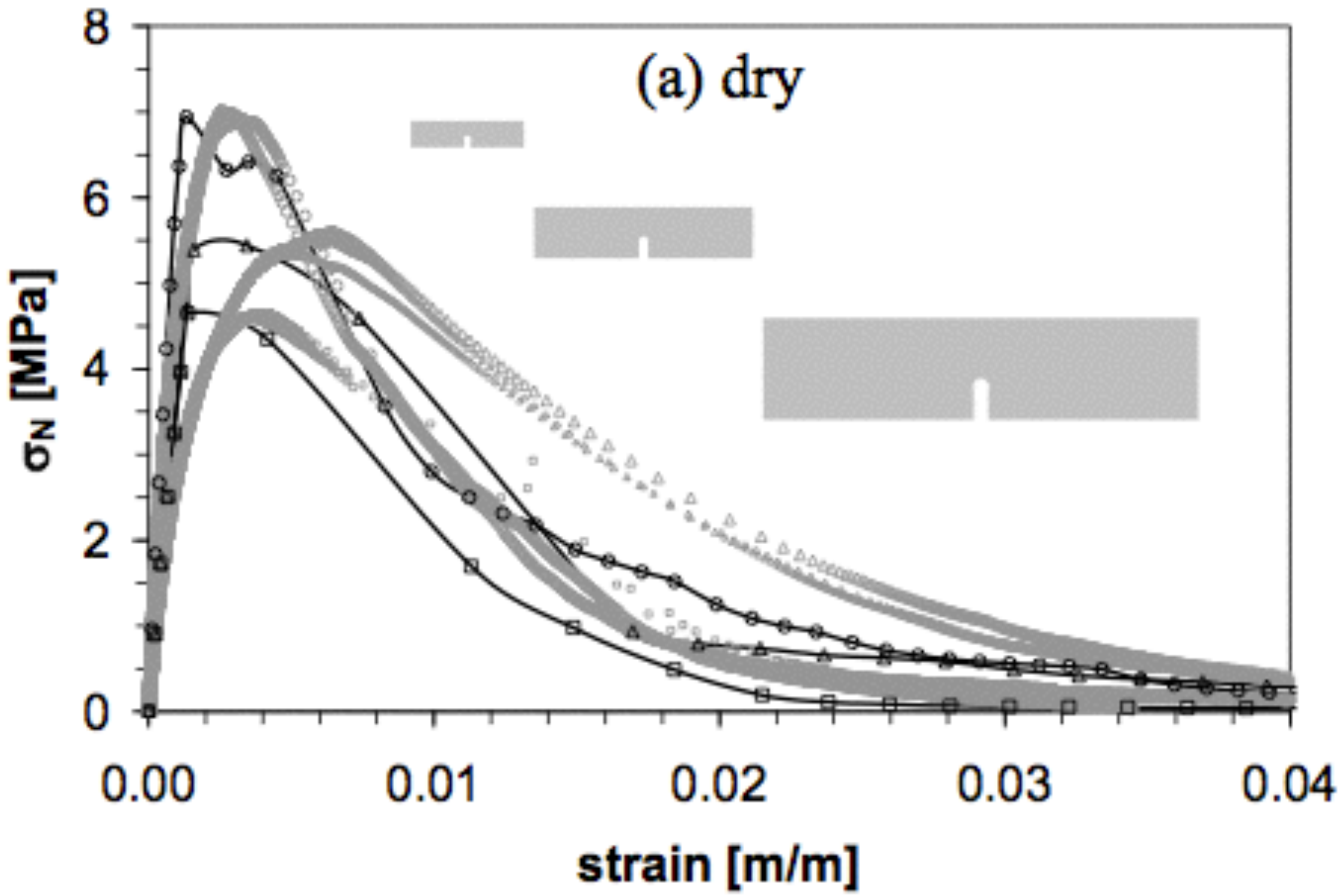


$$H(\mathbf{x}) = \begin{cases} +1 & \text{if } (\mathbf{x} - \mathbf{x}^*) \cdot \mathbf{n} \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

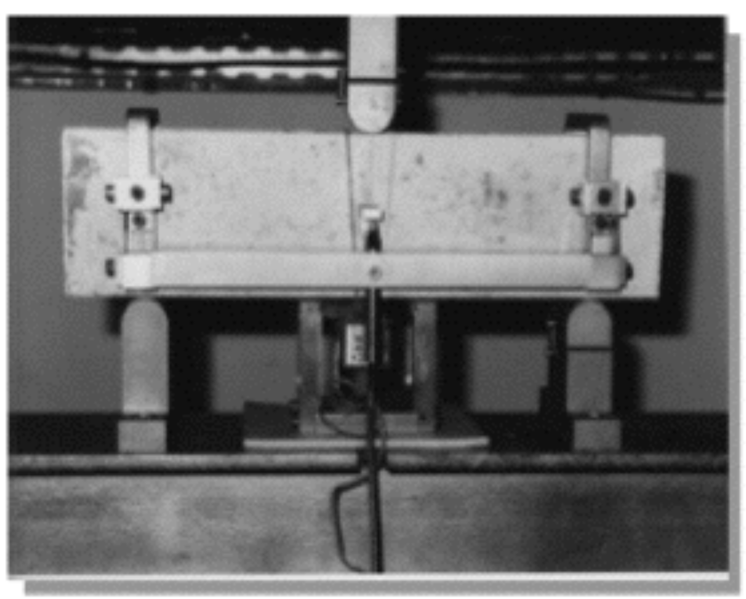
numerical integration

XFEM/Cohesive zones





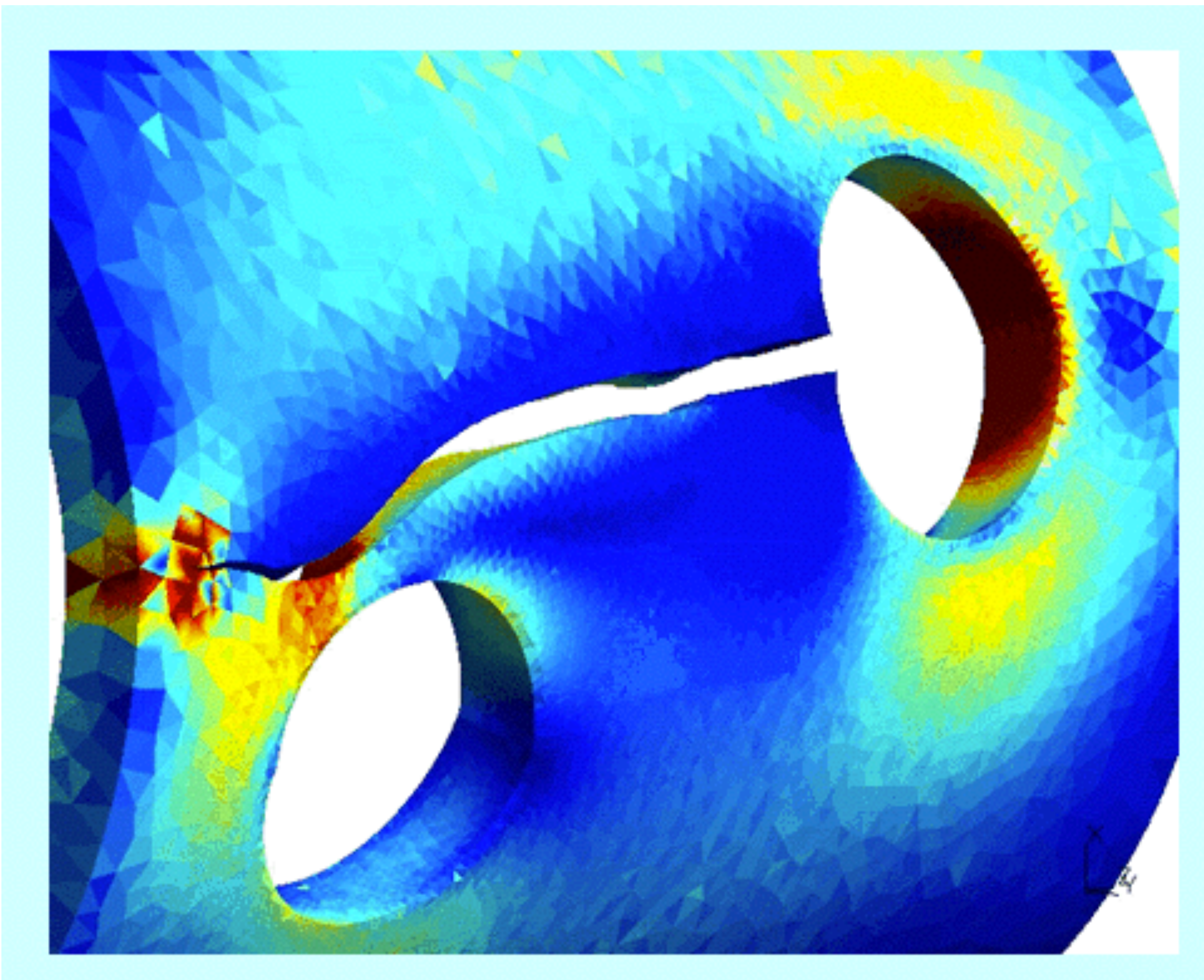
Size effect



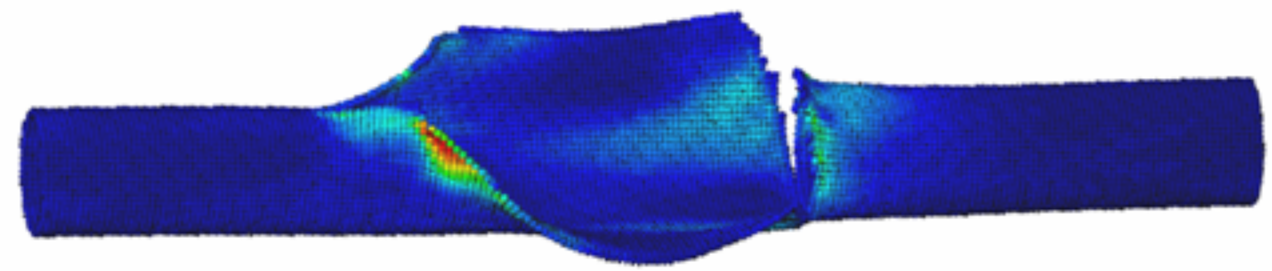
Usual lab tests (10 cm)

"Usual" structures (10m)

… convincing examples

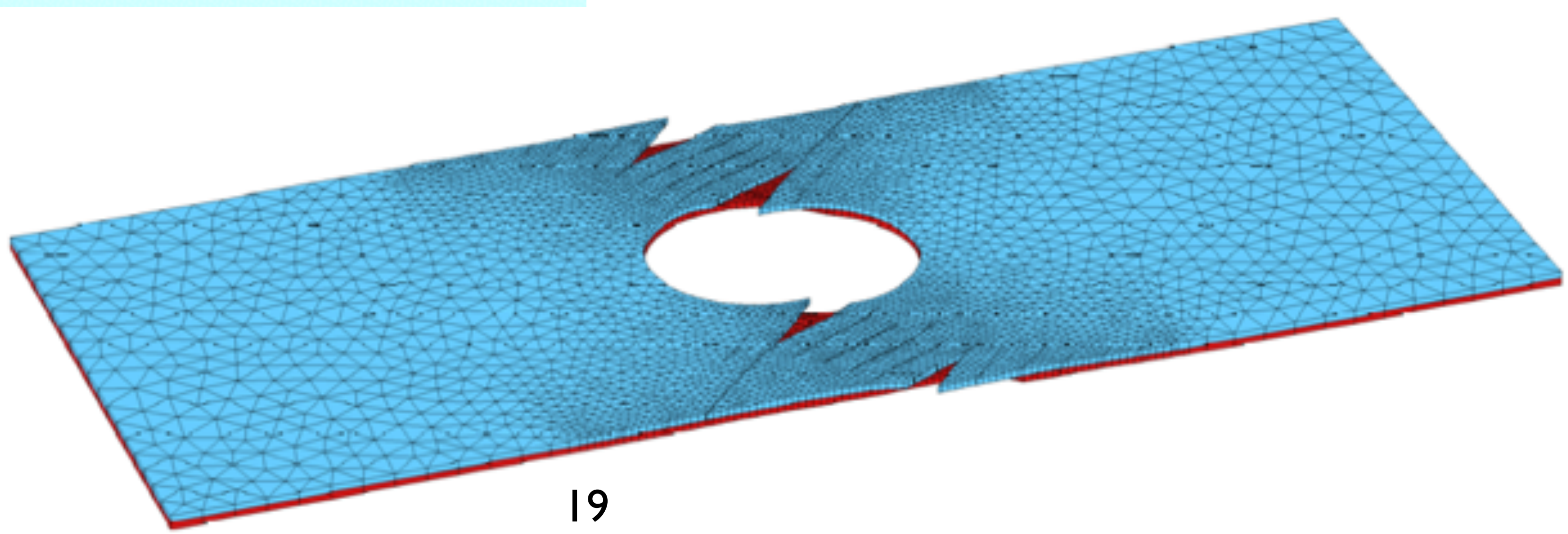


Northwestern Univ.



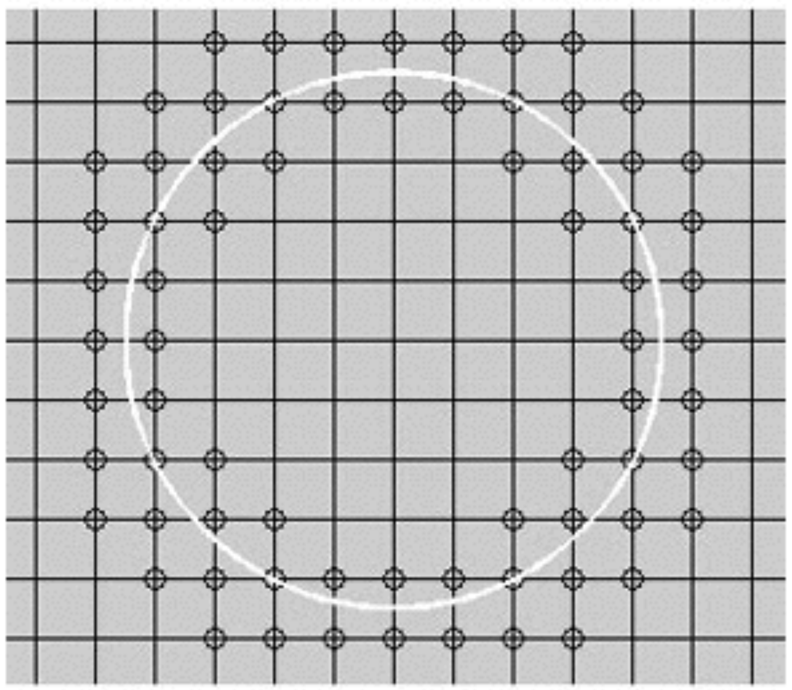
F.P. van der Mer, TU Delft

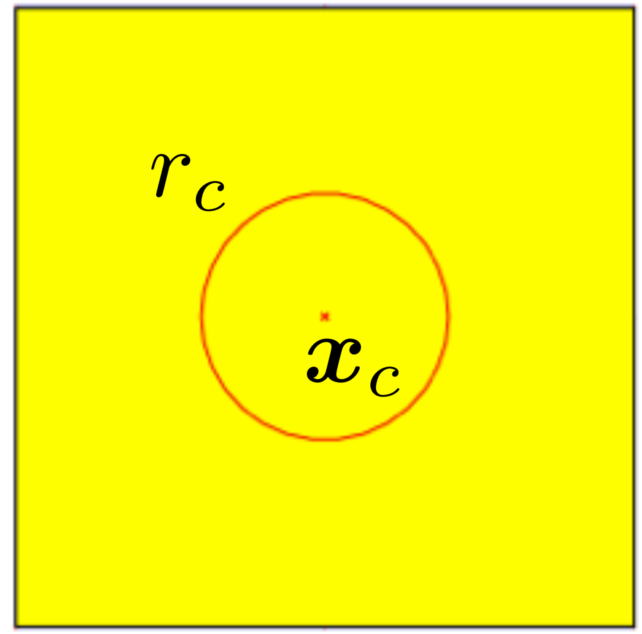
M. Duflot

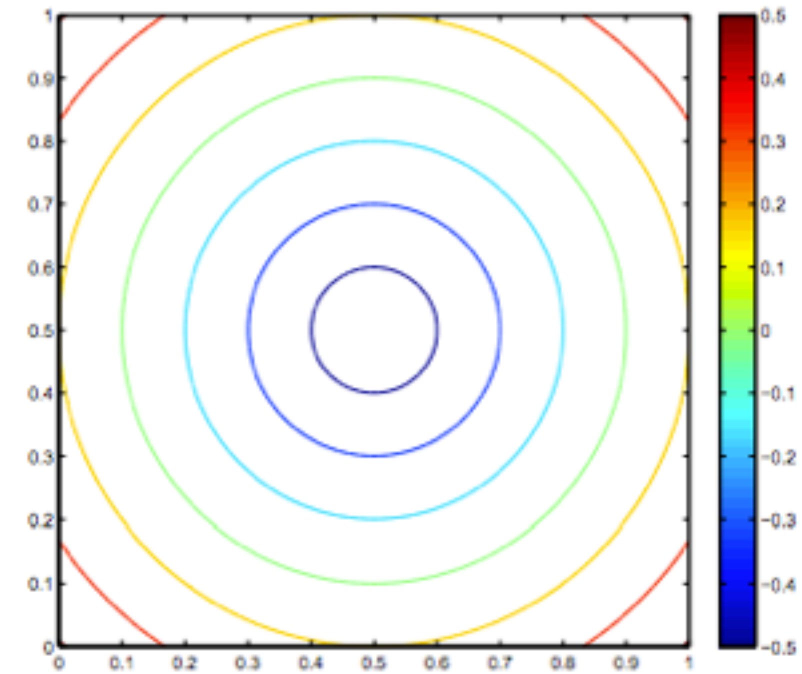


XFEM for material interfaces

Sukumar et al. 2002







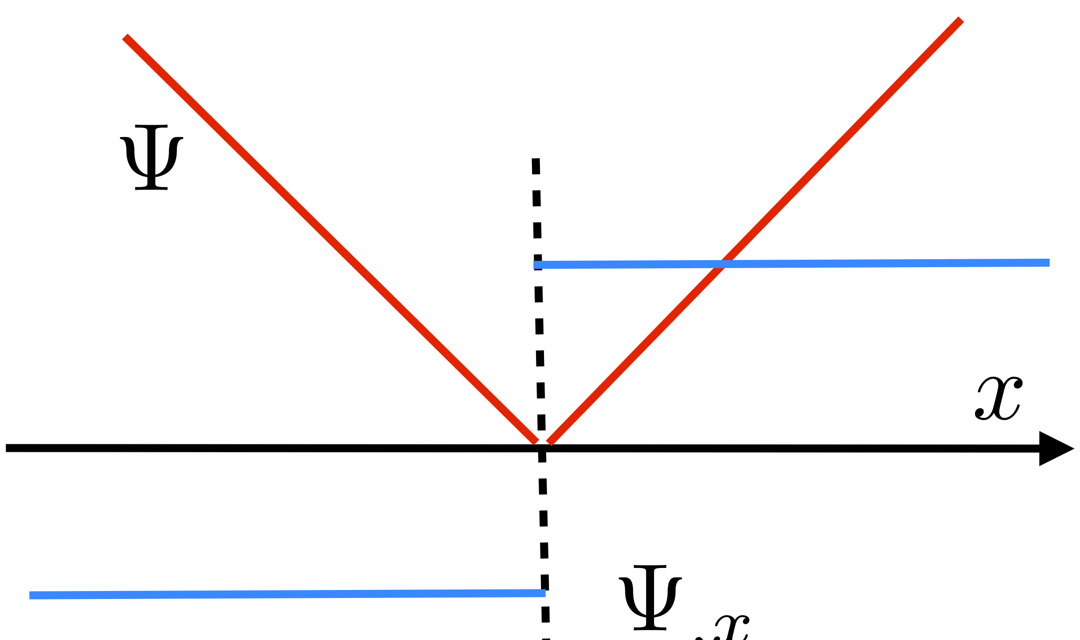
<u>across interface, strain field is discontinuous</u>

level set representation

abs-enrichment function $\psi = |\phi(x)|$

signed distance function

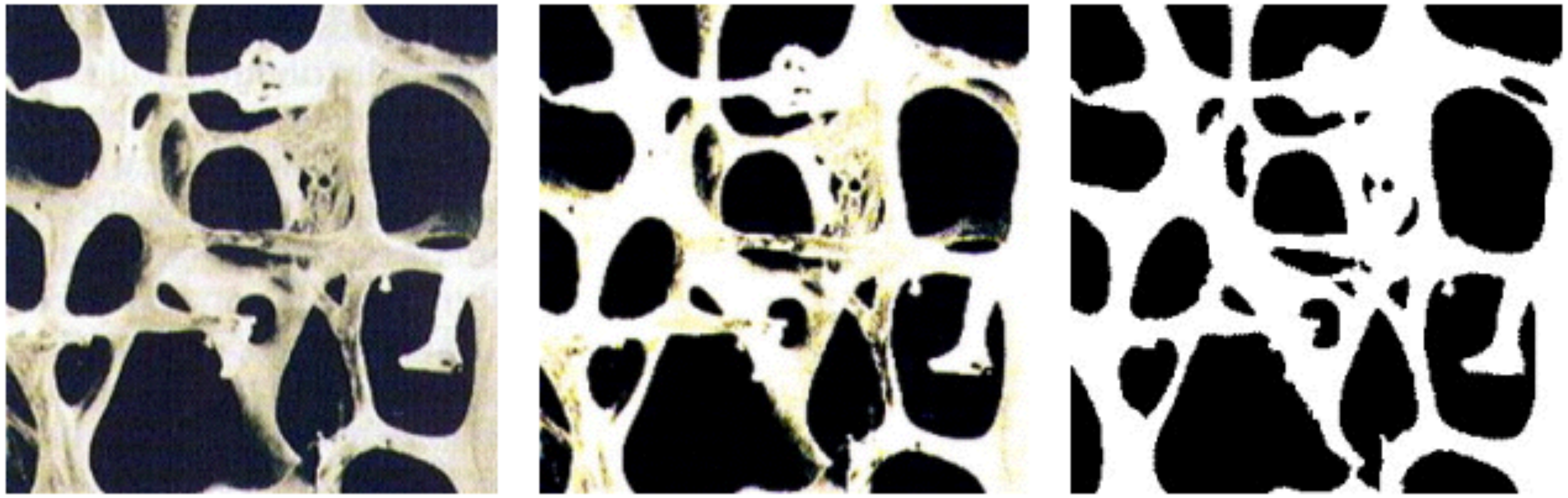
$$\phi = ||\mathbf{x} - \mathbf{x}_c|| - r_c$$

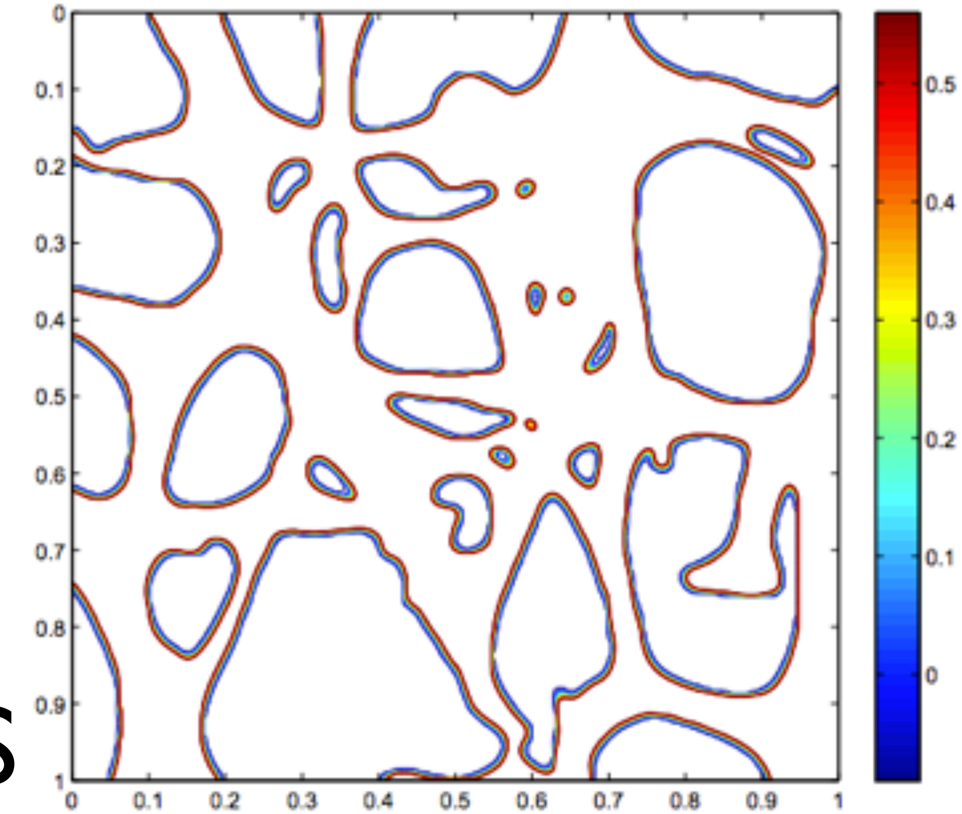


$$\phi(\mathbf{x}) = N_I(\mathbf{x})\phi_I$$

$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \mathcal{S}} N_I(\mathbf{x})\mathbf{u}_I + \sum_{J \in \mathcal{S}^c} N_J(\mathbf{x})\Psi(\mathbf{x})\mathbf{a}_J$$

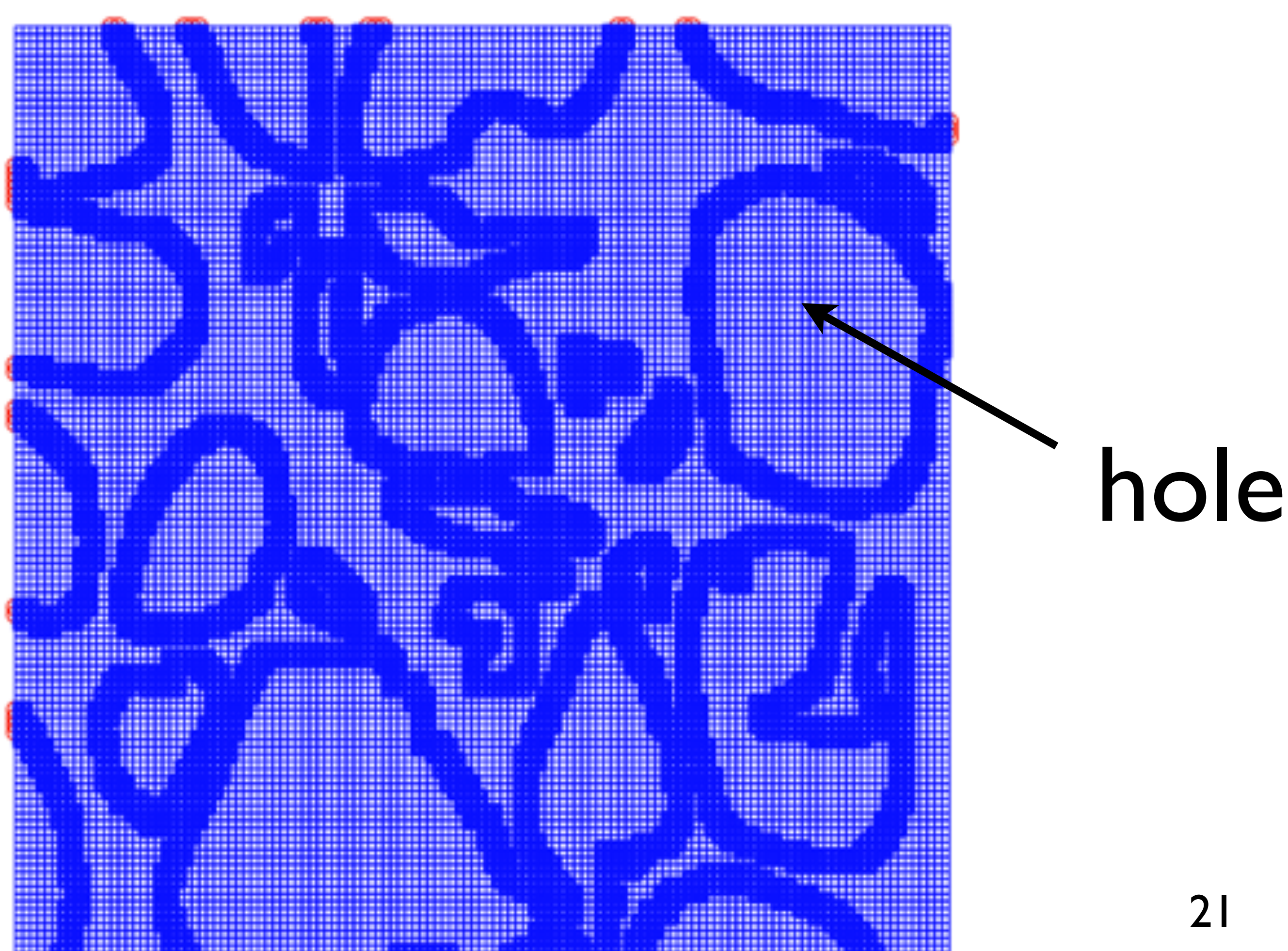
$\mathcal{S}^c \quad \phi_{\min}\phi_{\max} < 0$

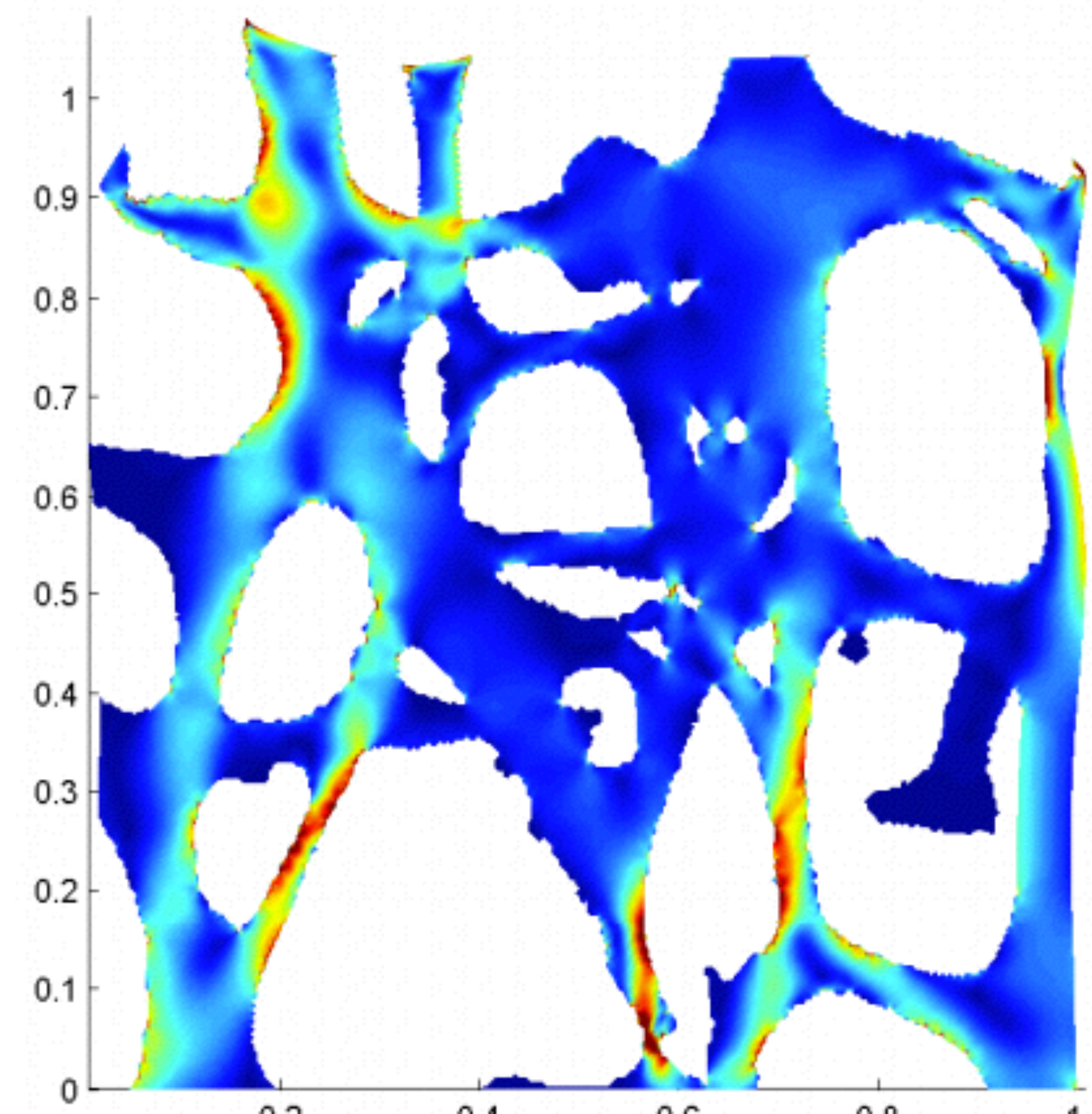




trabecular bone, PhD thesis, Tran, NUS

holes=extremely soft inclusions

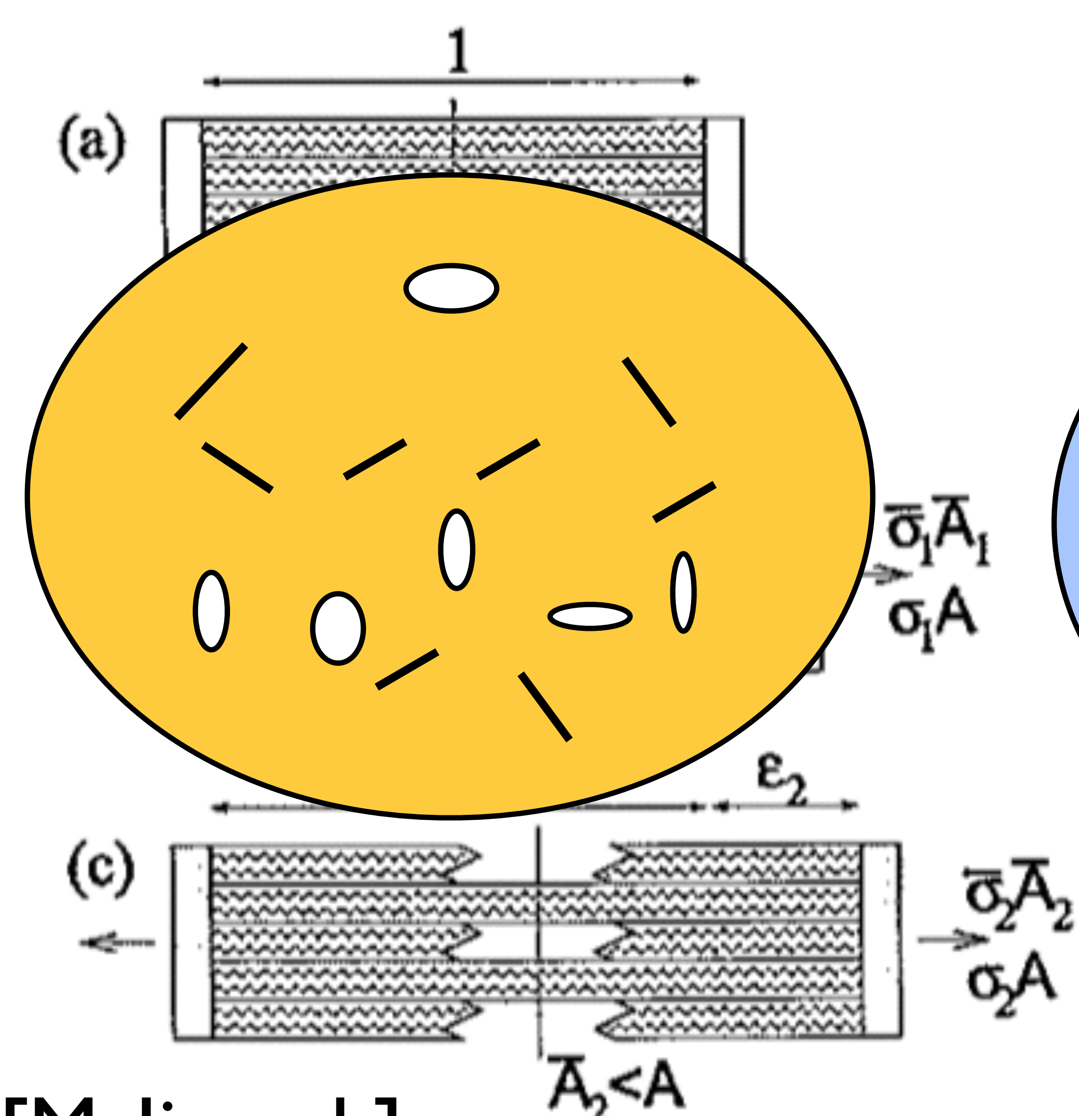




Continuum damage mechanics

Kachanov, 1958, Rabotnov 1969, Hult 1979

CDM is a constitutive theory that describes the progressive loss of material integrity due to the initiation, coalescence and propagation of microcracks, microvoids etc. These changes in the microstructure lead to the degradation of the material stiffness at the macroscale.



[M. Jirasek]

σ nominal stress A

$\bar{\sigma}$ …tress $\bar{A}$

$0 \leq \omega \leq 1$

$$\sigma = (1 - \omega) E \varepsilon$$

damage variable

$)\bar{\sigma},$ $\omega = 1 - \frac{\bar{A}}{A}$

damage variable

$\bar{\sigma} = E\varepsilon$

$$\sigma = (1 - \omega) E \varepsilon$$

Local damage model

<u>Isotropic</u> damage model

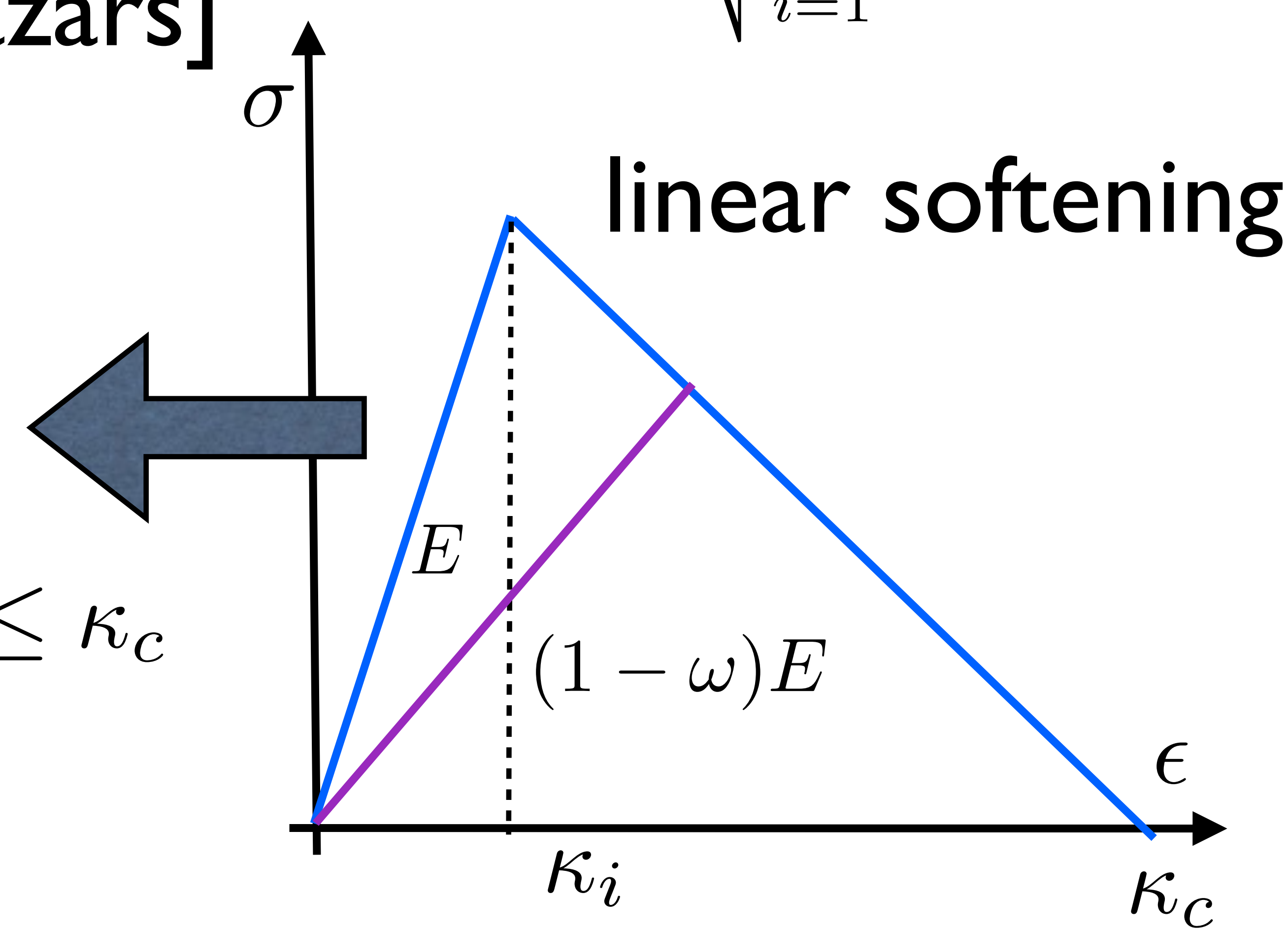
C : elasticity tensor

ϵ_{eq} : equivalent strain [-]

$$\boldsymbol{\sigma} = (1-\omega)\mathbf{C}\boldsymbol{\epsilon}$$
$$\omega = f(\epsilon_{\text{eq}})$$
$$\epsilon_{\text{eq}} = g(\boldsymbol{\epsilon})$$

Tensile failure [Mazars]

$$\epsilon_{\text{eq}} = \sqrt{\sum_{i=1}^{3} \langle \epsilon_i \rangle^2}$$



Damage evolution law

$$\omega = \begin{cases} 0 & \text{if } \kappa < \kappa_i \\ 1 - \frac{\kappa_i}{\kappa}\frac{\kappa_c - \kappa}{\kappa_c - \kappa_i} & \text{if } \kappa_i \leq \kappa \leq \kappa_c \\ 1 & \text{if } \kappa > \kappa_c \end{cases}$$

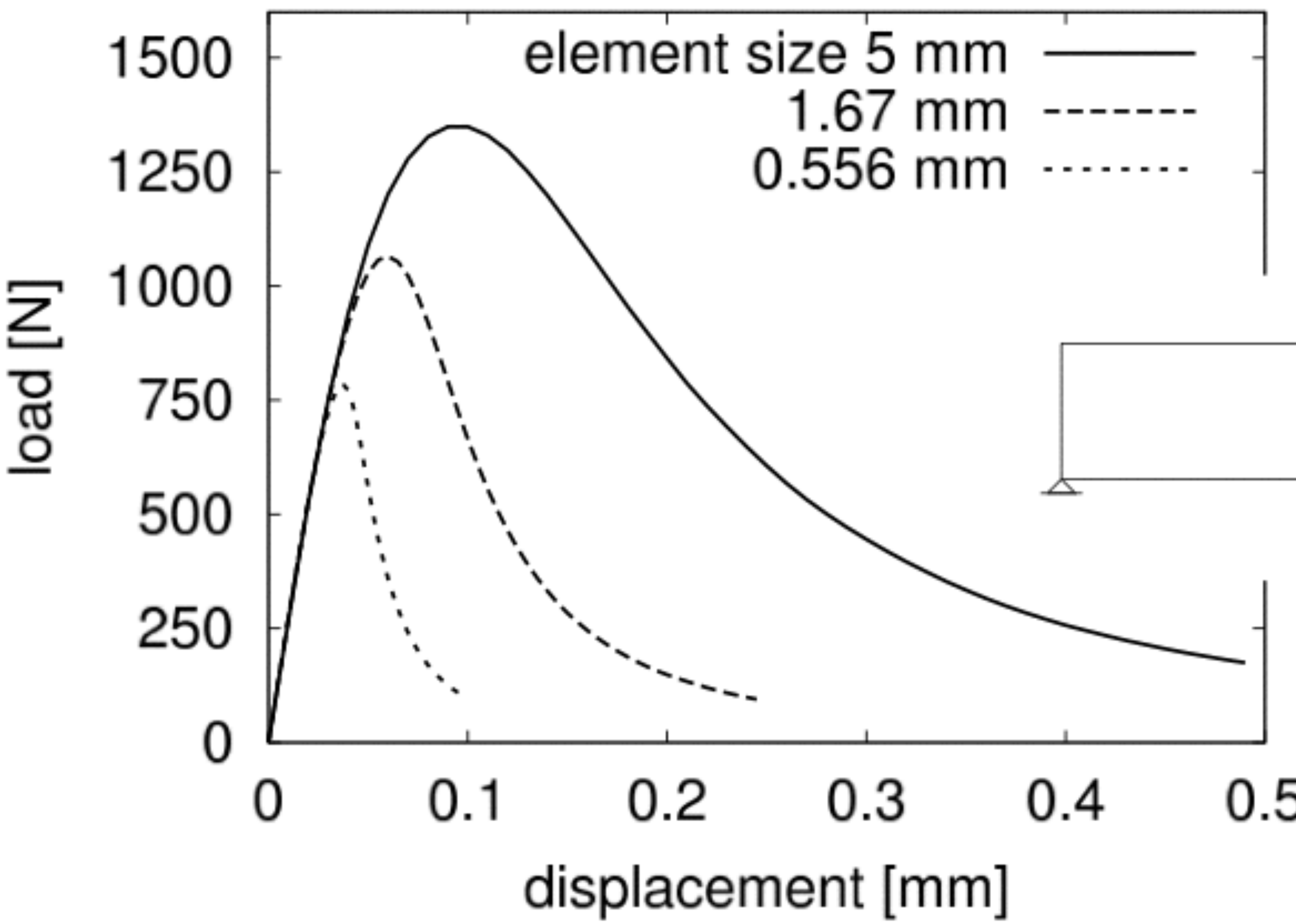
Irreversibility of failure

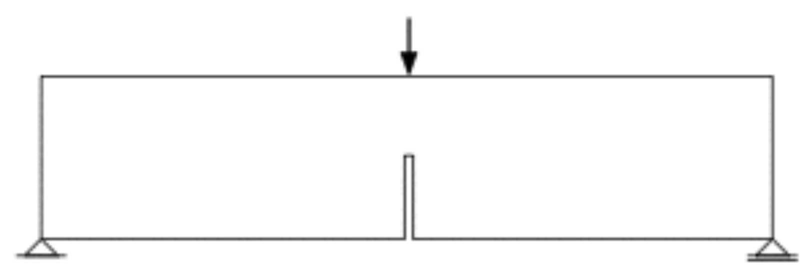
$$\kappa = \max \epsilon_{\text{eq}}$$

stress update: explicit and simple

Local damage model

In the early 1980s it was found that FE solutions of softening damage do not converge upon mesh refinement, Z. Bazant, 1984.





Isotropic damage model

$$\boldsymbol{\sigma} = (1-\omega)\mathbf{C}\boldsymbol{\epsilon}$$

$$\omega = f(\epsilon_{\mathrm{eq}})$$

$$\epsilon_{\mathrm{eq}} = g(\boldsymbol{\epsilon})$$

No energy dissipation !!!

Softening plastic models: also suffer from mesh sensitivity.

Nonlocal damage model

Cabot and Bazant, 1987

$$\boldsymbol{\sigma} = (1-\omega)\mathbf{C}\boldsymbol{\epsilon}$$

$$\omega = f(\bar{\epsilon}_{\text{eq}}) \qquad 0 \leq \omega \leq 1$$

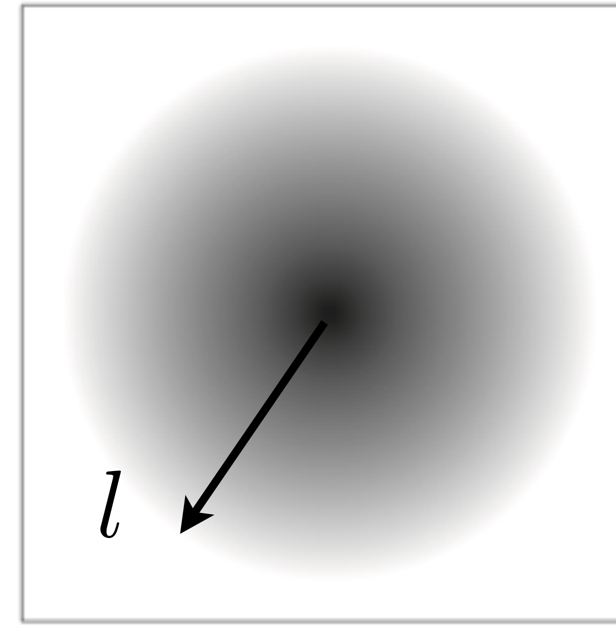
$$\bar{\epsilon}_{\text{eq}}(\mathbf{x}) = \int_{\Omega} \alpha(\mathbf{x}-\xi)\boldsymbol{\epsilon}_{\text{eq}}(\xi)d\xi$$

nonlocal eqv. strain

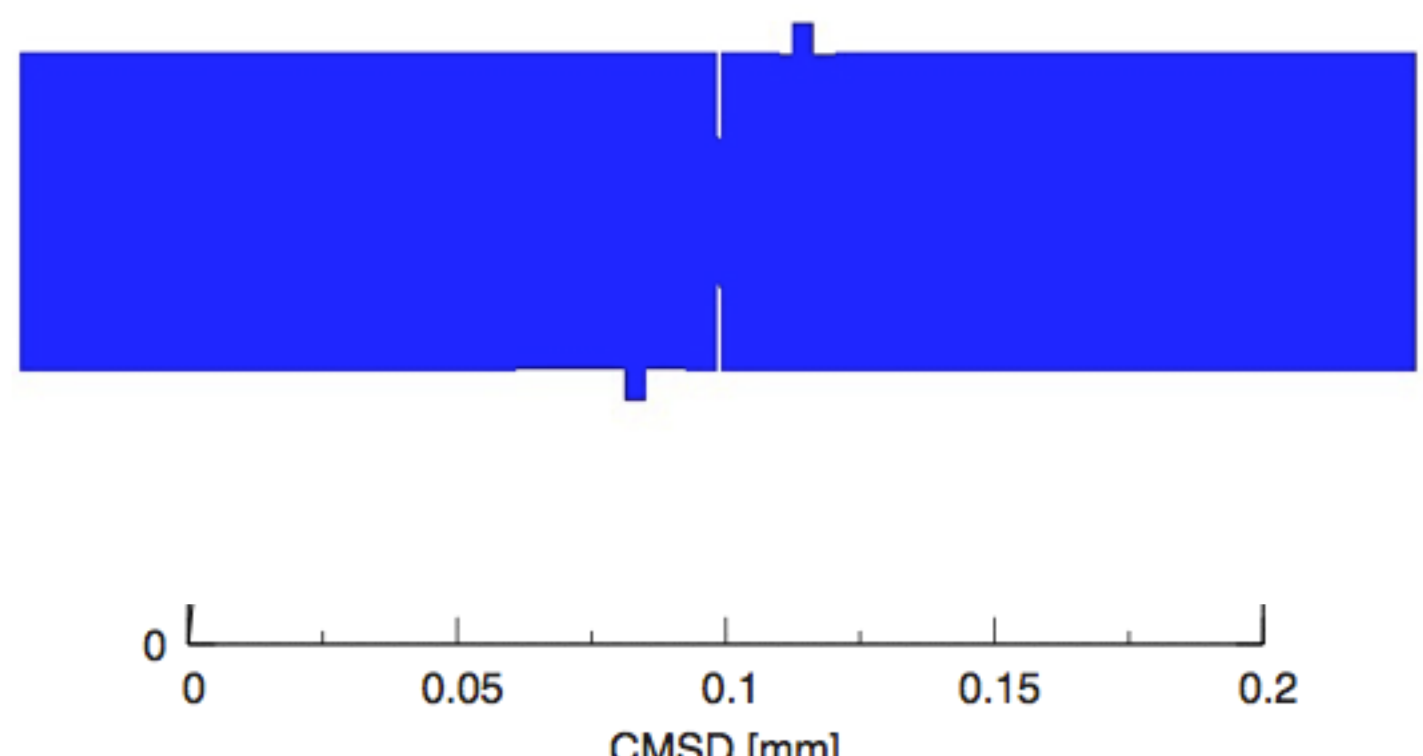
$$\alpha(r) = \exp\left(-\frac{r^2}{2l^2}\right)$$

?

l is the length scale



SEN beam



Gradient damage model

$$\boldsymbol{\sigma} = (1-\omega)\mathbf{C}\boldsymbol{\epsilon}$$

$$\omega = f(\bar{\epsilon}_{\text{eq}}) \qquad 0 \le \omega \le 1$$

$$\bar{\epsilon}_{\text{eq}}(\mathbf{x}) = \int_{\Omega} \alpha(\mathbf{x}-\xi)\boldsymbol{\epsilon}_{\text{eq}}(\xi)d\xi$$

$$\alpha(r) = \exp\left(-\frac{r^2}{2l^2}\right)$$

secant matrix

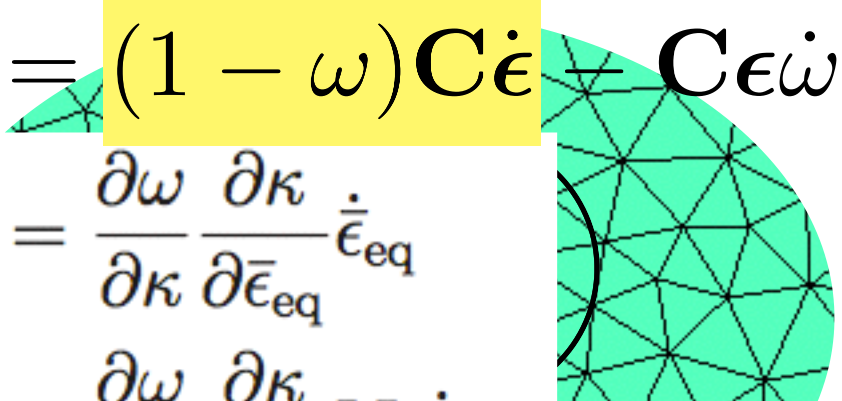
$$\boldsymbol{\sigma} = (1-\omega)\mathbf{C}\boldsymbol{\epsilon}$$

$$\omega = f(\bar{\epsilon}_{\text{eq}})$$

$$\bar{\epsilon}_{\text{eq}} - c\nabla^2\bar{\epsilon}_{\text{eq}} = \epsilon_{\text{eq}}$$

$$c = \frac{l^2}{2}$$

$$\dot{\boldsymbol{\sigma}} = (1-\omega)\mathbf{C}\dot{\boldsymbol{\epsilon}} - \mathbf{C}\boldsymbol{\epsilon}\dot{\omega}$$



Microplane Damage Models (Z. Bazant)

Implicit GD model

Peerlings et al., 1996

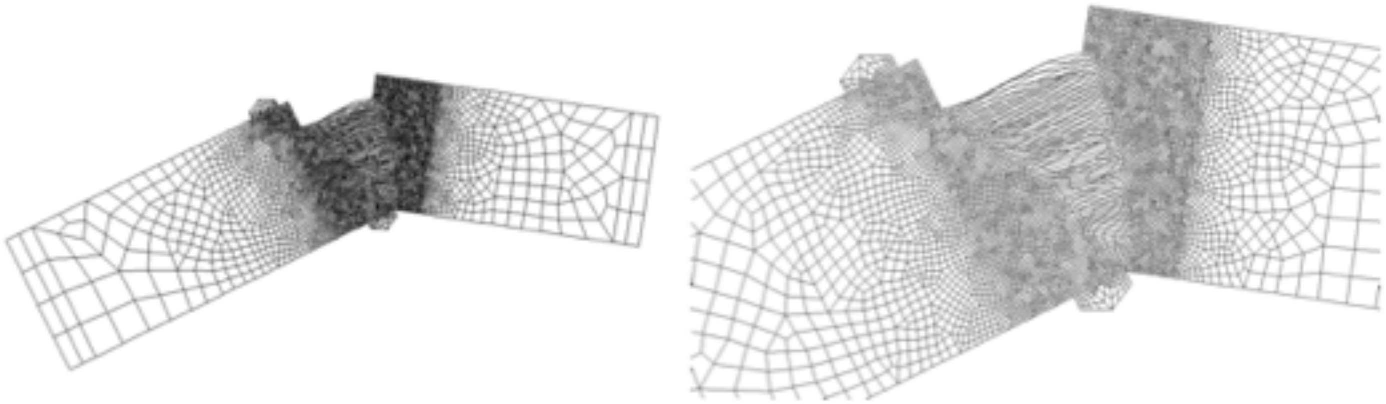
$$\dot{\omega} = \frac{\partial\omega}{\partial\kappa}\frac{\partial\kappa}{\partial\bar{\epsilon}_{\text{eq}}}\dot{\bar{\epsilon}}_{\text{eq}} = \frac{\partial\omega}{\partial\kappa}\frac{\partial\kappa}{\partial\bar{\epsilon}_{\text{eq}}}\mathbf{N}_{\epsilon}\dot{\bar{\boldsymbol{\epsilon}}}_{\text{eq}}$$

$$-\begin{bmatrix} \mathbf{K}_{\epsilon u} & \mathbf{K}_{\epsilon\epsilon} \end{bmatrix} \begin{Bmatrix} \delta\mathbf{d}^{(i)} \\ \delta\bar{\boldsymbol{\epsilon}}_{\text{eq}}^{(i)} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_{\text{int,u}} \\ \mathbf{f}_{\text{int},\epsilon} \end{Bmatrix}^{(i-1)} - \begin{Bmatrix} \mathbf{f}_{\text{ext,u}} \\ \mathbf{0} \end{Bmatrix}^{(i-1)}$$

displacements

uivalent strain

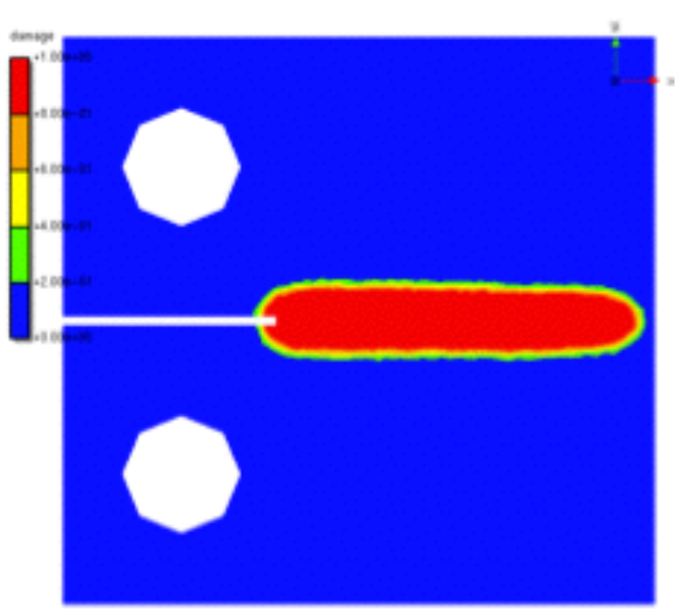
Continuous vs. discontinuous description



(a) (b)

+ easy to implement (2D/3D)
+ one single constitutive law
+ <u>standard elements</u>
- incorrect final stage of failure
- evolving length scale

- hard to implement (3D)
- two separate constitutive laws
- <u>enriched elements</u>
+ correct final stage of failure

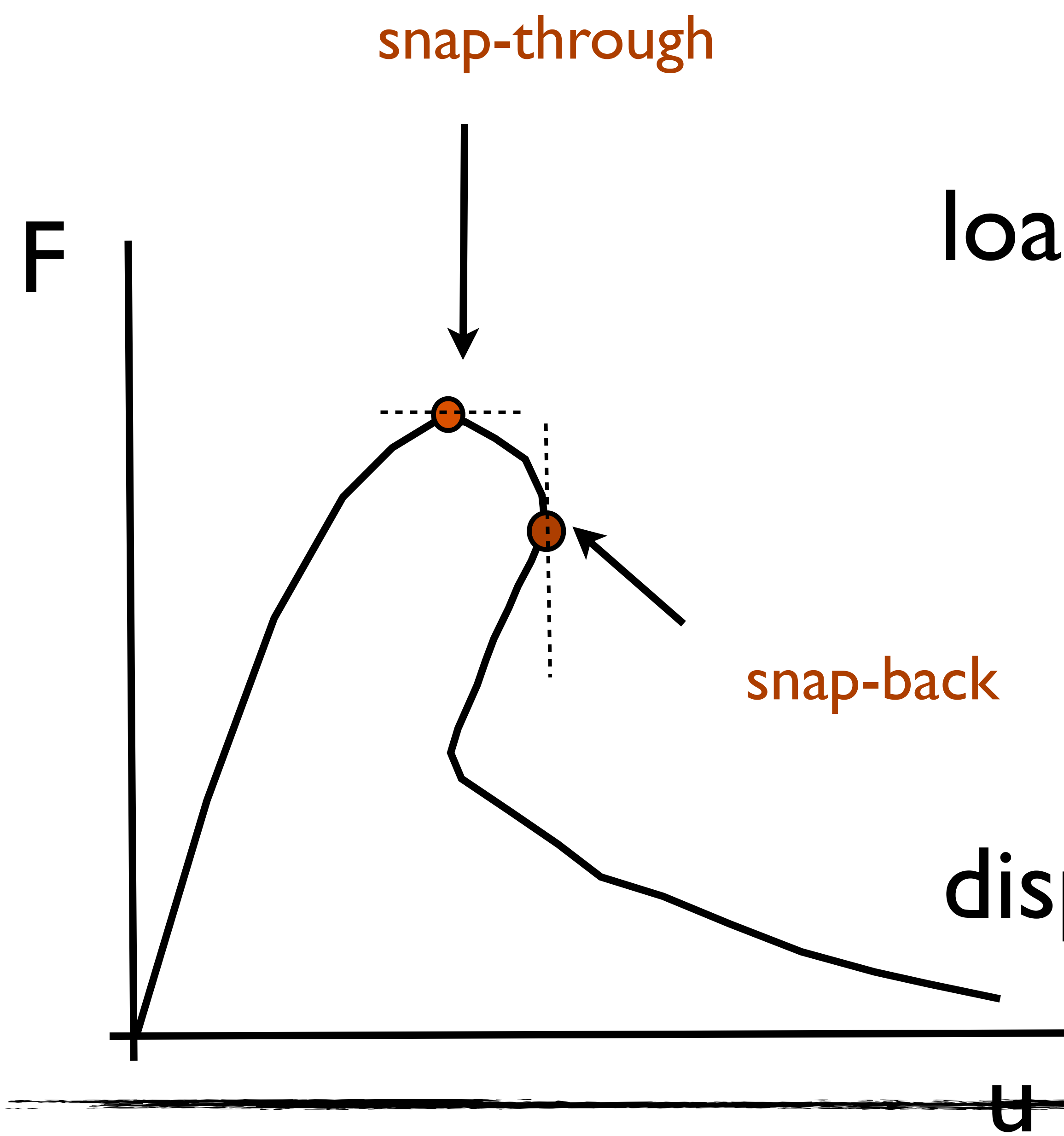


bests of both worlds: <u>combined continuous-discontinuous approaches</u>

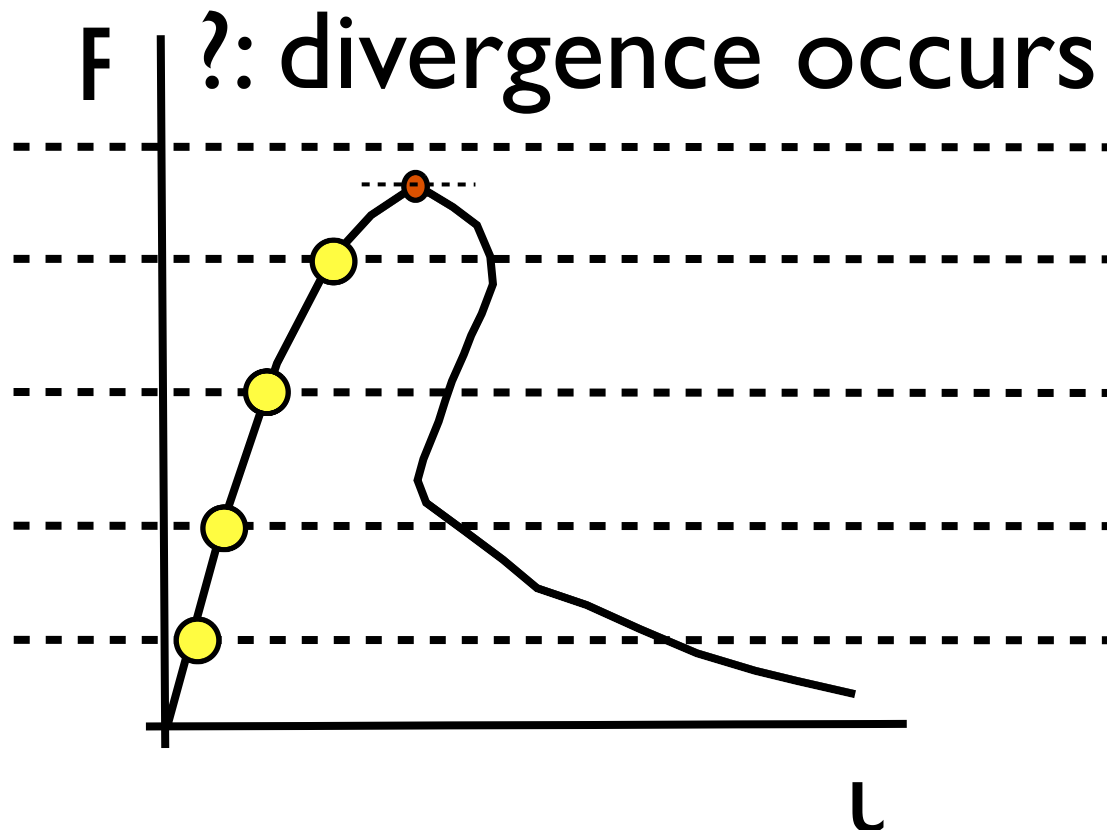
(Dr. Nguyen Dinh Giang, Univ. Sydney)

Solution strategies

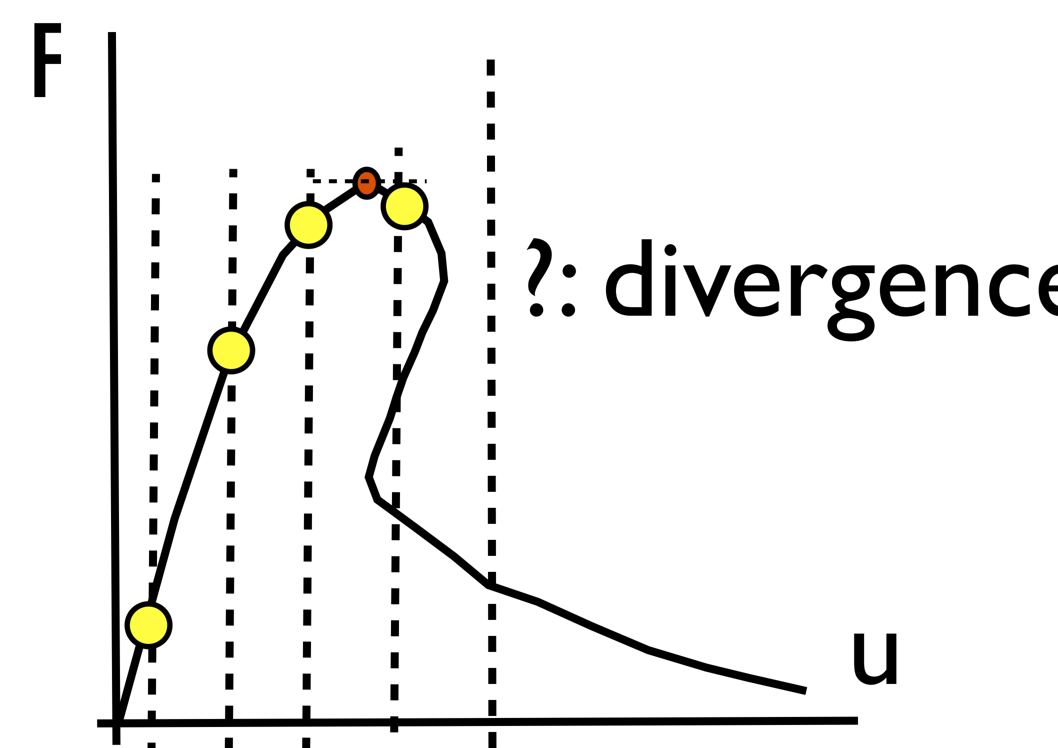
For a **quasi-static analysis** of softening solids, one encounters cases...



load control



disp control



Incremental-iterative procedure

Path-following methods

Riks 1972

$$\left[\begin{array}{c} \mathbf{f}^{\text{int}}(\mathbf{u}) - \lambda\mathbf{g} \\ \phi(\mathbf{u}, \lambda) \end{array}\right] = 0$$

$\mathbf{f}^{\text{ext}} = \lambda\mathbf{g}$ ← reference load vector

λ load factor

Newton-Raphson $\phi(\mathbf{u}, \lambda)$ arc-length/constraint function

$$\left[\begin{array}{c} \mathbf{f}^{\text{int}}(\mathbf{u}_{(k)}) - \lambda_{(k)}\mathbf{g} \\ \phi(\mathbf{u}_{(k)}, \lambda_{(k)}) \end{array}\right] + \left[\begin{array}{cc} \mathbf{K} & -\mathbf{g} \\ \mathbf{v}^{\mathrm{T}} & w \end{array}\right]^{(k)} \cdot \left[\begin{array}{c} \Delta\mathbf{u} \\ \Delta\lambda \end{array}\right] = 0$$

where

$$\mathbf{K} = \frac{\partial \mathbf{f}^{\text{int}}}{\partial \mathbf{u}}, \quad \mathbf{v} = \frac{\partial \phi}{\partial \mathbf{u}}, \quad w = \frac{\partial \phi}{\partial \lambda}$$

$$\longrightarrow \quad \left[\begin{array}{c} \Delta\mathbf{u} \\ \Delta\lambda \end{array}\right] = \left[\begin{array}{c} \mathbf{u}_I \\ 0 \end{array}\right] - \frac{\mathbf{v}^{\mathrm{T}}\mathbf{u}_I + \phi}{\mathbf{v}^{\mathrm{T}}\mathbf{u}_{II} + w}\left[\begin{array}{c} \mathbf{u}_{II} \\ 1 \end{array}\right]$$

$$\mathbf{u}_I = \mathbf{K}^{-1}\mathbf{r}, \quad \mathbf{u}_{II} = \mathbf{K}^{-1}\mathbf{g}$$

correction $\left[\begin{array}{c} \mathbf{u} \\ \lambda \end{array}\right]^{(k+1)} = \left[\begin{array}{c} \mathbf{u} \\ \lambda \end{array}\right]^{(k)} + \left[\begin{array}{c} \Delta\mathbf{u} \\ \Delta\lambda \end{array}\right]$

Energy control

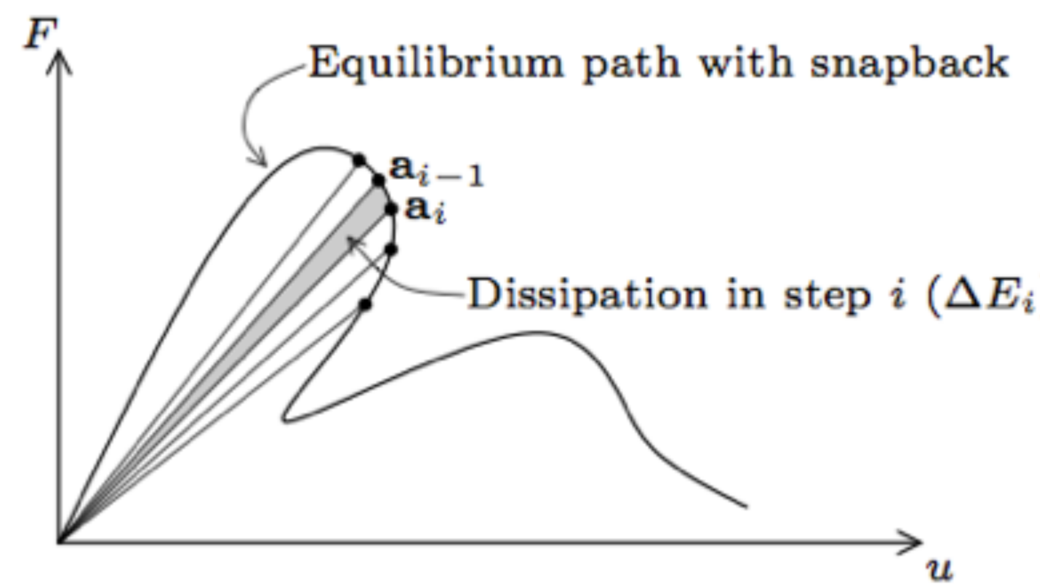
$$\boldsymbol{\epsilon} = \mathbf{Ba} \qquad \mathbf{f}^{\text{int}} = \int_\Omega \mathbf{B}^{\text{T}}\boldsymbol{\sigma}$$

Gutierrez 2004

equilibrium

$$V = \frac{1}{2}\int_\Omega \boldsymbol{\epsilon}^{\text{T}}\boldsymbol{\sigma} = \frac{1}{2}\int_\Omega \mathbf{a}^{\text{T}}\mathbf{B}^{\text{T}}\boldsymbol{\sigma} = \frac{1}{2}\mathbf{a}^{\text{T}}\mathbf{f}^{\text{int}} = \frac{1}{2}\lambda\mathbf{a}^{\text{T}}\mathbf{g}$$

$$\dot{V} = \frac{1}{2}\lambda\dot{\mathbf{a}}^{\text{T}}\mathbf{g} + \frac{1}{2}\dot{\lambda}\mathbf{a}^{\text{T}}\mathbf{g}$$



Energy release rate $\quad \dot{V} - \lambda\dot{\mathbf{a}}^{\text{T}}\mathbf{g}$

$$G = \frac{1}{2}\lambda\dot{\mathbf{a}}^{\text{T}}\mathbf{g} - \frac{1}{2}\dot{\lambda}\mathbf{a}^{\text{T}}\mathbf{g}$$

$$\boxed{G > 0}$$

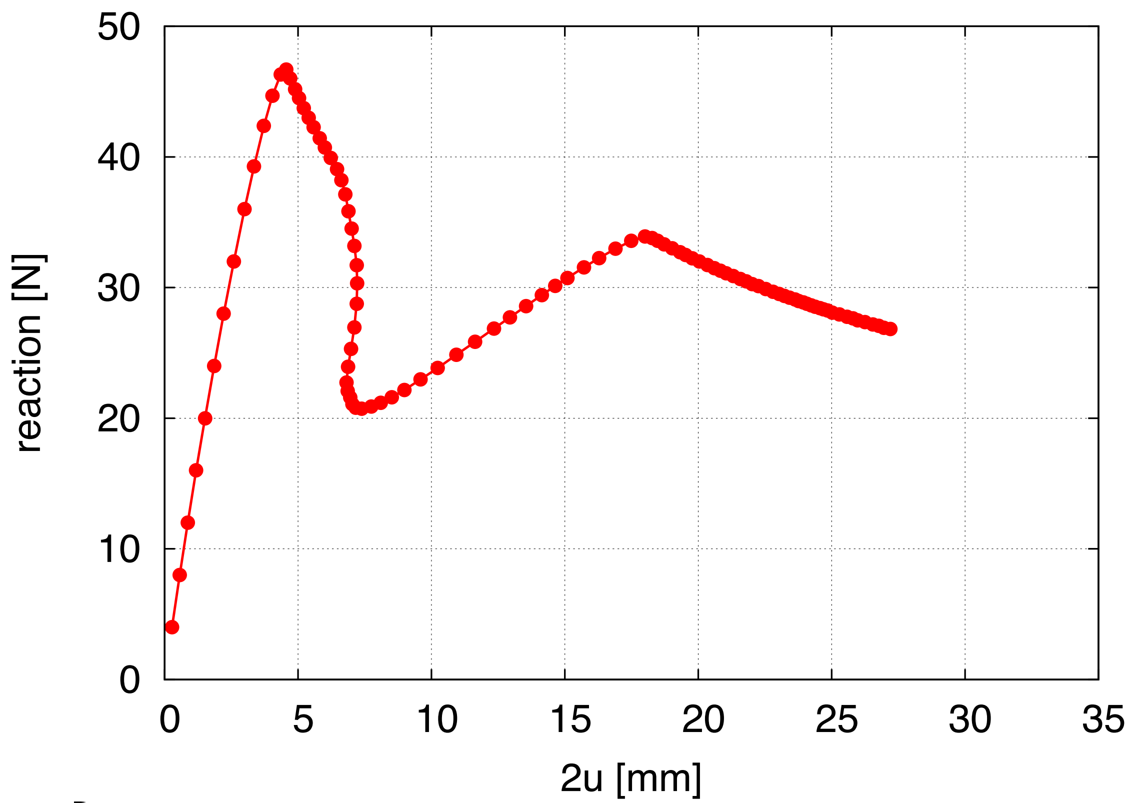
Arc-length function

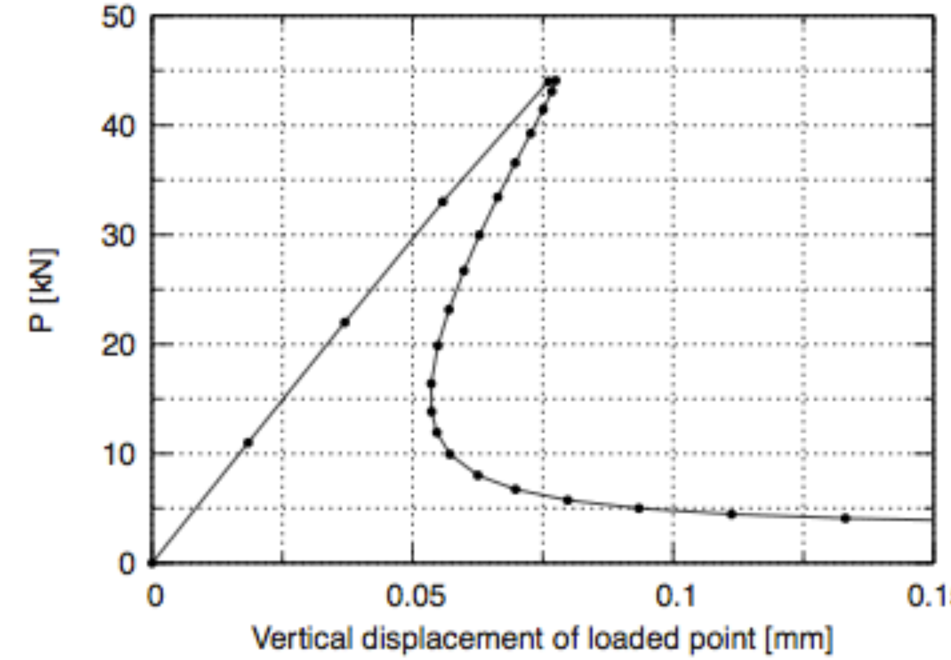
predefined amount of energy to be released [Nm]

$$\phi = \frac{1}{2}\left[\lambda^{(n)}(\mathbf{a}^{\text{T}}_{(n+1)} - \mathbf{a}^{\text{T}}_{(n)}) - \Delta\lambda^{(n)}\mathbf{a}^{\text{T}}_{(n)}\right]\mathbf{g} - \Delta\tau = 0$$

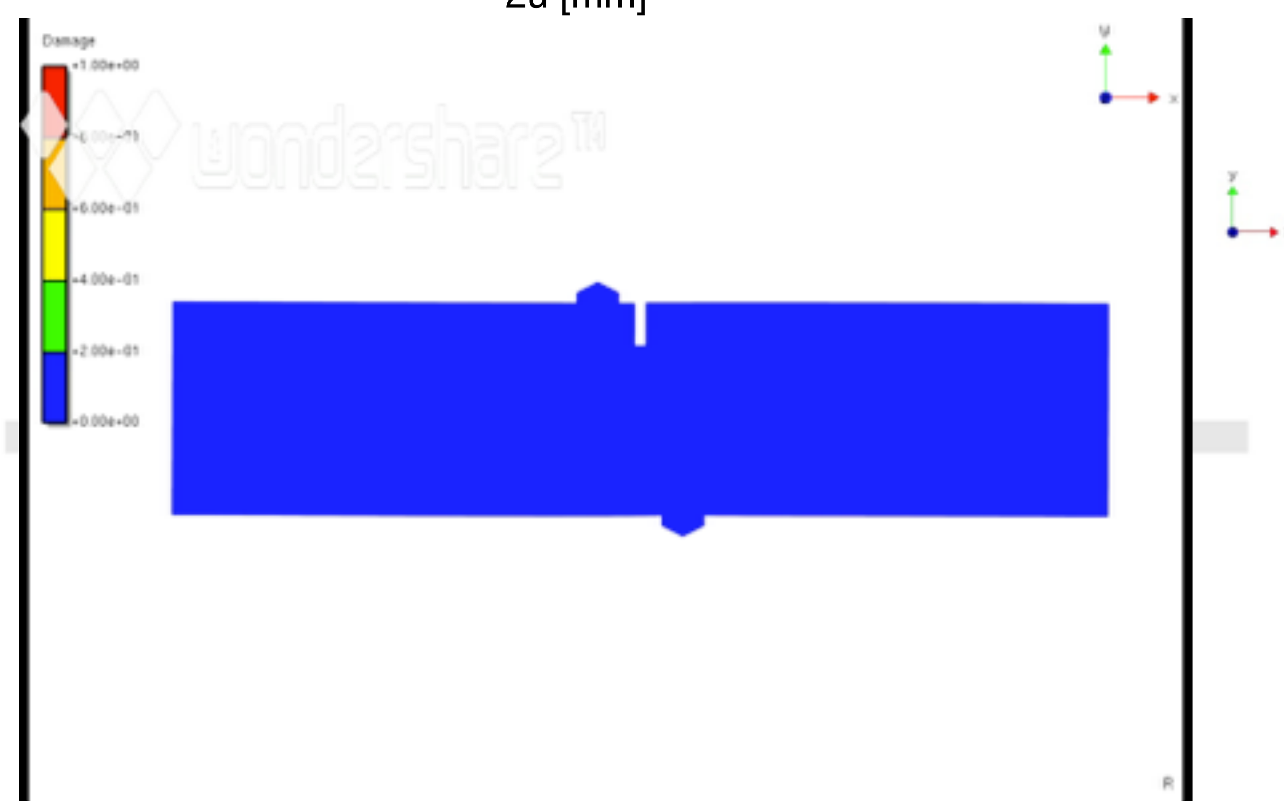
forward Euler

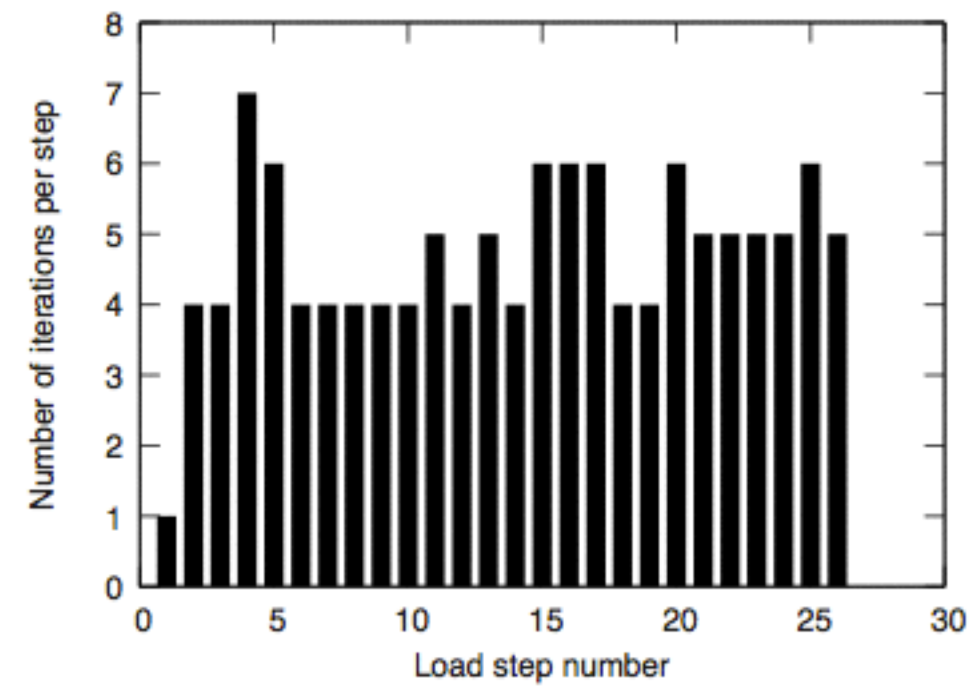
Energy based arc-length control





(a)

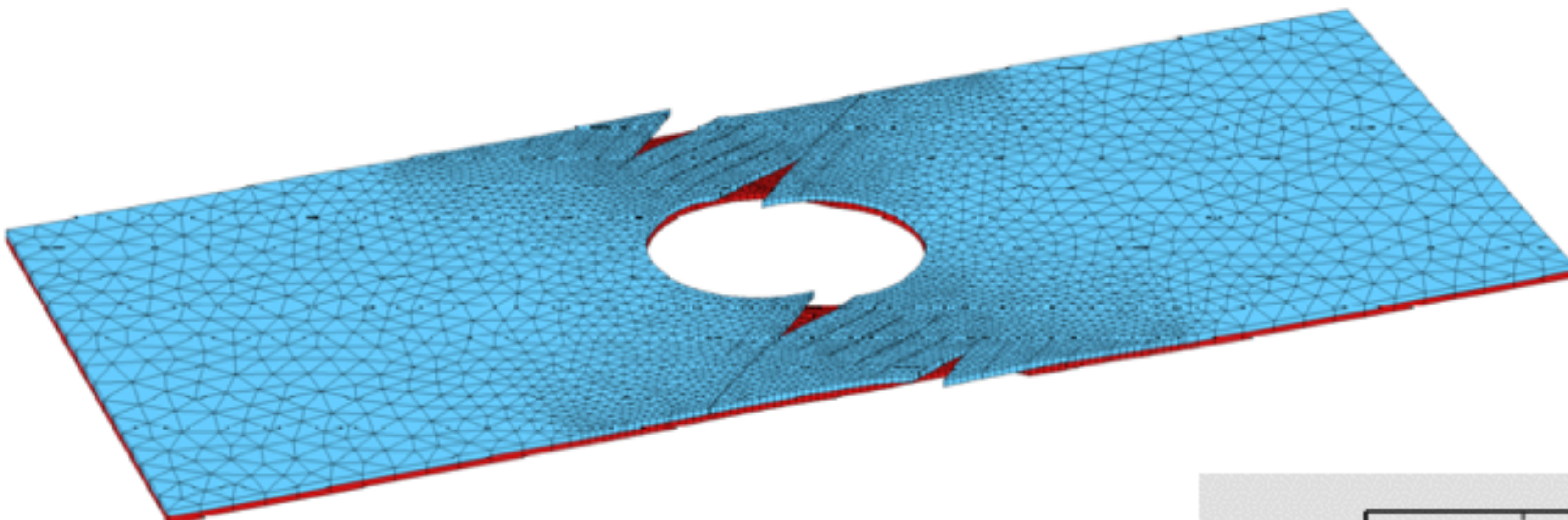


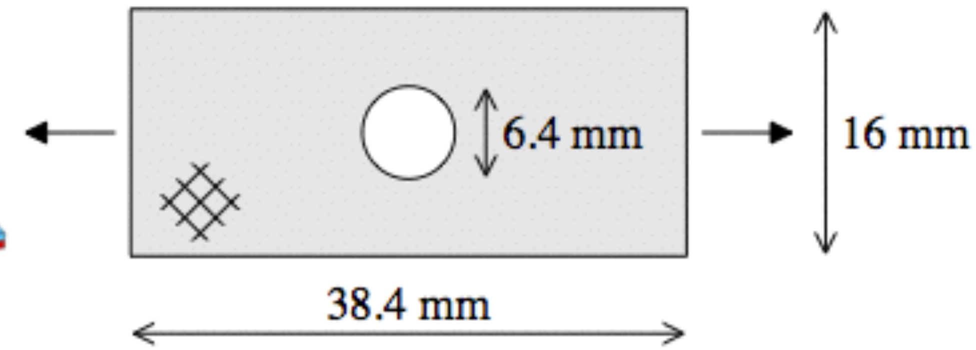


… and here we are

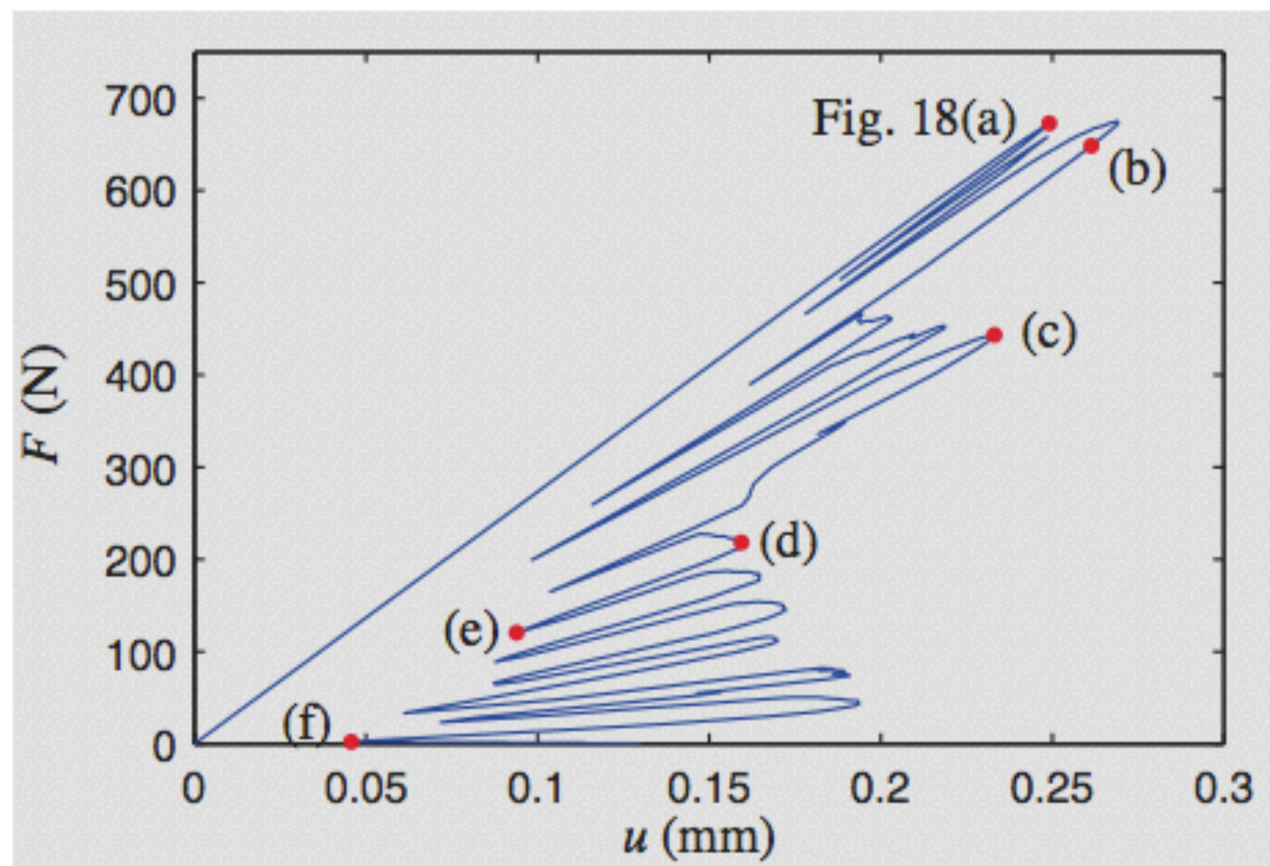
complex failure mechanism in composites

$[\pm 45^o]$





- matrix cracking
- delamination of plies

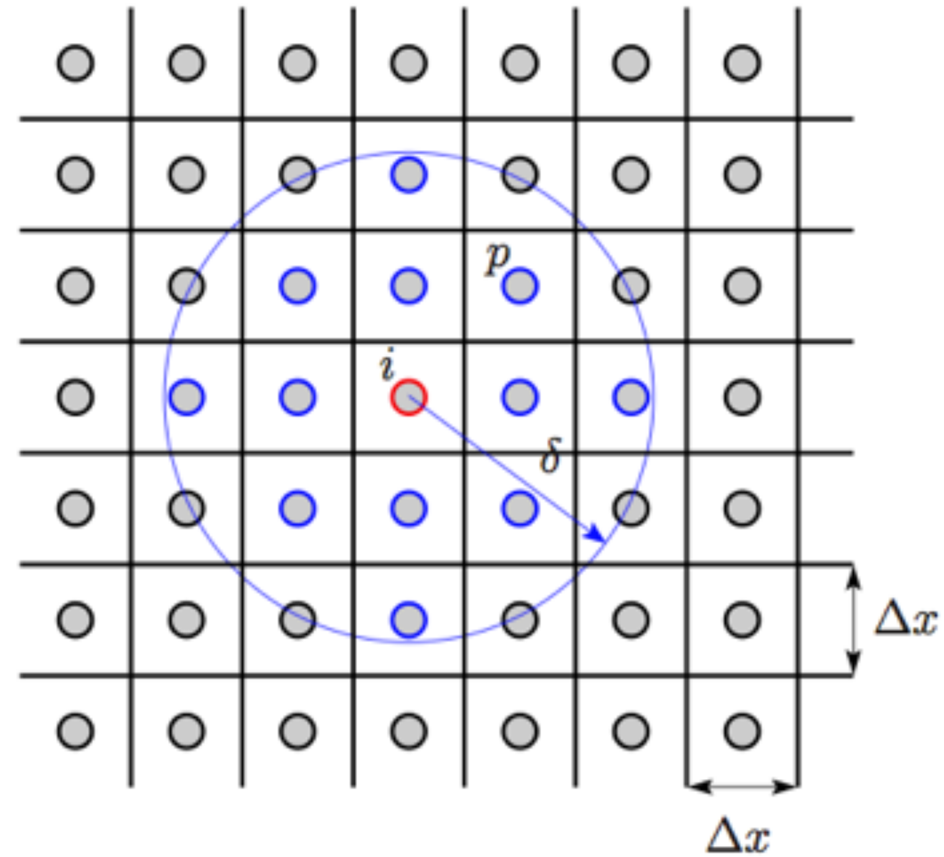


F.P. van der Mer
EFM, 2008

Peridynamics

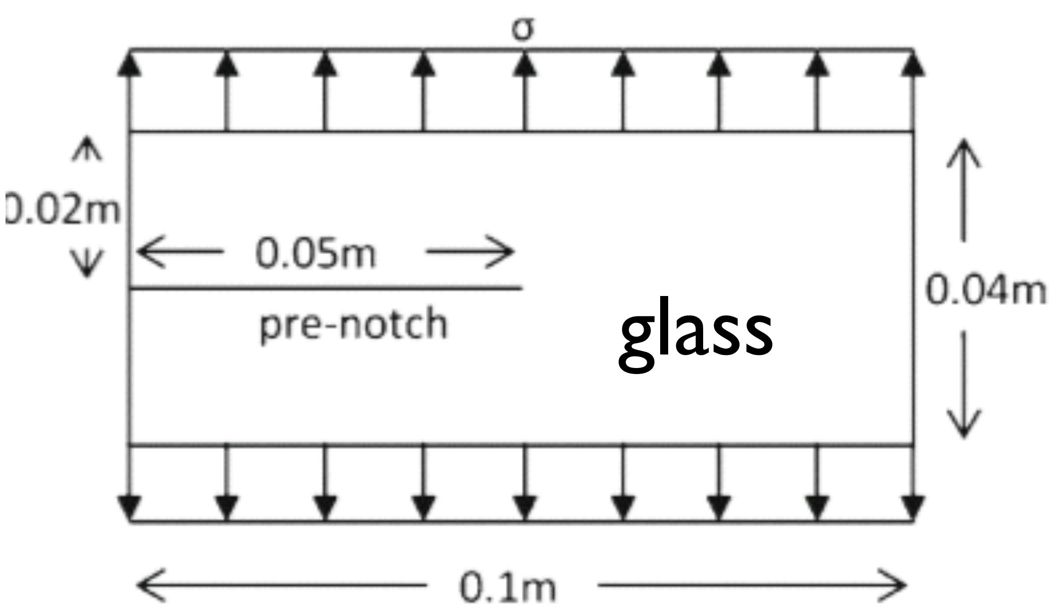
S. Silling 2000

$$\rho_i \ddot{\mathbf{u}}_i^n = \sum_{p \in \mathcal{F}_i} \mathbf{f}(\mathbf{u}_p^n - \mathbf{u}_i^n, \mathbf{x}_p - \mathbf{x}_i) V_p - \mathbf{b}_i^n \equiv \tilde{\mathbf{f}}_i^n$$



time integration: Verlet integration

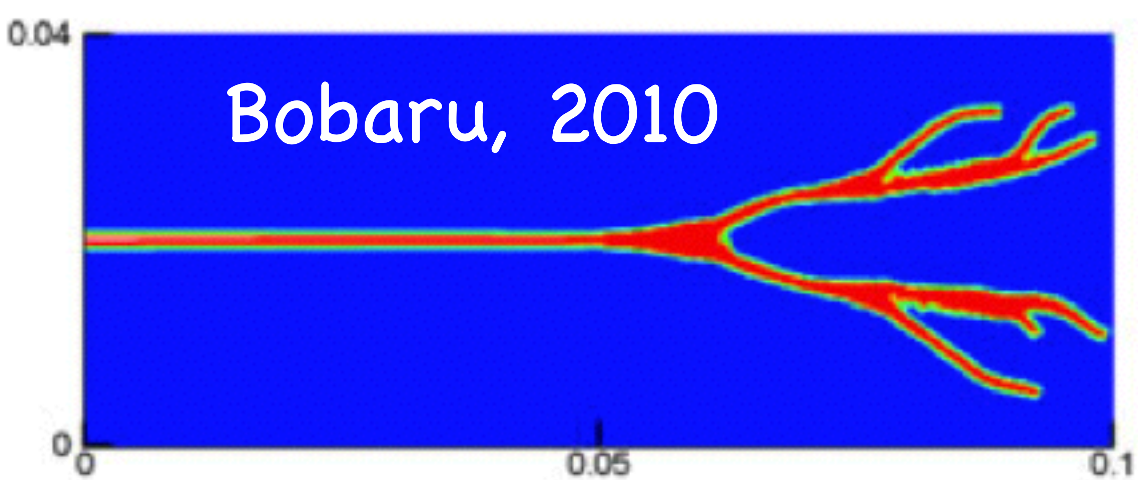
continuum version of MD (molecular dynamics)

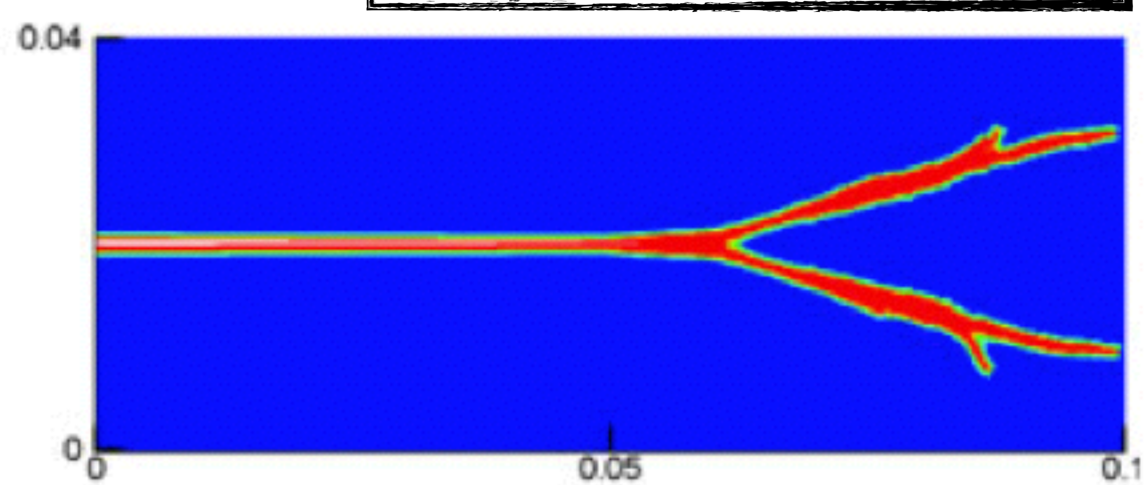


XFEM can do this as well but would require genius programmers (2D)

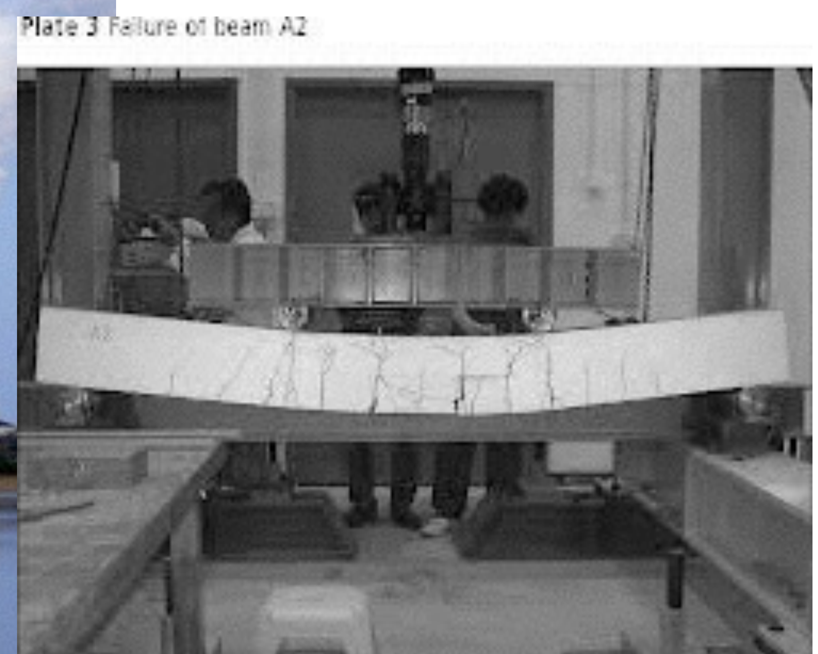
See phase field models for similar capacities

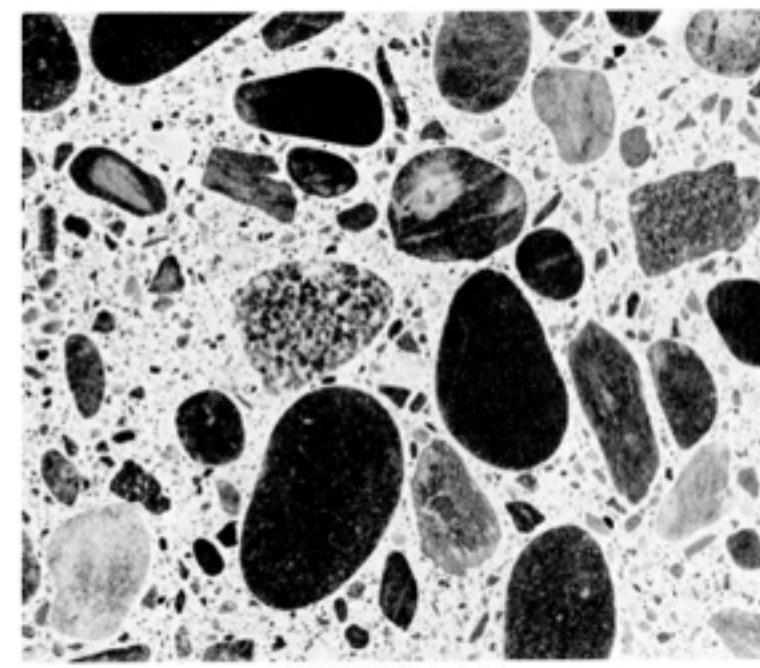
crack branching





Multiscale methods





multiple length scales

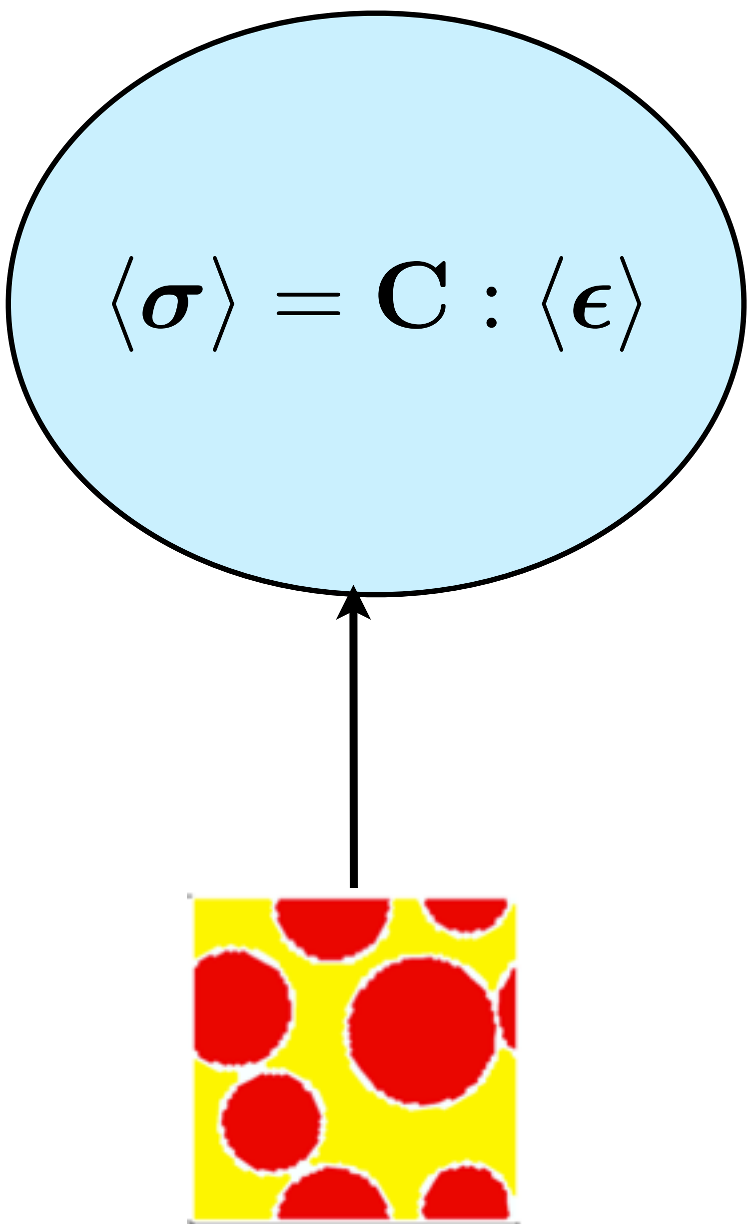
Multiscale models:

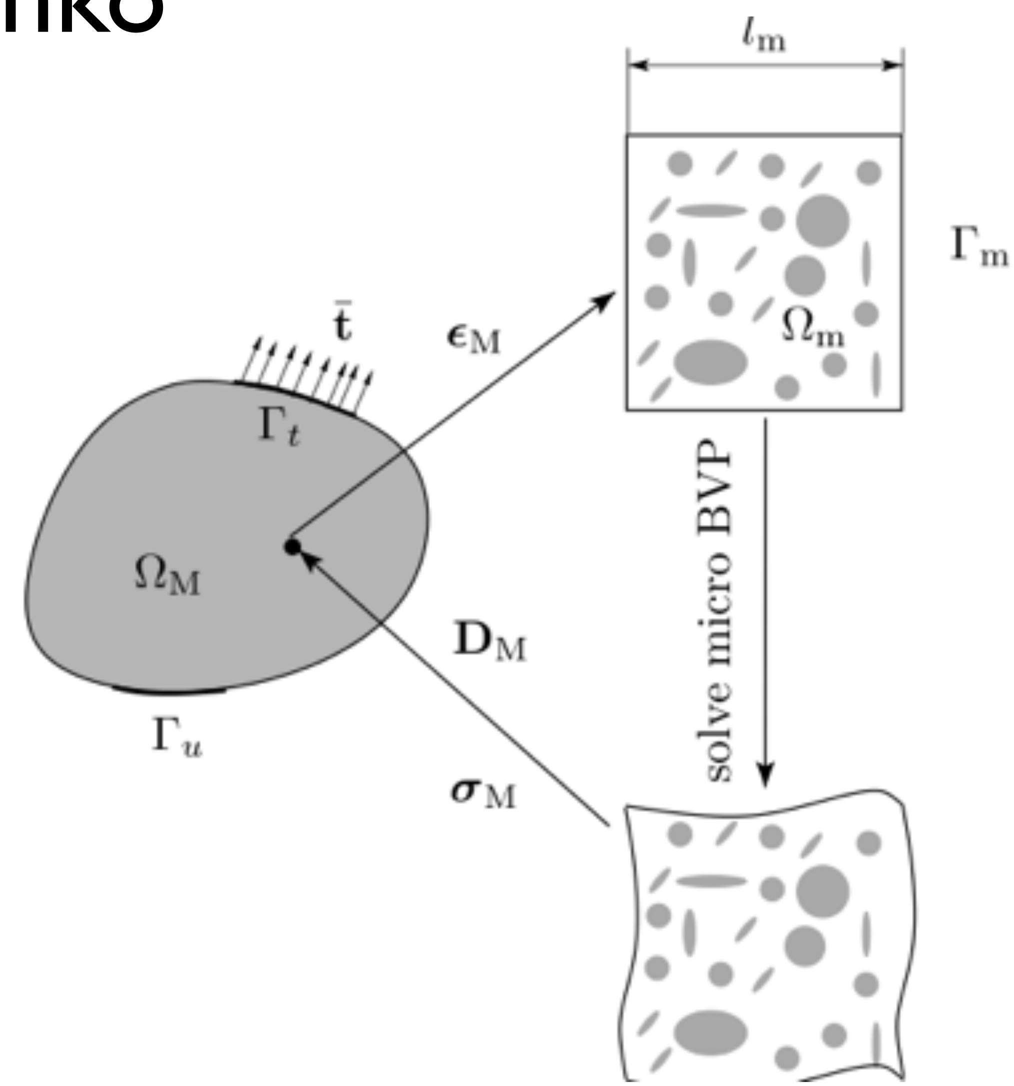
- better constitutive models
- design new materials

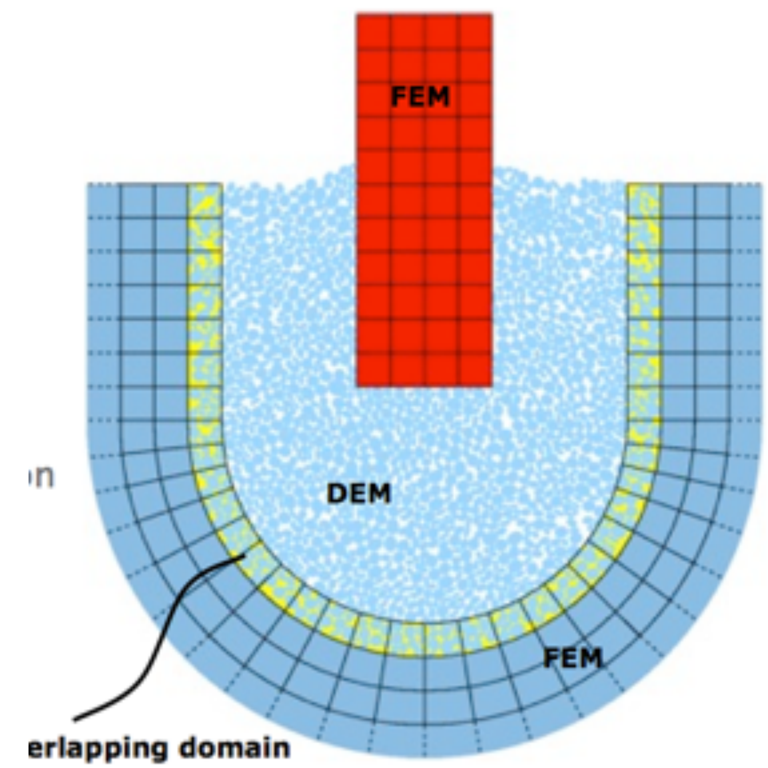
Classification

After Ted Belytschko

ARLEQUIN method







pile installation
Wriggers,2011

hierarchical methods

semi-concurrent

concurrent method

Arlequin method

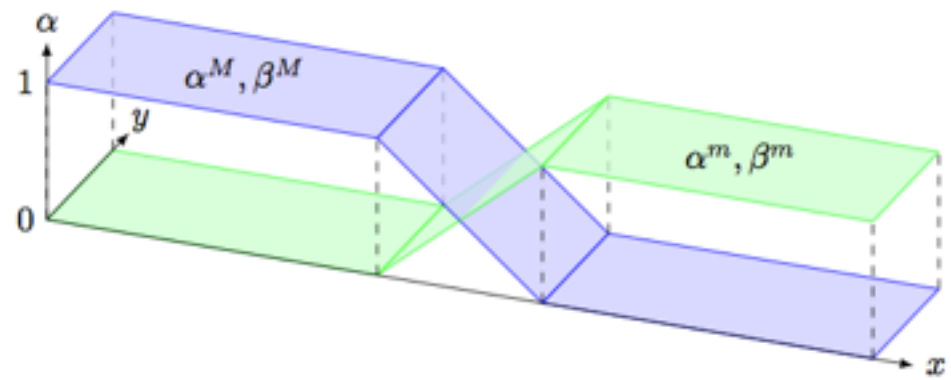
[H. Ben Dhia, 1998]

- partition of unity for energy in gluing zone

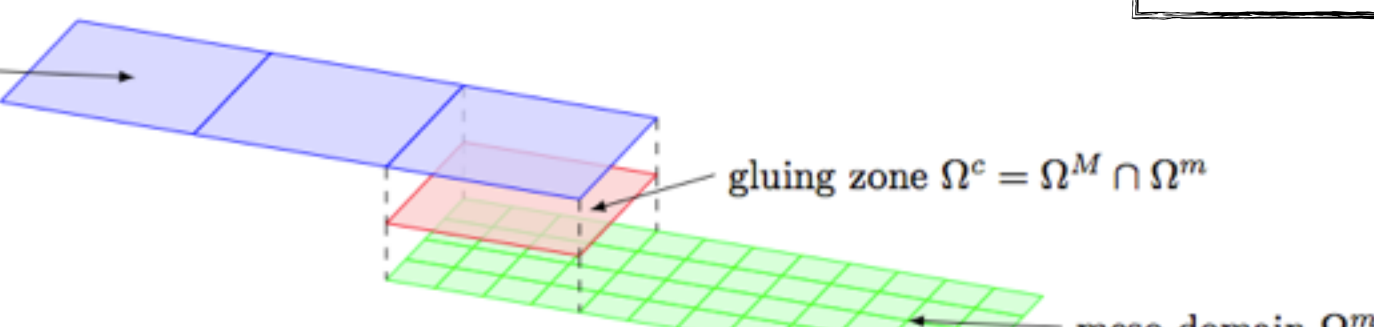
$$\alpha^M + \alpha^m = 1$$

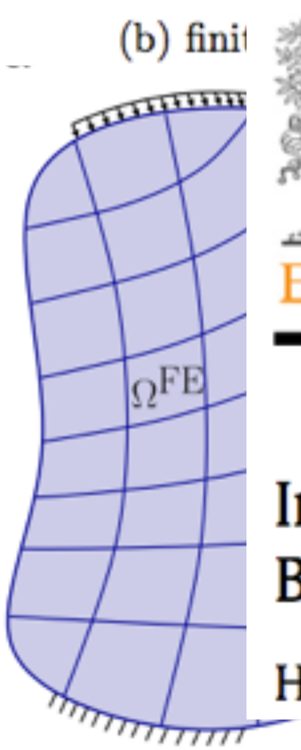
- Lagrange multipliers to glue two models

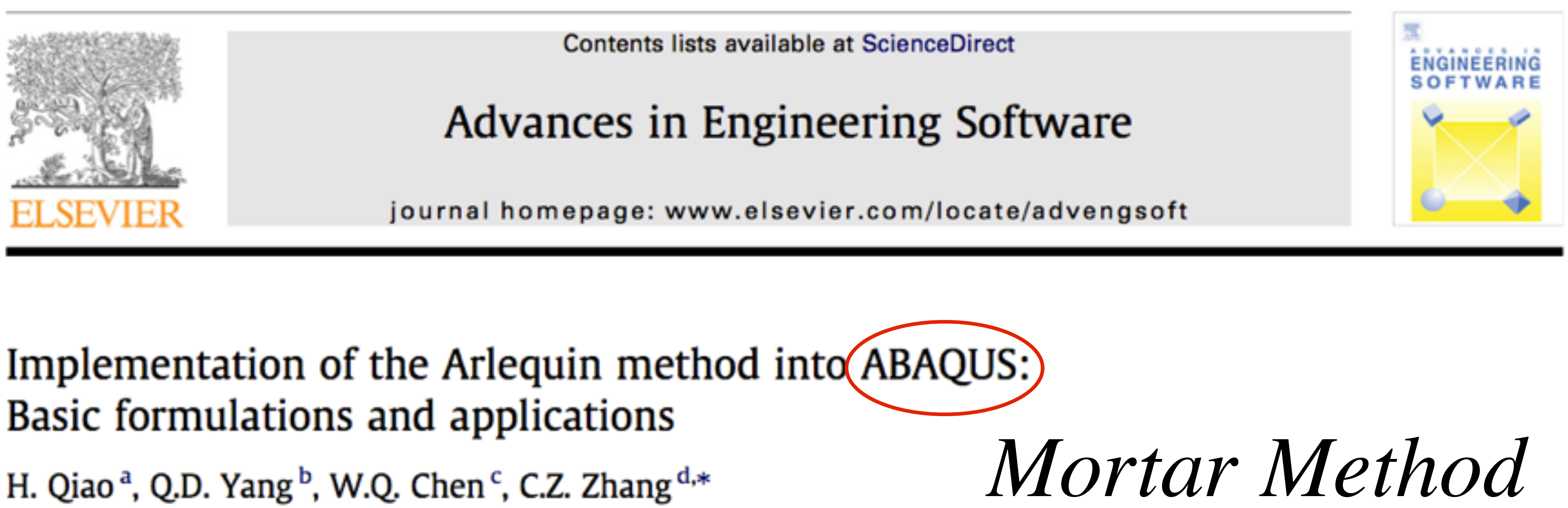
a multi-scale/multi-model method



(a) arlequin weight functions







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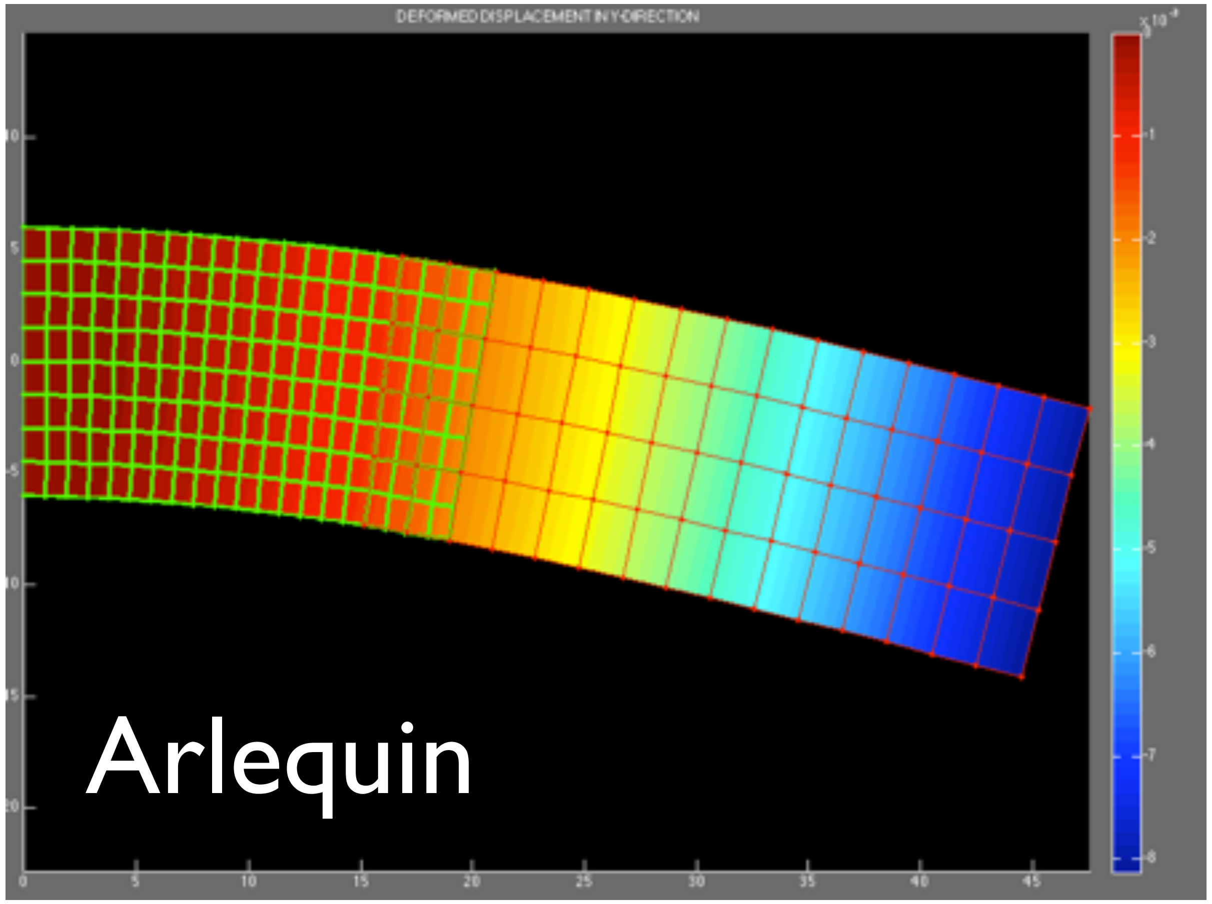
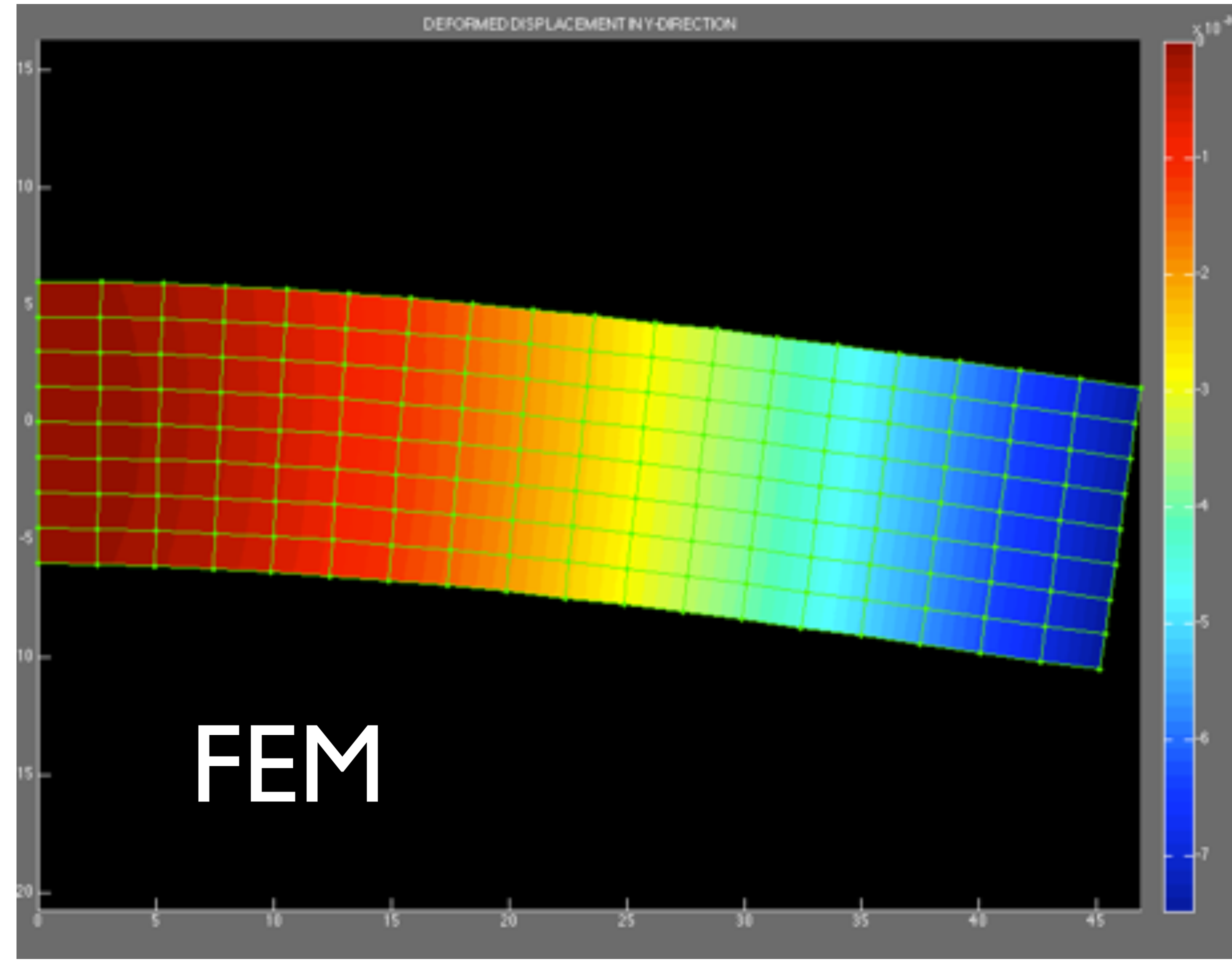
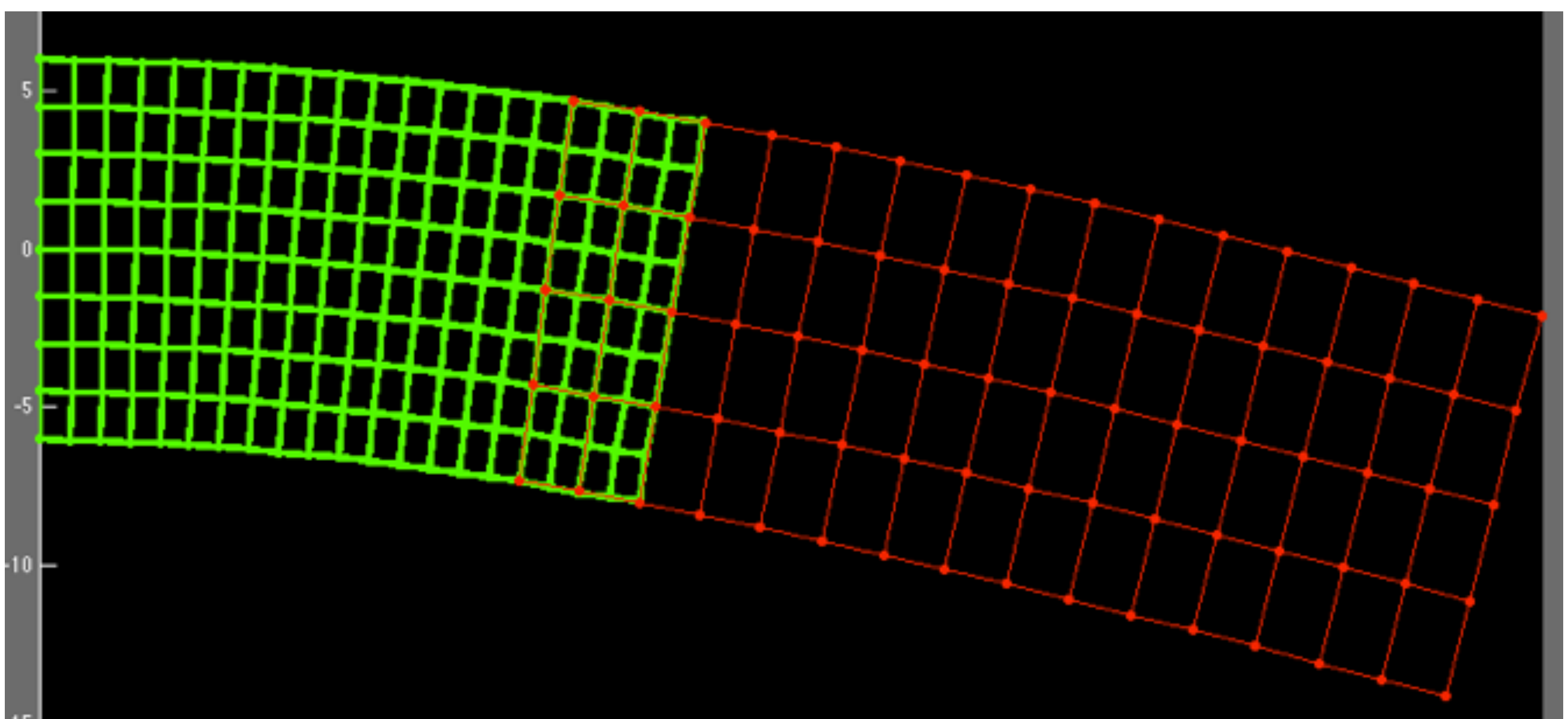
Implementation of the Arlequin method into ABAQUS: Basic formulations and applications

H. Qiao [a], Q.D. Yang [b], W.Q. Chen [c], C.Z. Zhang [d,*]

Mortar Method



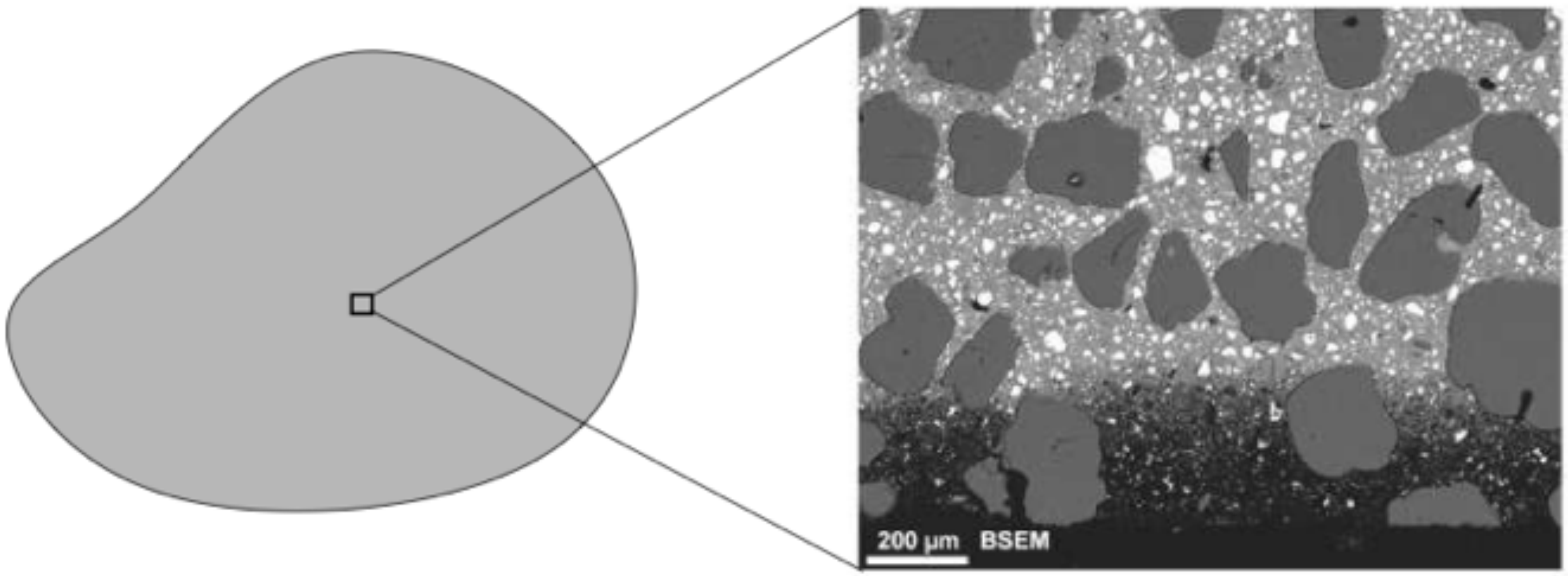




work in progress

Heterogeneous materials

macroscopically homogeneous but microscopically heterogeneous



macroscopic length scale   microscopic length scale

macroscopic behavior depends on

- size, shape
- spatial distribution
- volume fraction
- mechanical properties

of the constituents.

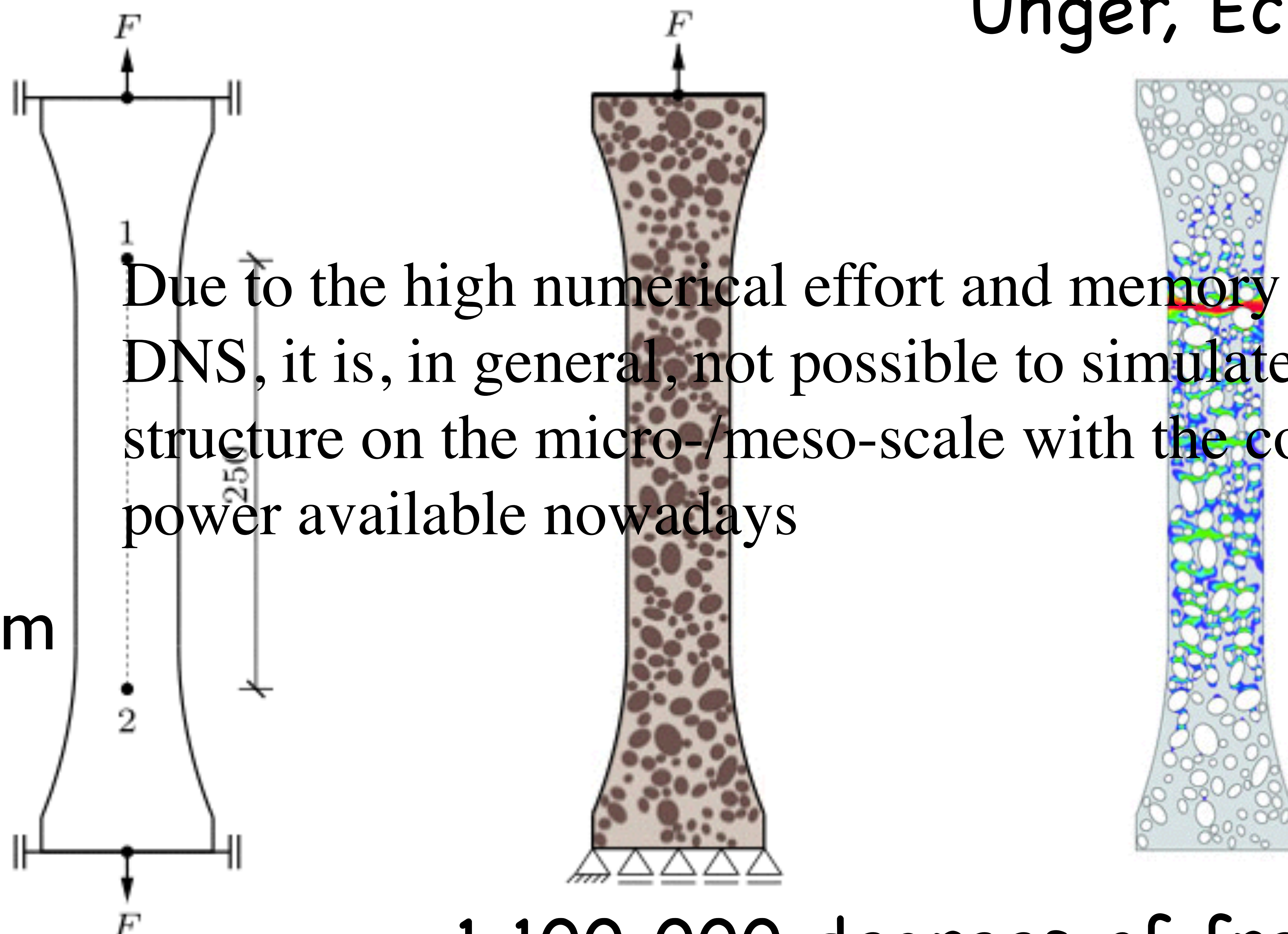
phenomenological constitutive models $\boldsymbol{\sigma} = f(\epsilon, \alpha)$

two many params

the identification of these parameters is generally difficult

Direct Numerical Simulation (DNS)

Unger, Eckard, 2011



Due to the high numerical effort and memory demand of DNS, it is, in general, not possible to simulate the full structure on the micro-/meso-scale with the computational power available nowadays

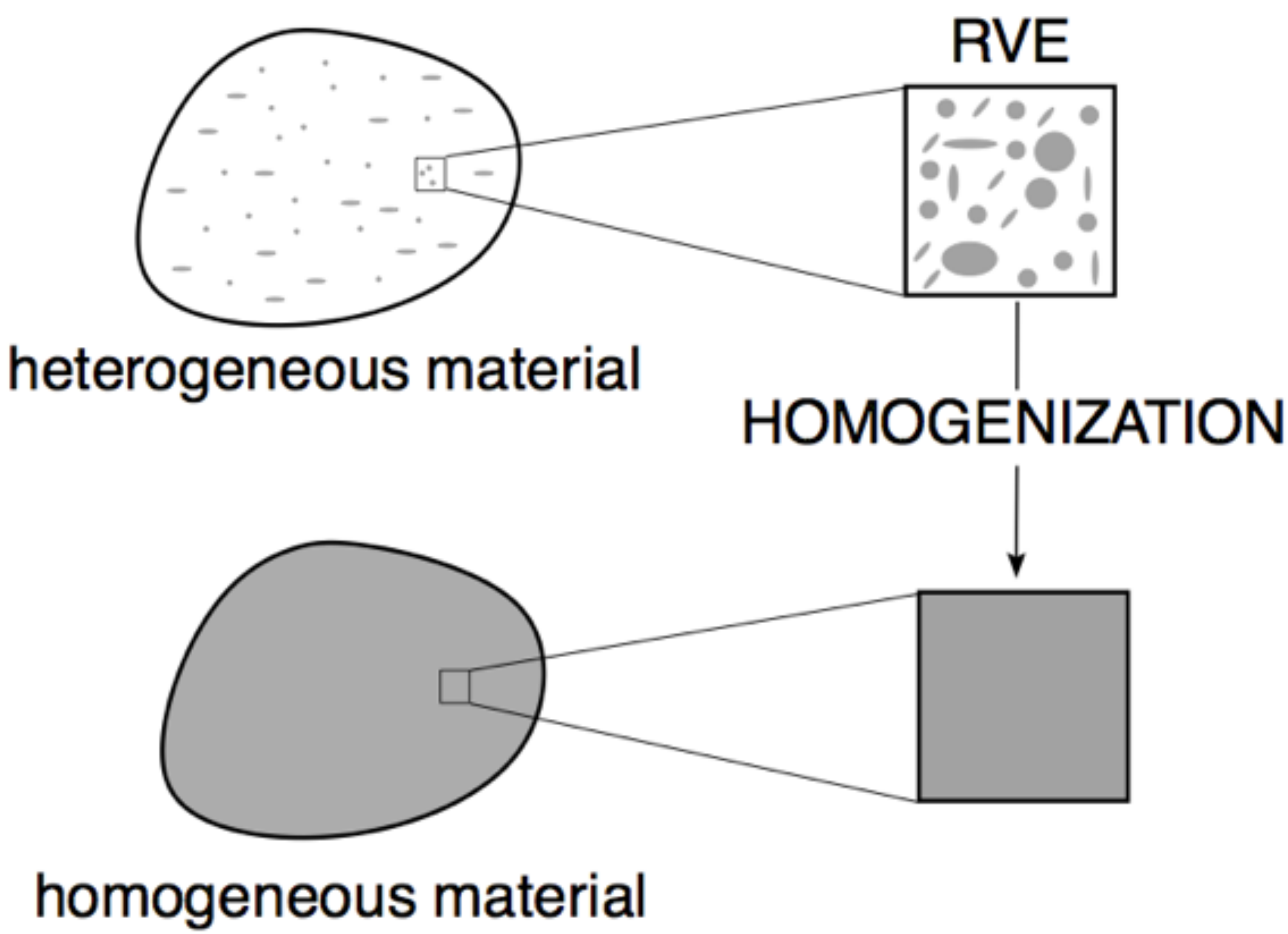
44 cm

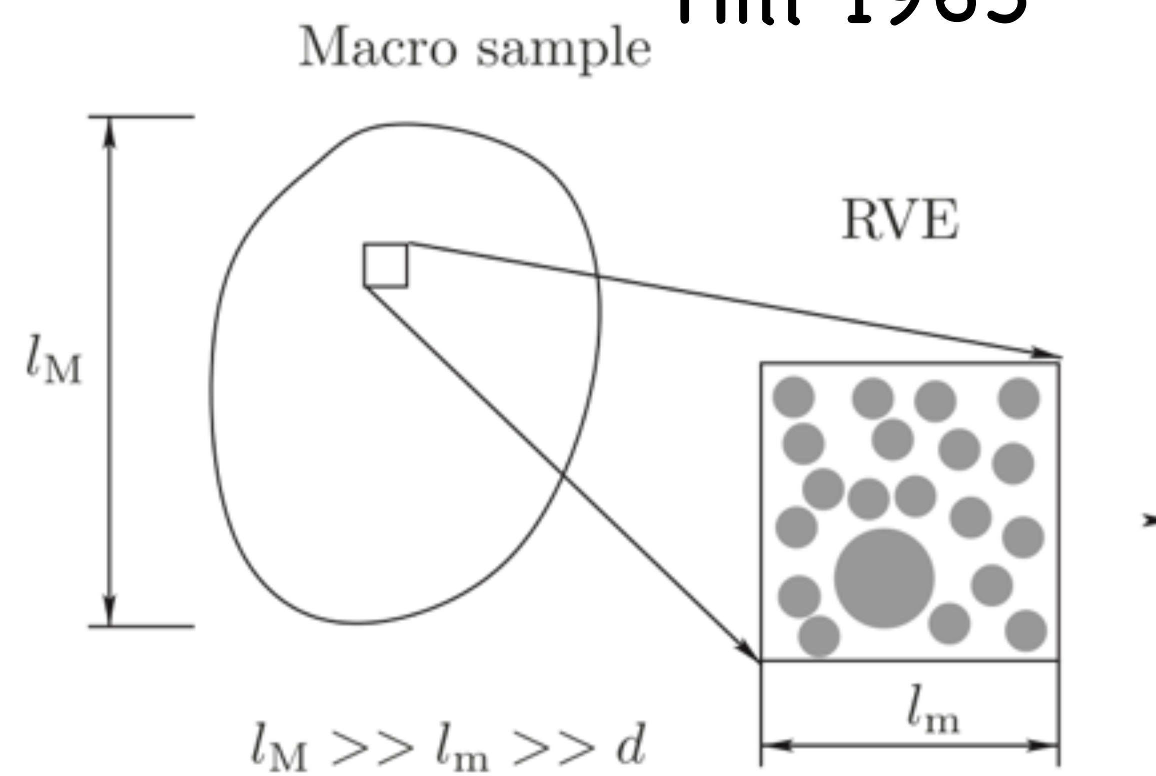
1 100 000 degrees of freedom

Homogenization

Homogenization = replace a heterogeneous material with an **equivalent homogeneous** material.

Voigt, 1910
Reuss 1929
Hill 1965





separation of scales

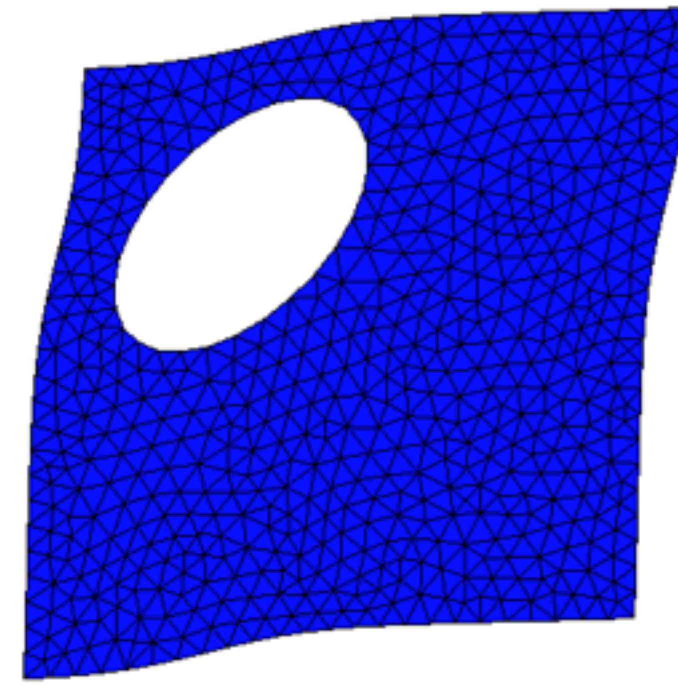
RVE=Representative Volume Element

Homogenization

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C} : \langle \boldsymbol{\epsilon} \rangle$$

bottom-up approach

1



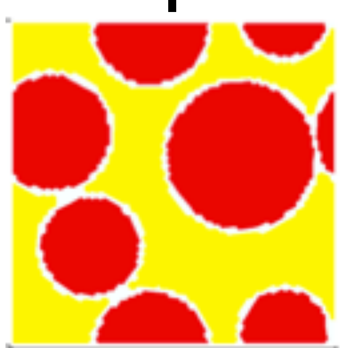
FEM

2

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{|\Omega_{\mathrm{m}}|} \int_{\Omega_{\mathrm{m}}} \boldsymbol{\sigma}_{\mathrm{m}} \mathrm{d}\Omega$$

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{|\Omega_{\mathrm{m}}|} \int_{\Omega_{\mathrm{m}}} \boldsymbol{\epsilon}_{\mathrm{m}} \mathrm{d}\Omega$$

RVE



6 independent loads are needed to determine 36 constants → $\mathbf{C}$ effective properties

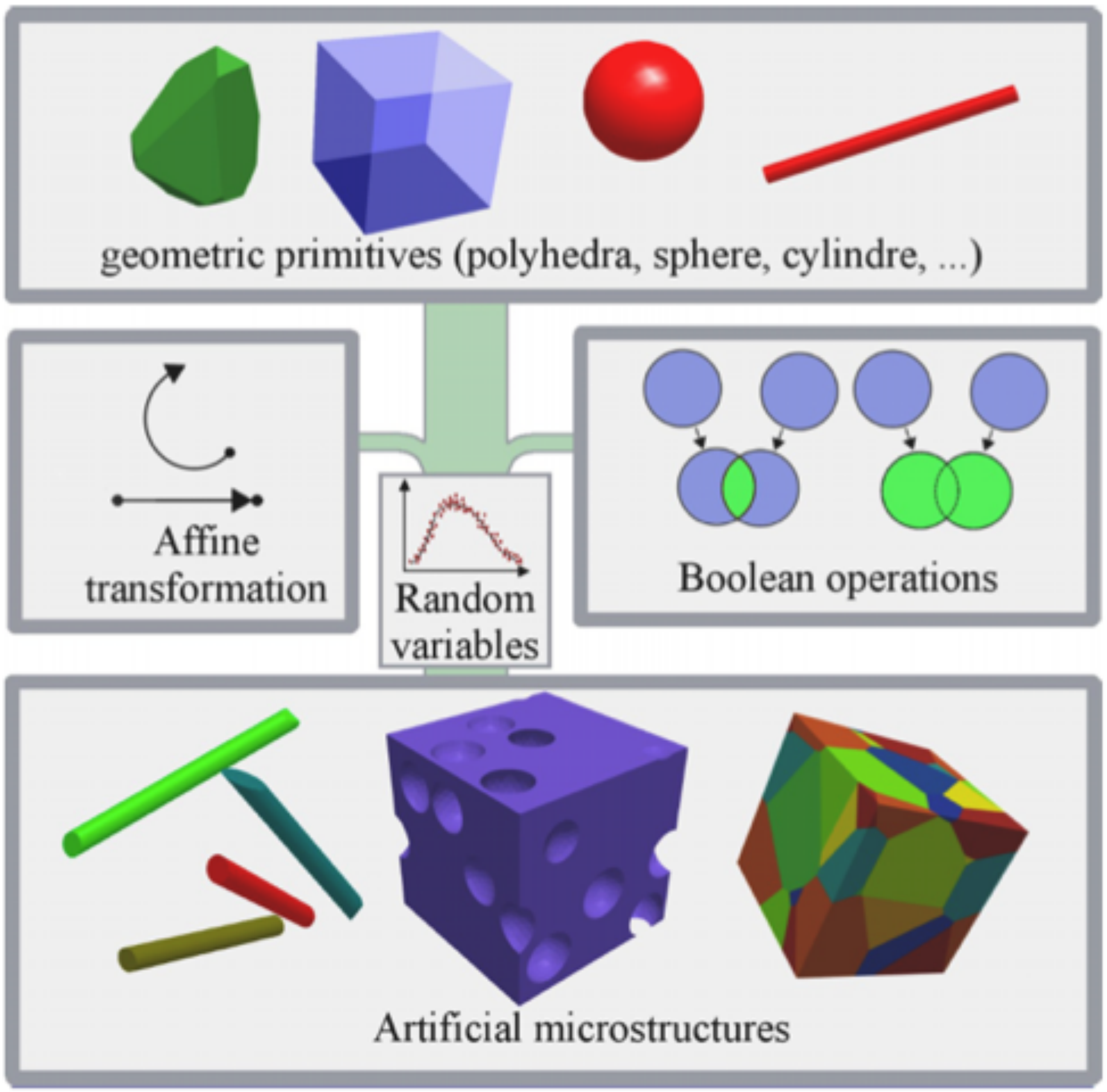
$$\begin{Bmatrix} \langle\sigma_{11}\rangle_\Omega \\ \langle\sigma_{22}\rangle_\Omega \\ \langle\sigma_{33}\rangle_\Omega \\ \langle\sigma_{12}\rangle_\Omega \\ \langle\sigma_{23}\rangle_\Omega \\ \langle\sigma_{13}\rangle_\Omega \end{Bmatrix} = \begin{bmatrix} E^*_{1111} & E^*_{1122} & E^*_{1133} & E^*_{1112} & E^*_{1123} & E^*_{1113} \\ E^*_{2211} & E^*_{2222} & E^*_{2233} & E^*_{2212} & E^*_{2223} & E^*_{2213} \\ E^*_{3311} & E^*_{3322} & E^*_{3333} & E^*_{3312} & E^*_{3323} & E^*_{3313} \\ E^*_{1211} & E^*_{1222} & E^*_{1233} & E^*_{1212} & E^*_{1223} & E^*_{1213} \\ E^*_{2311} & E^*_{2322} & E^*_{2333} & E^*_{2312} & E^*_{2323} & E^*_{2313} \\ E^*_{1311} & E^*_{1322} & E^*_{1333} & E^*_{1312} & E^*_{1323} & E^*_{1313} \end{bmatrix} \begin{Bmatrix} \langle\epsilon_{11}\rangle_\Omega \\ \langle\epsilon_{22}\rangle_\Omega \\ \langle\epsilon_{33}\rangle_\Omega \\ 2\langle\epsilon_{12}\rangle_\Omega \\ 2\langle\epsilon_{23}\rangle_\Omega \\ 2\langle\epsilon_{13}\rangle_\Omega \end{Bmatrix}$$

o constitutive model

simple plasticity

Artificial microstructures

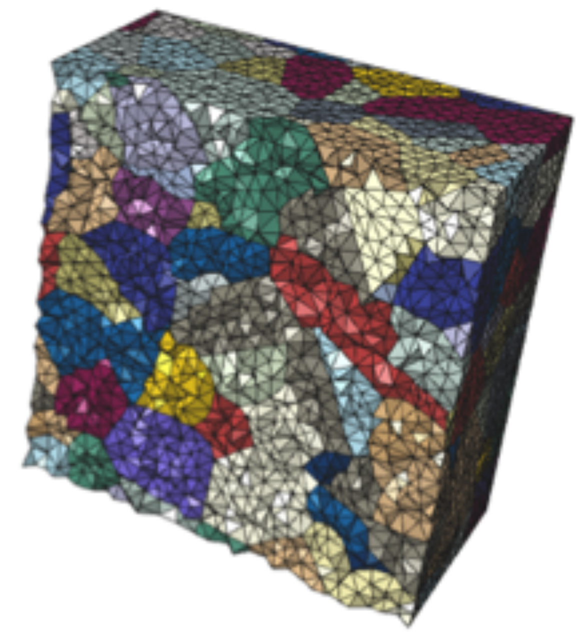
Real microstructures: hard to obtain and not meshable



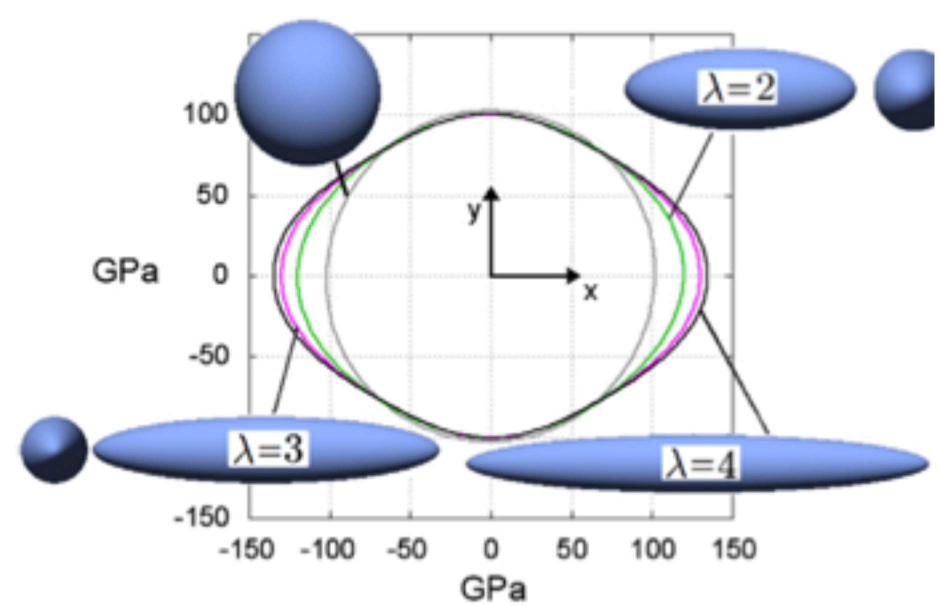
F. Fritzen 2010

Statistically equivalent to real microstructures

Easy to discretized into finite elements

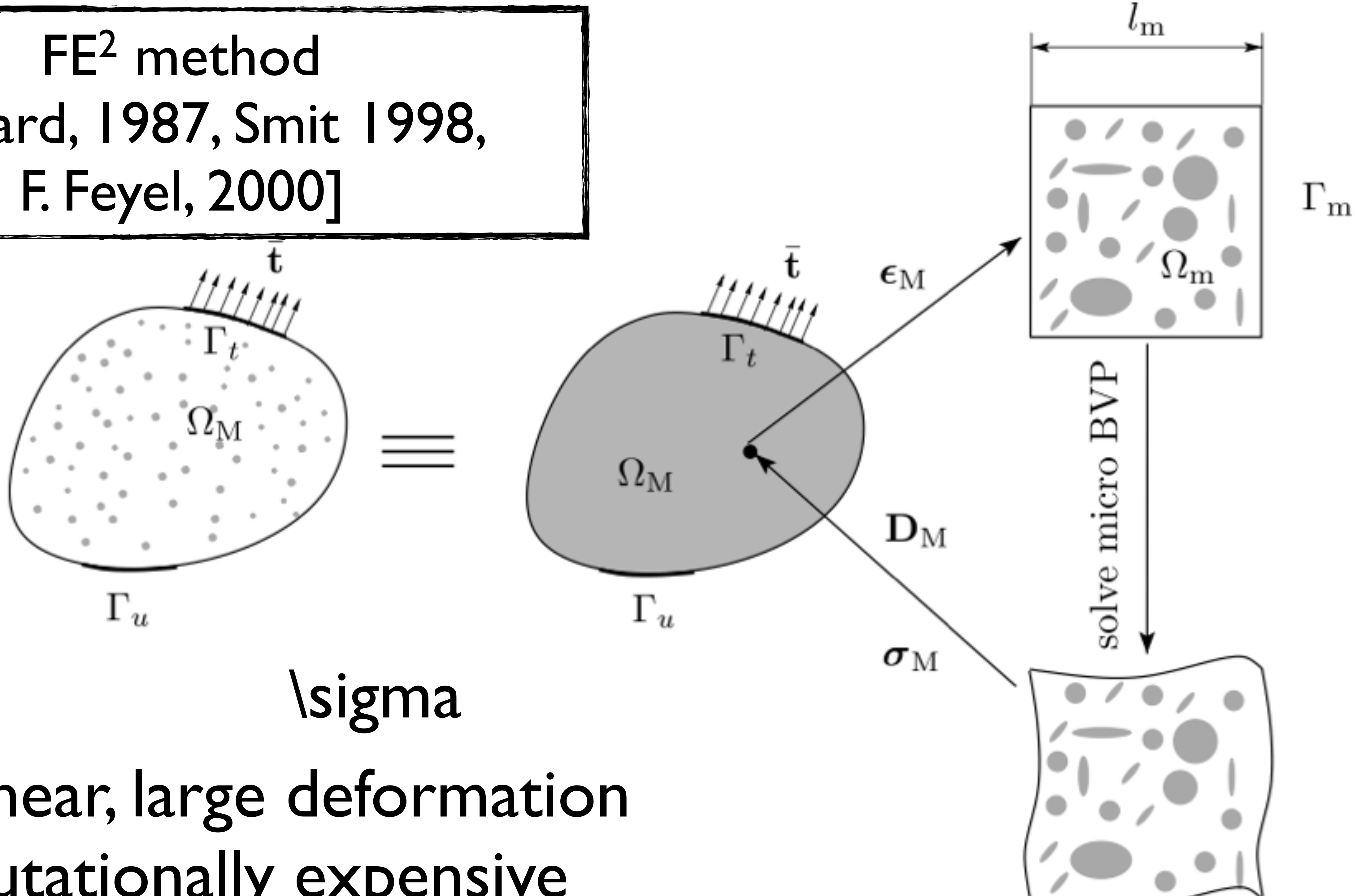


Build tailor made materials



Computational Homogenization

FE^2 method
[Renard, 1987, Smit 1998,
F. Feyel, 2000]

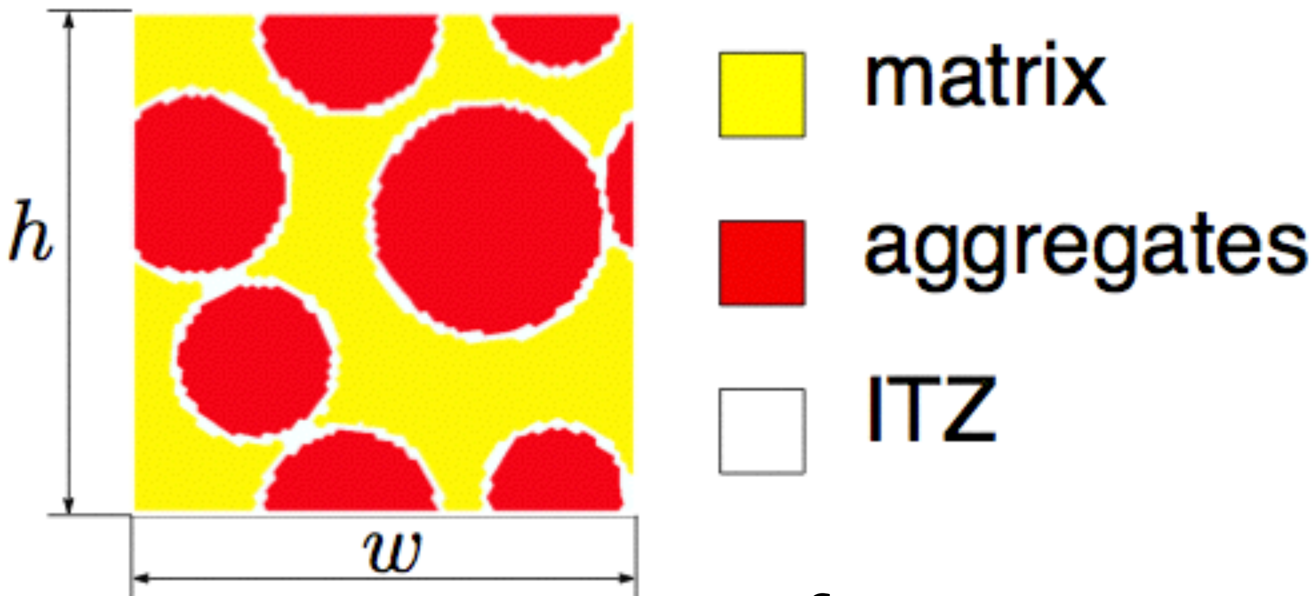


\sigma

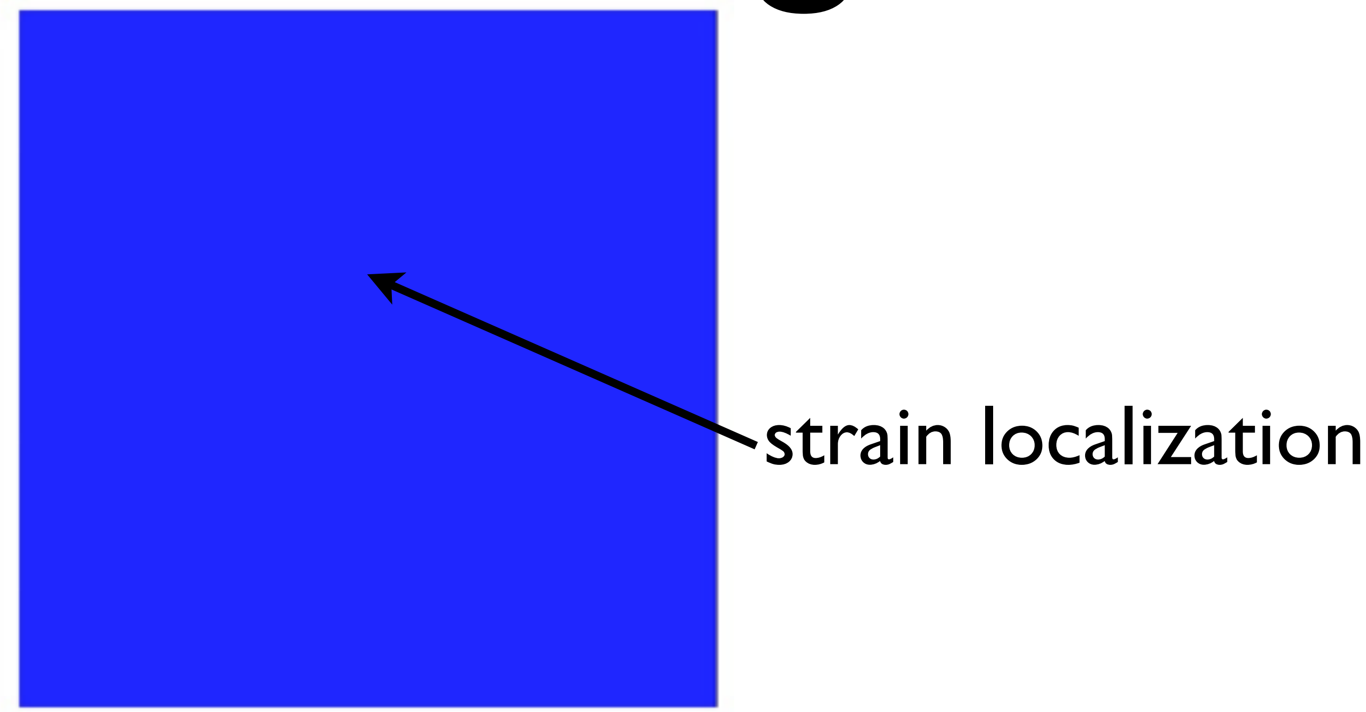
+ nonlinear, large deformation
- computationally expensive
- 2D problems at laboratory scale
- not always robust!!!

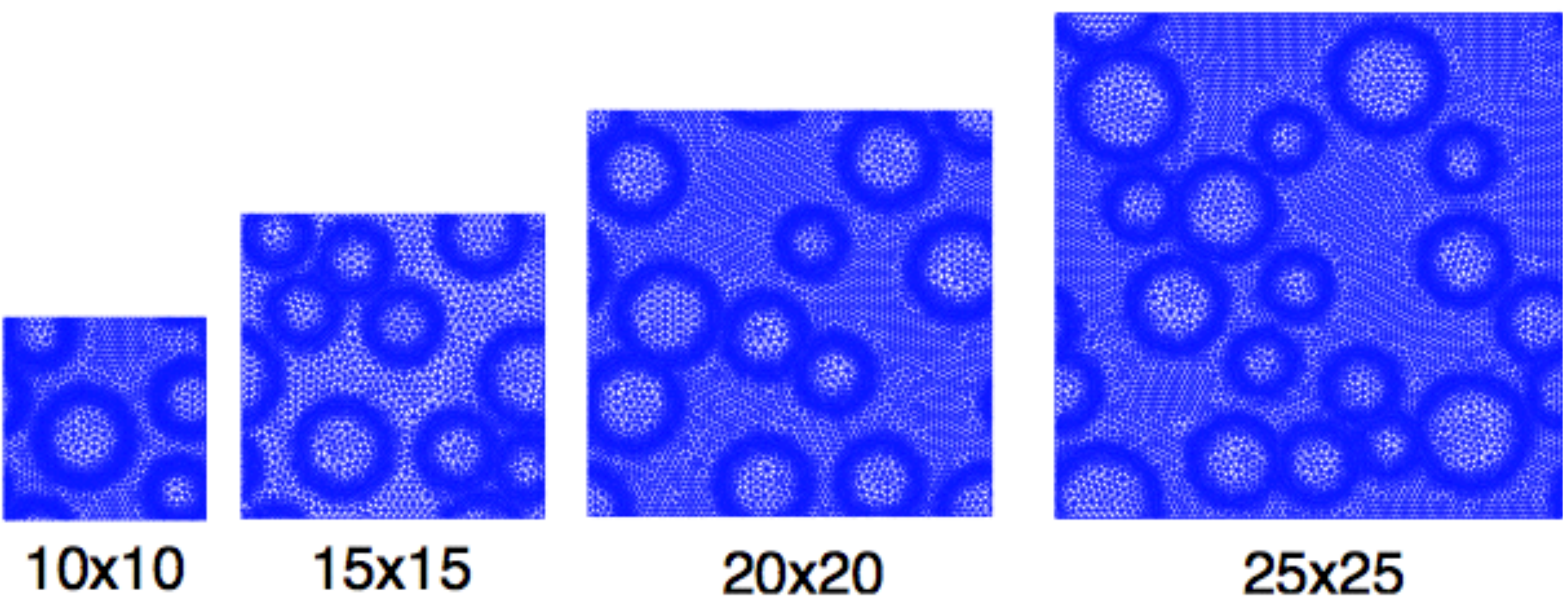
Micro problems are solved in parallel

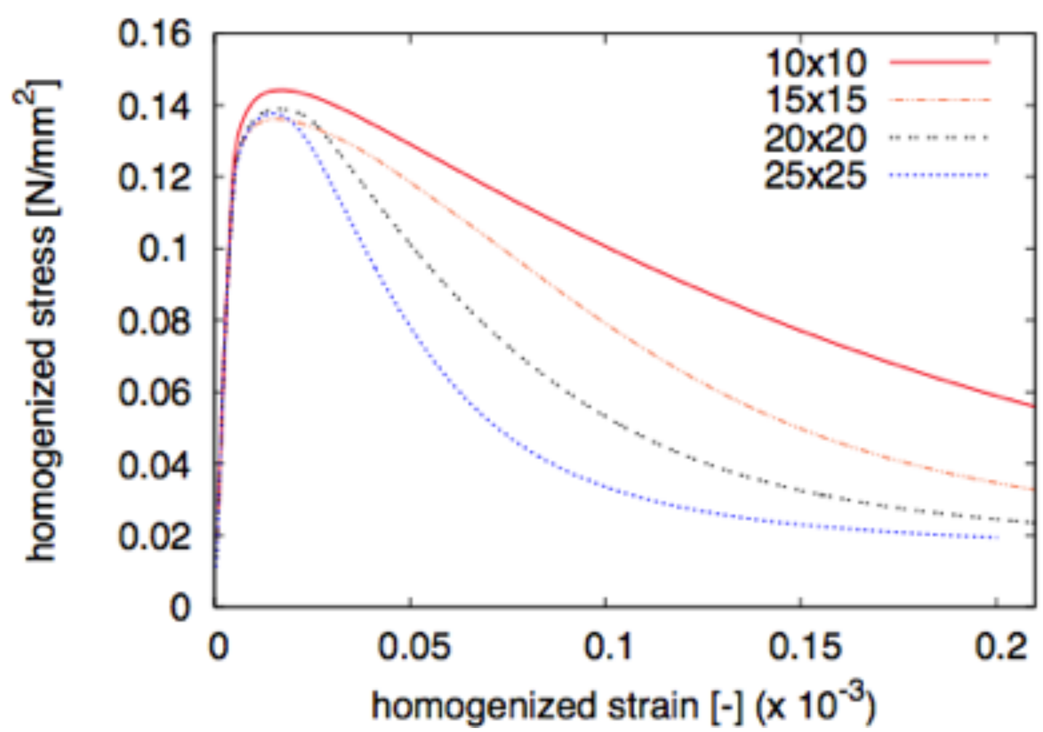
Troubles with softening RVEs



meso-structure of concrete







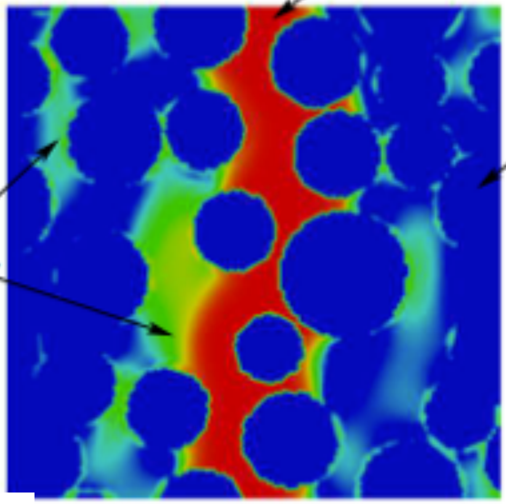
- RVE does not exist for softening materials
- CH cannot be applied for softening materials

Failure zone averaging

Ω_e: elastic domain

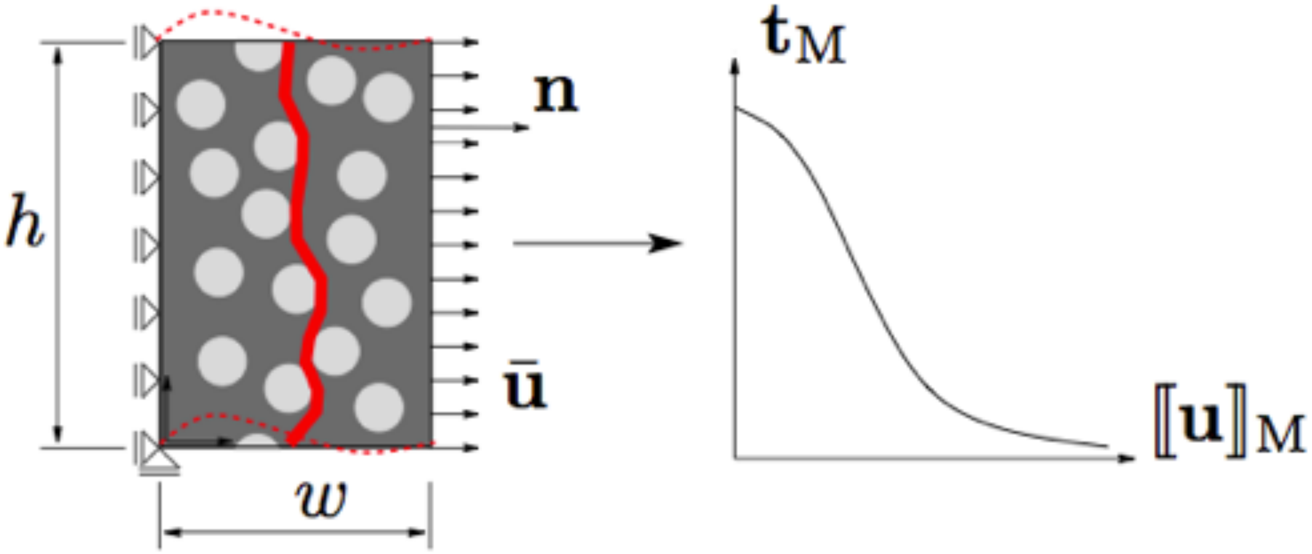
Ω_d: active damaged domain

Ω_{du}: inactive damaged domain



$$\Omega_d = \{\mathbf{x} \in \Omega_m \mid \omega(\mathbf{x}) > 0, f(\mathbf{x}) = 0\}$$

$$\langle \boldsymbol{\sigma} \rangle_{dam} = \frac{1}{|\Omega_d|} \int_{\Omega_d} \boldsymbol{\sigma}_m d\Omega_d, \quad \langle \boldsymbol{\epsilon} \rangle_{dam} = \frac{1}{|\Omega_d|} \int_{\Omega_d} \boldsymbol{\epsilon}_m d\Omega_d$$



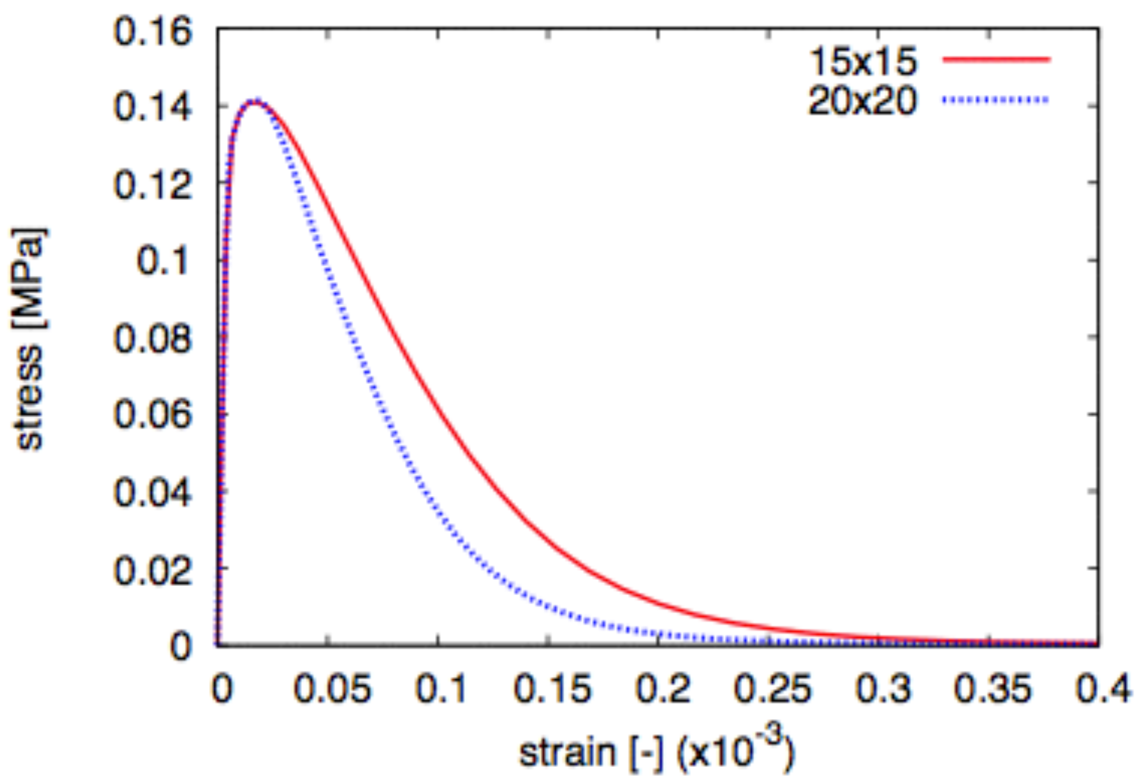
$$\mathbf{t}_M = \frac{1}{h} \boldsymbol{\sigma}_M \cdot \mathbf{n}$$

$$\mathbf{u}_{dam} = \langle \boldsymbol{\epsilon} \rangle_{dam} \cdot (l\mathbf{n}), \quad l = |\Omega_d| / h$$

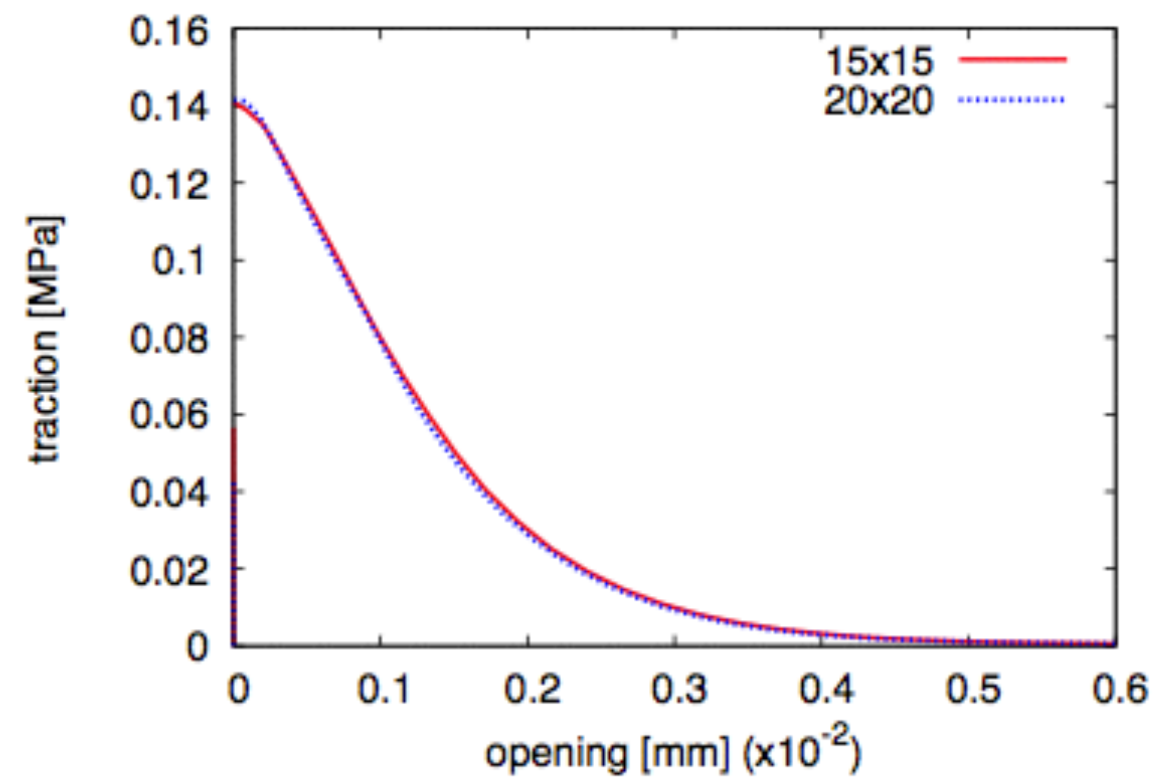
$$[\![\mathbf{u}]\!]_M = \mathbf{u}_{dam} - \mathring{\mathbf{u}}_{dam}$$

Nguyen et al, 2010

standard averaging



new averaging

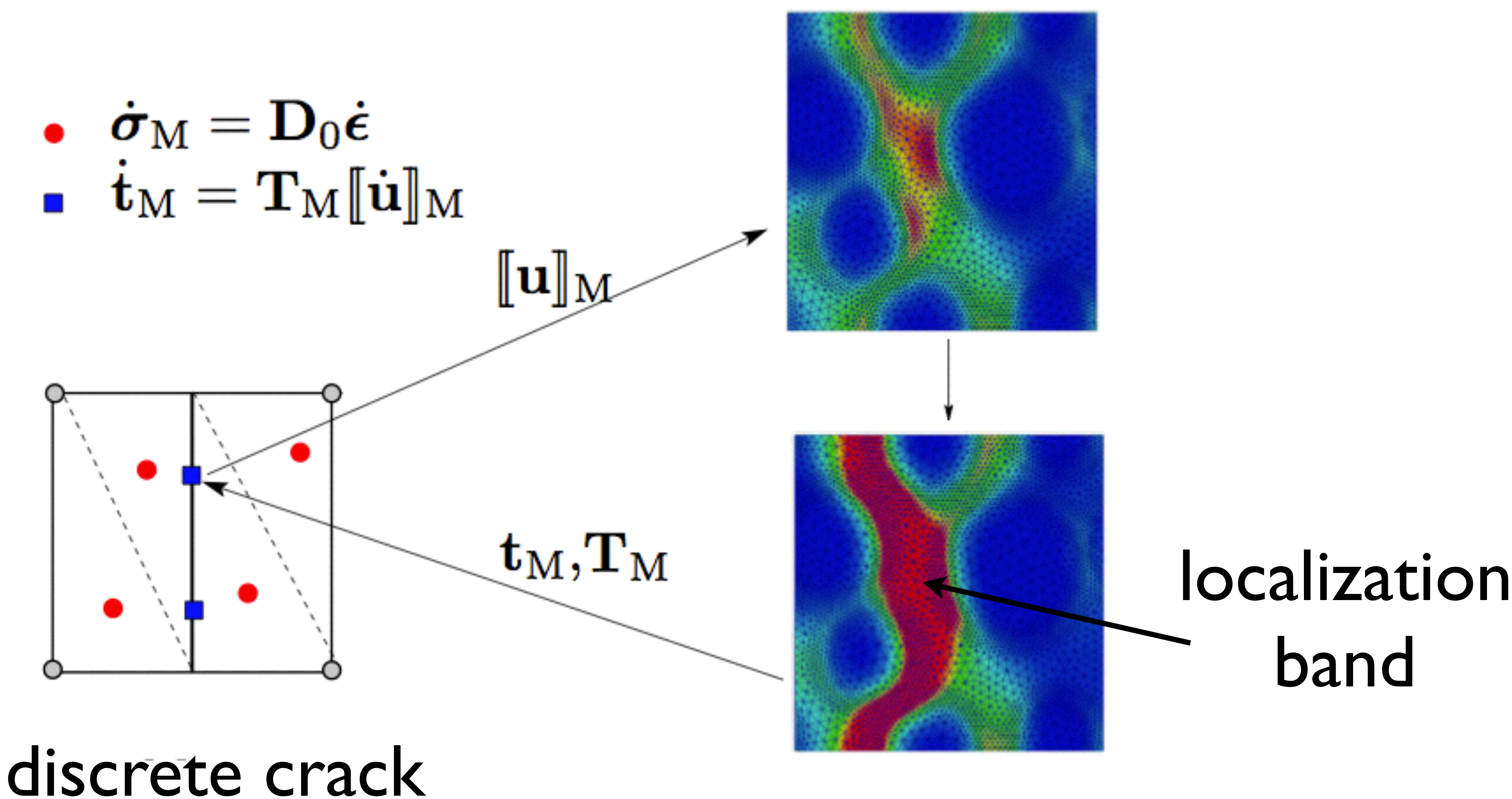


→ RVE does exist for softening materials by using the failure zone averaging technique

Discontinuous CH model

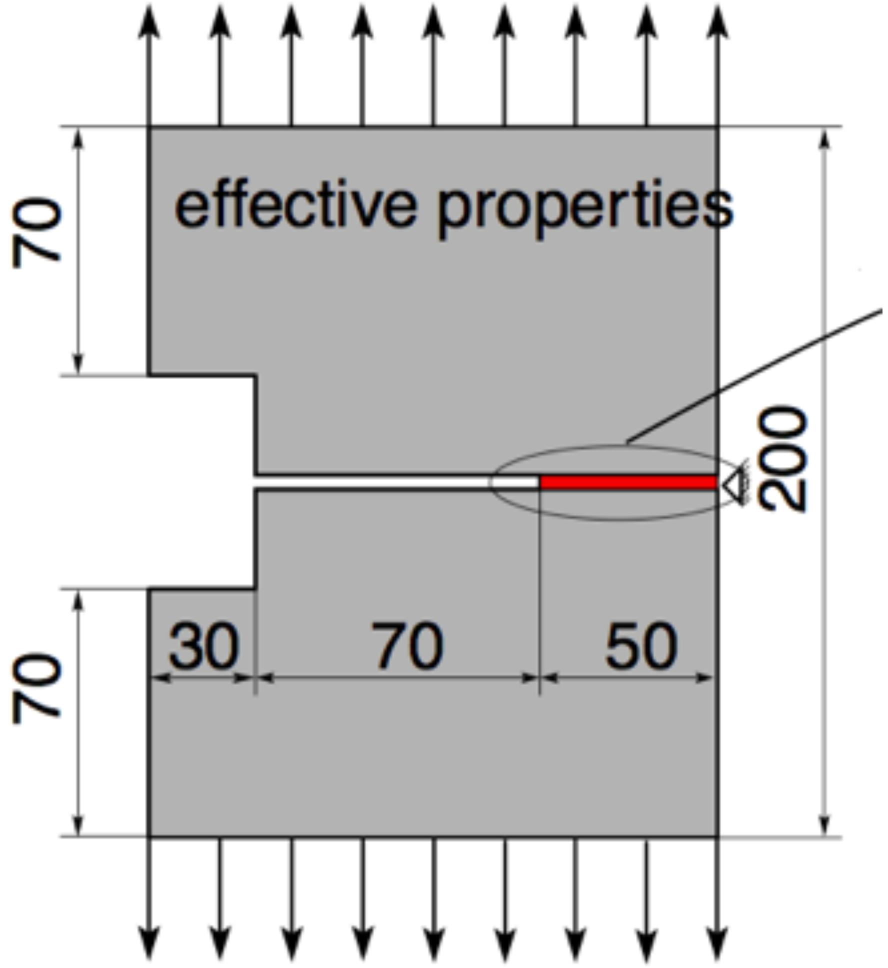
MACRO

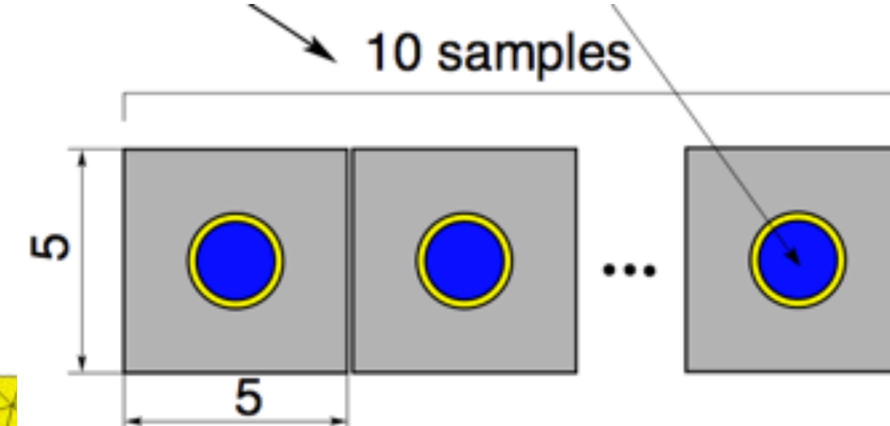
MICRO

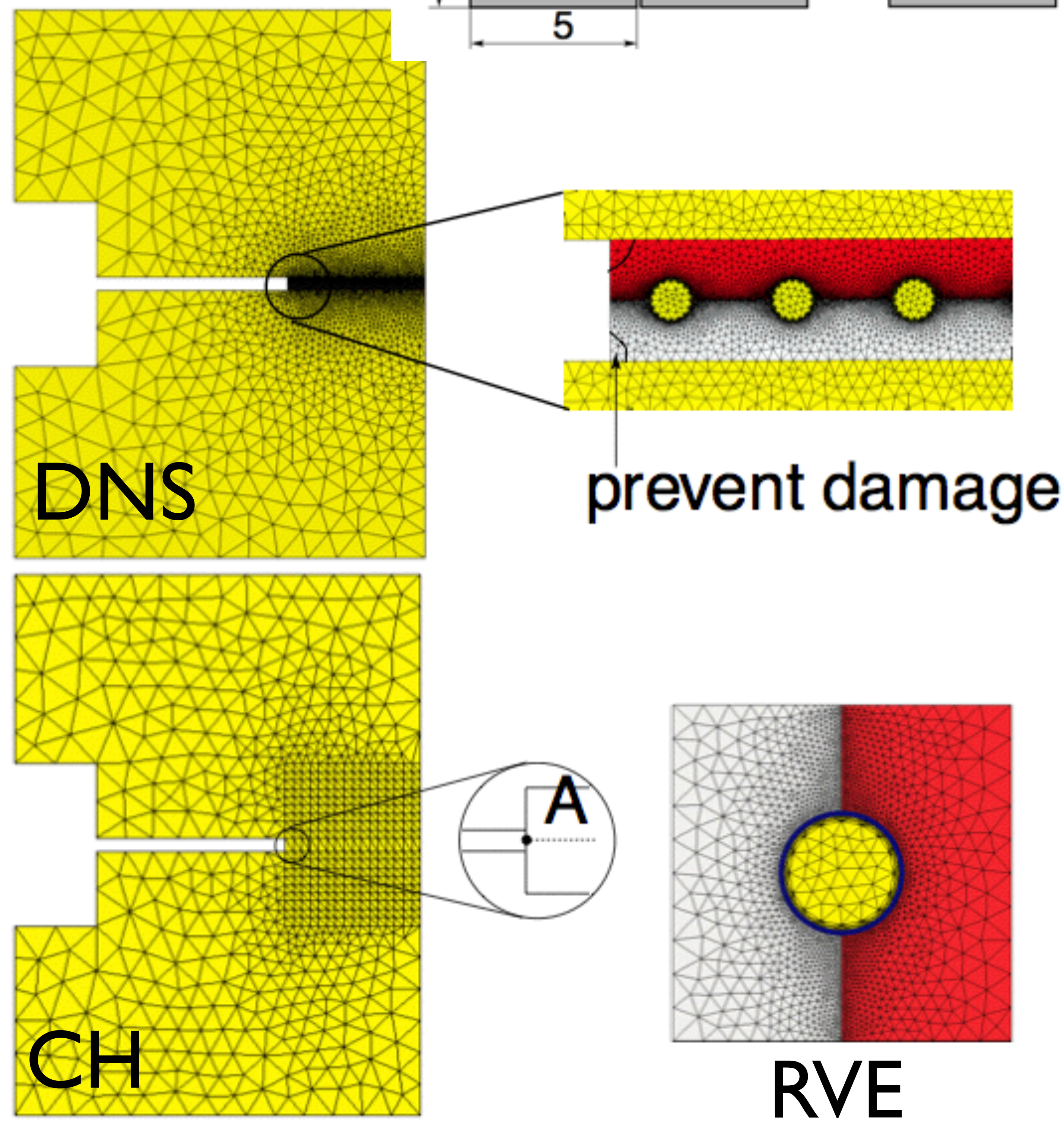


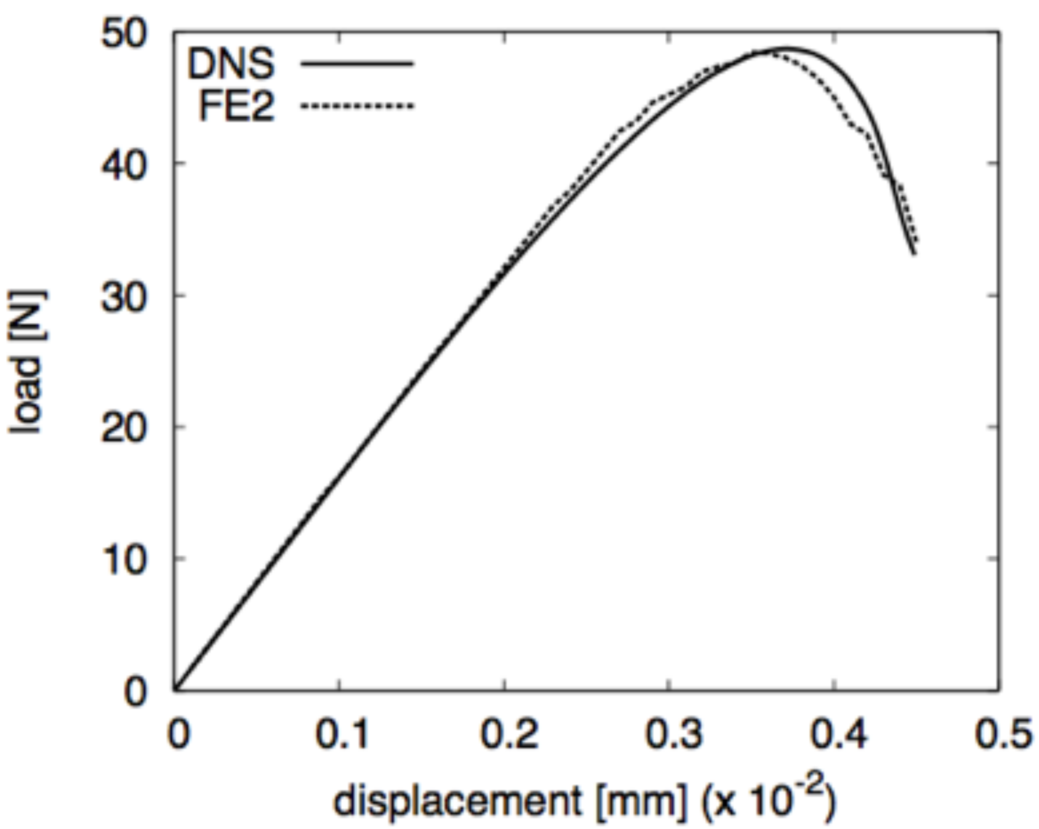
Nguyen et al, 2011

Example

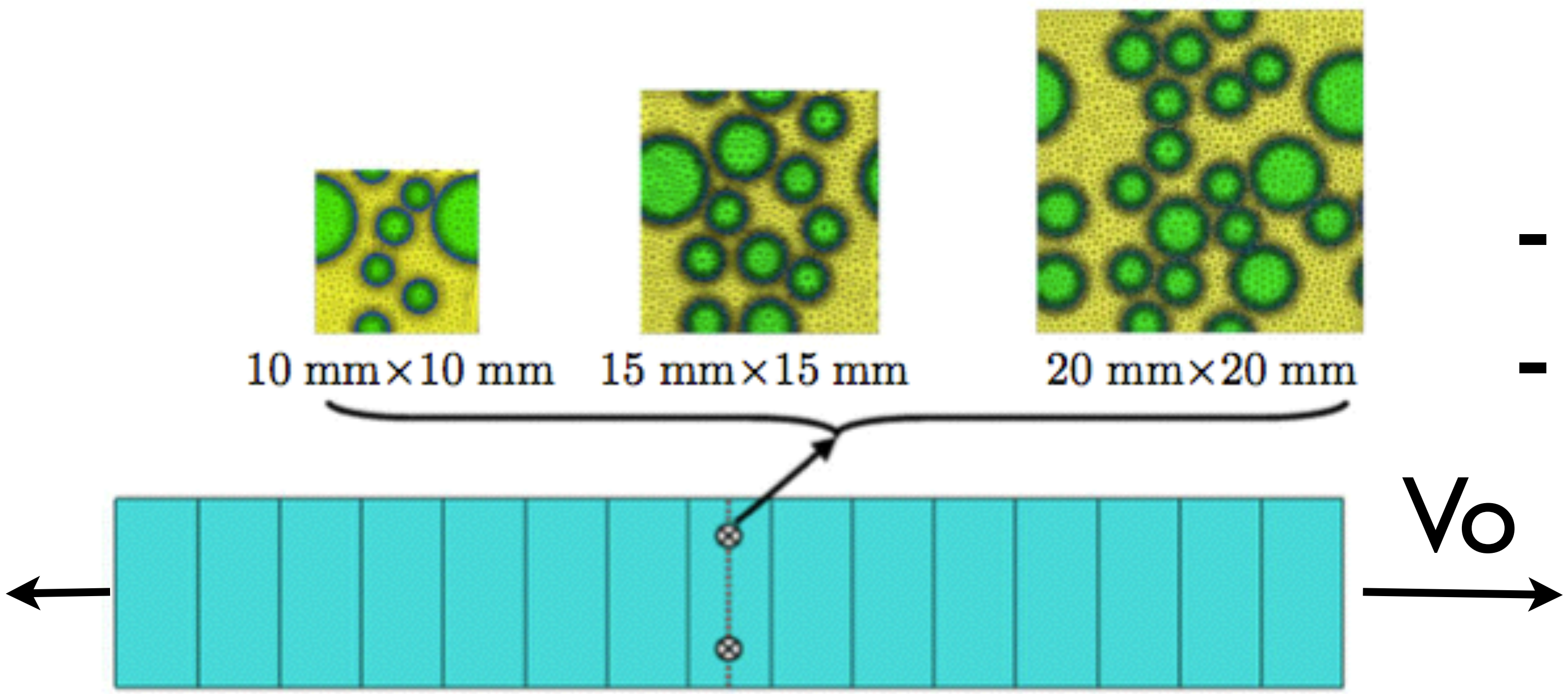

effective properties
70
70
200
30
70
50


10 samples
5
5
...

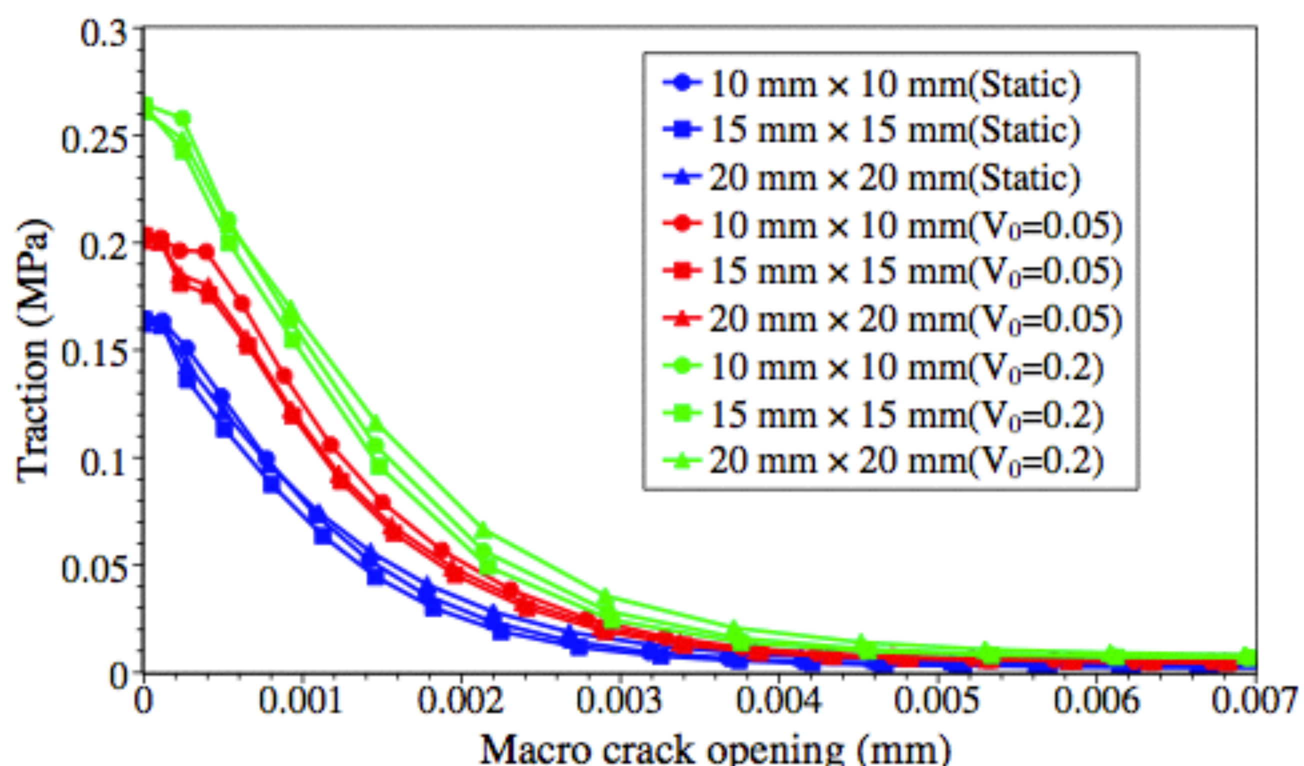

DNS
prevent damage
CH
A
RVE


DNS
FE2
load [N]
displacement [mm] (x 10^-2)
0
10
20
30
40
50
0
0.1
0.2
0.3
0.4
0.5

Dynamic discontinuous CH model



- macro: implicit dynamics
- micro: quasi-static



A. Karamnejad, Nguyen, Sluys, 2012

More information

Archives of Computational Methods in Engineering
March 2009, Volume 16, Issue 1, pp 31-75

Multiscale Methods for Composites: A Review

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VINH PHU NGUYEN, MARTIJN STROEVEN, and LAMBERTUS JOHANNES SLUYS, *J. Multiscale Modelling* **03**, 229 (2011). DOI: 10.1142/S1756973711000509

MULTISCALE CONTINUOUS AND DISCONTINUOUS MODELING OF HETEROGENEOUS MATERIALS: A REVIEW ON RECENT DEVELOPMENTS

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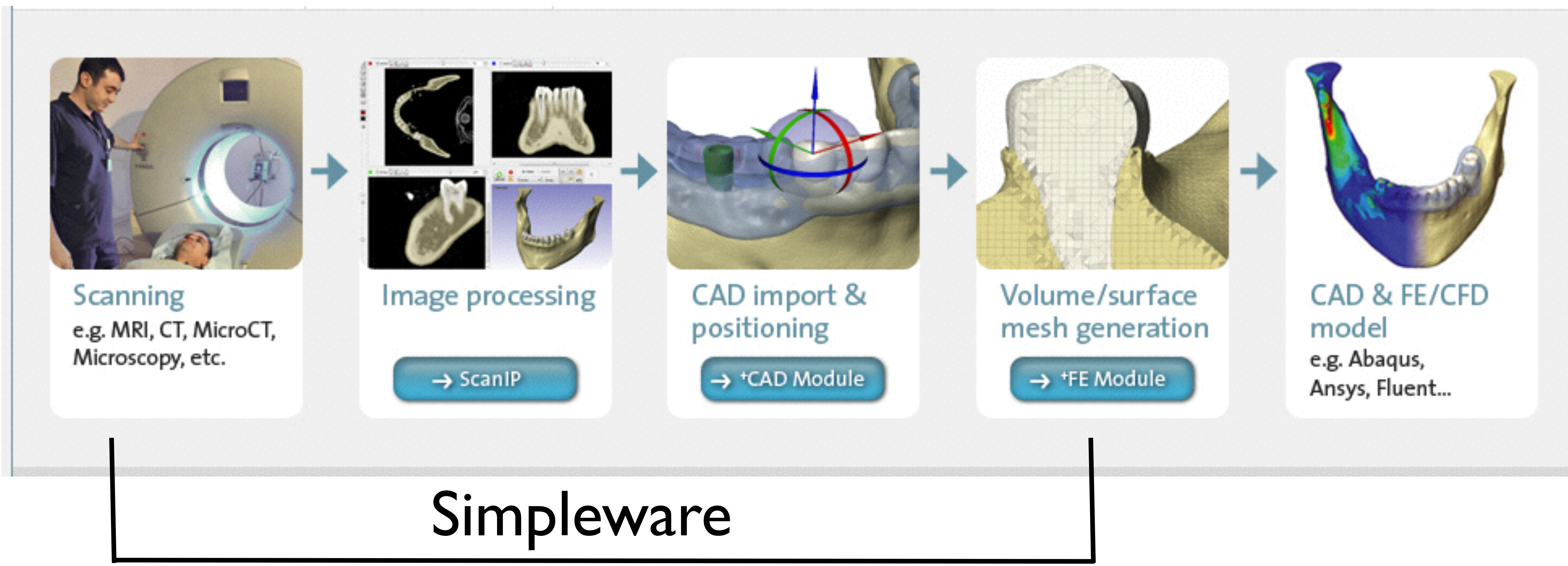
Image-based modeling

Traditional FE analysis

Geometry (CAD) ⟶ Mesh ⟶ FE solver

There are many cases in which such CAD geometries are not available. However, image data are so ready: medicine, material sciences...

(1) Industry

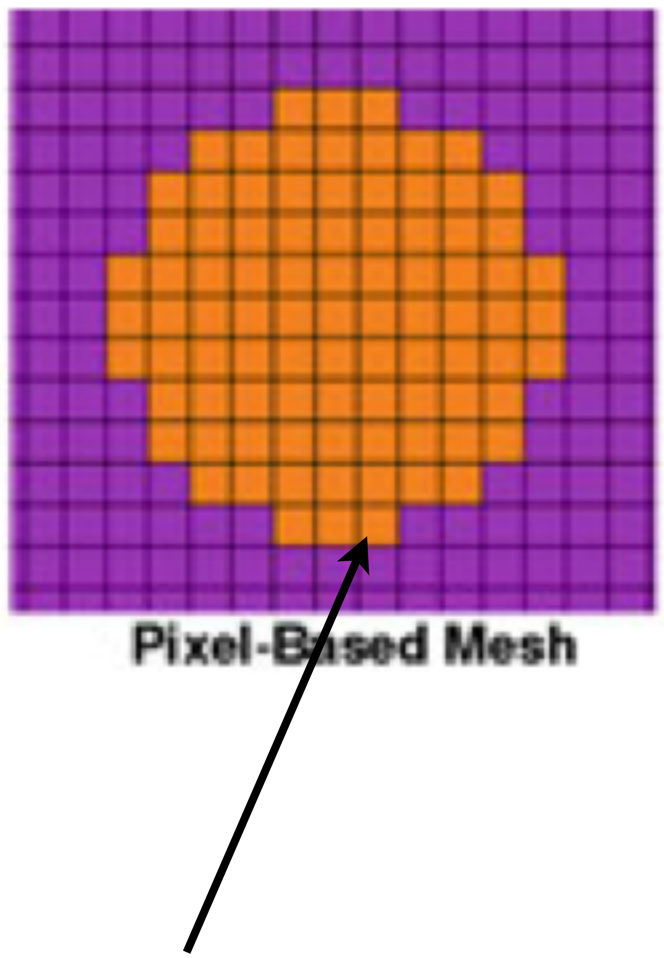


See also the FREE program OOF2, NIST, USA

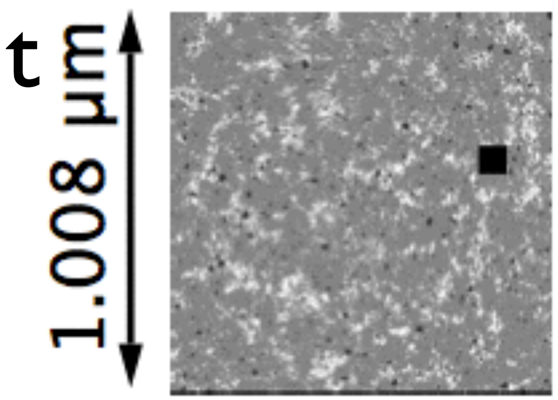
(2) universities — microstructure of cement paste

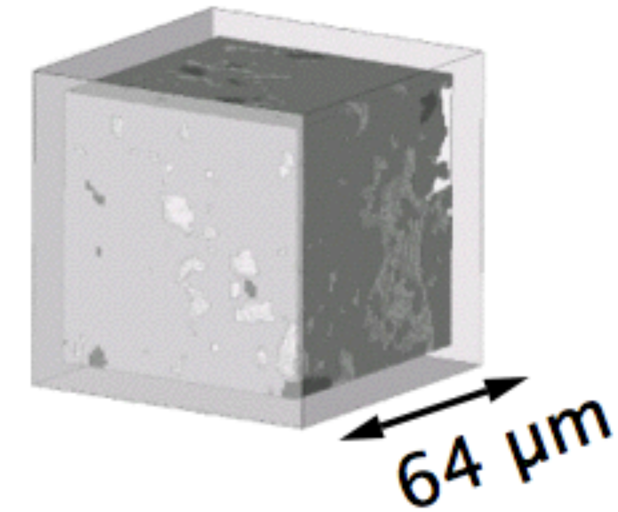
voxel based method

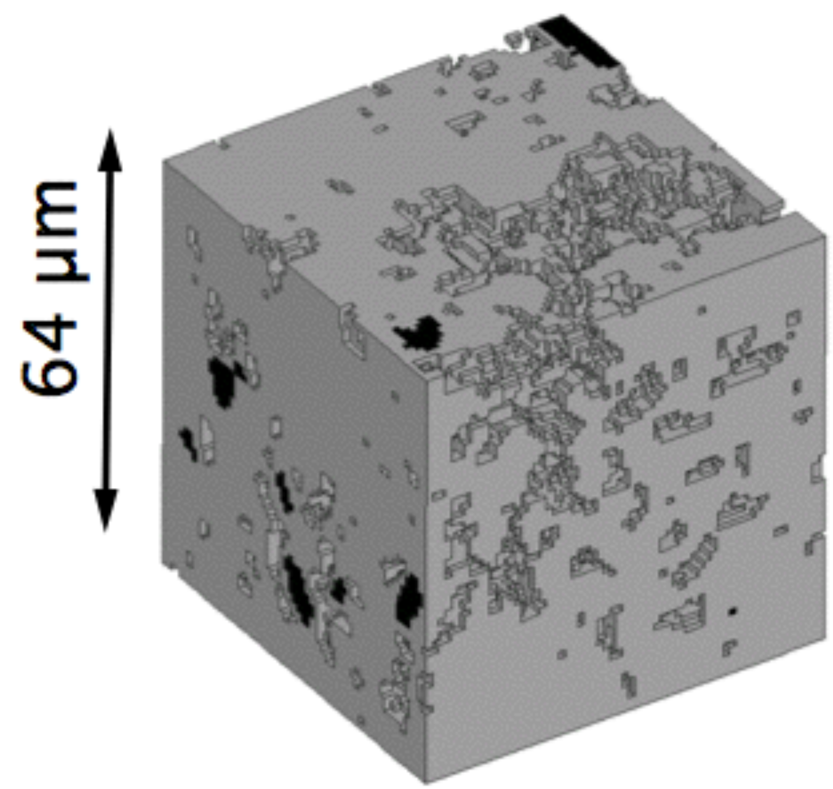
each voxel = one finite element



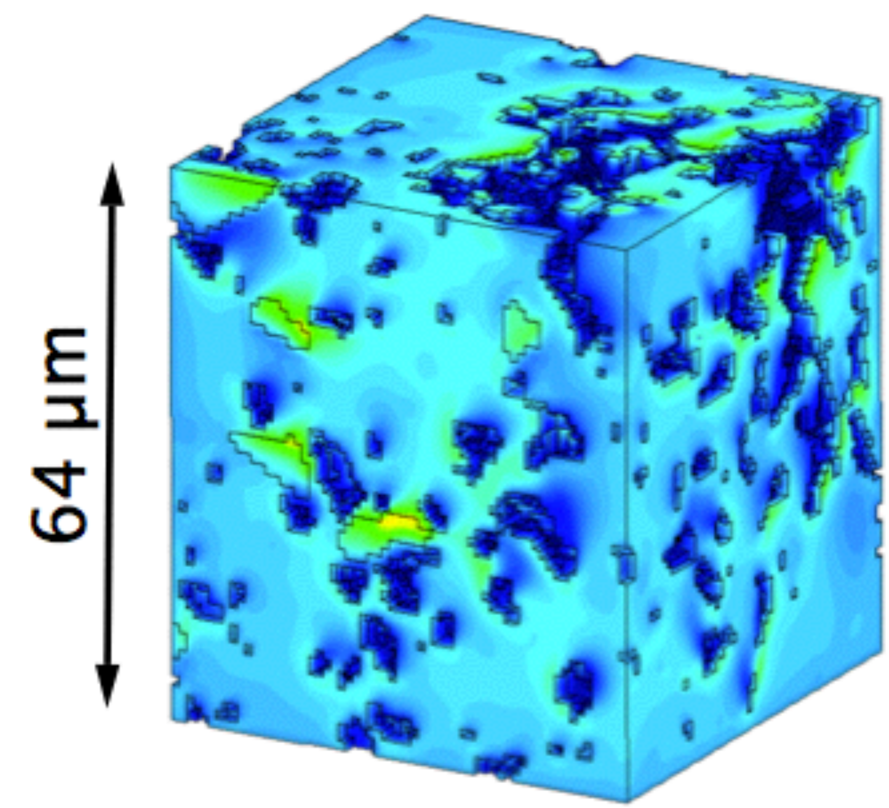
zig-zag boundary







64^3 hexahedron elements

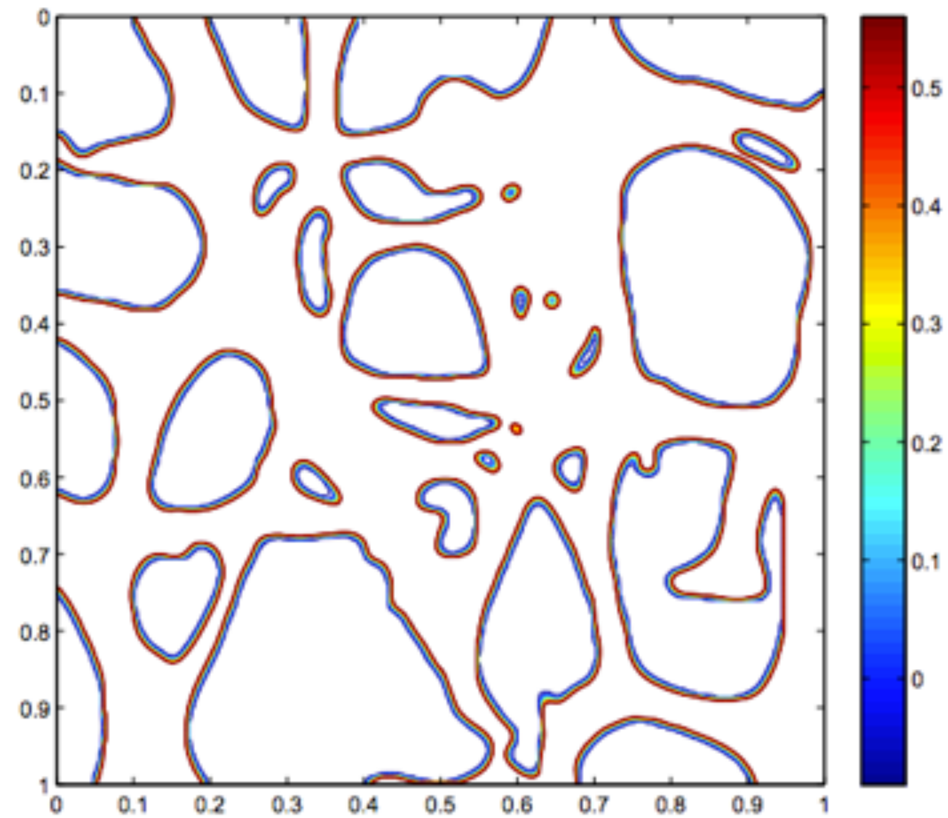


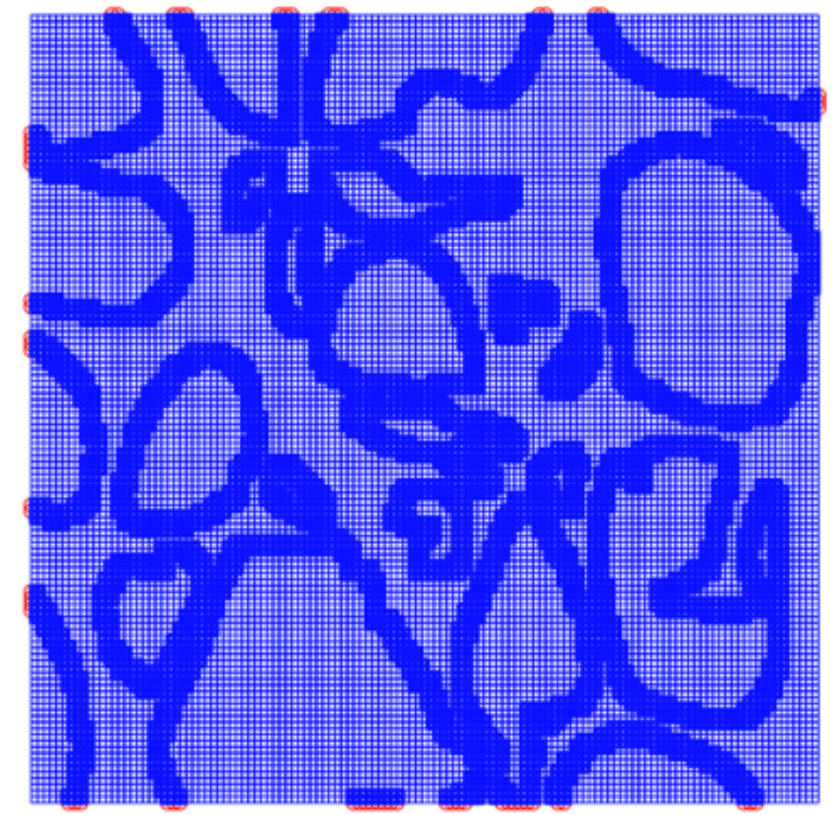
820 000 DOFs

- incorrect volume fraction
- images with high resolution are required
- too large problem size!!!

P. Wriggers

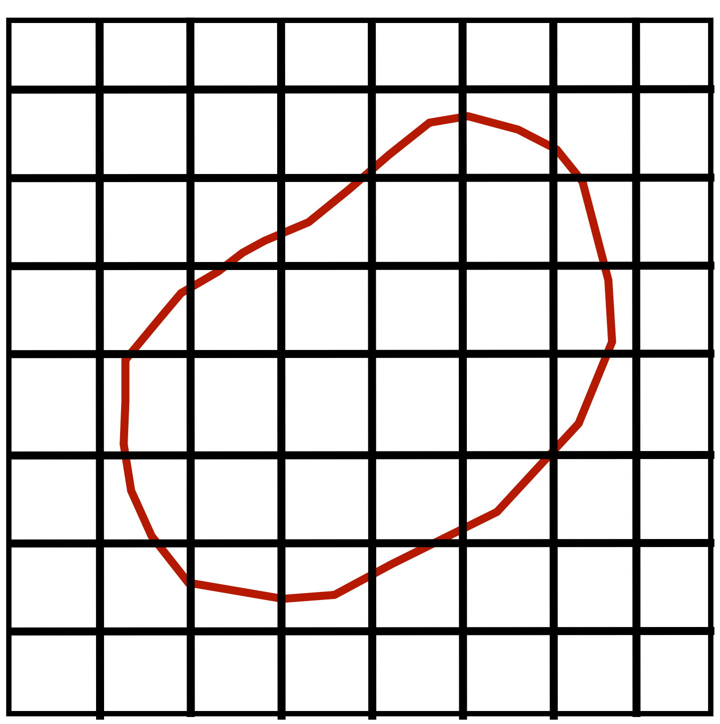
Level set/XFEM

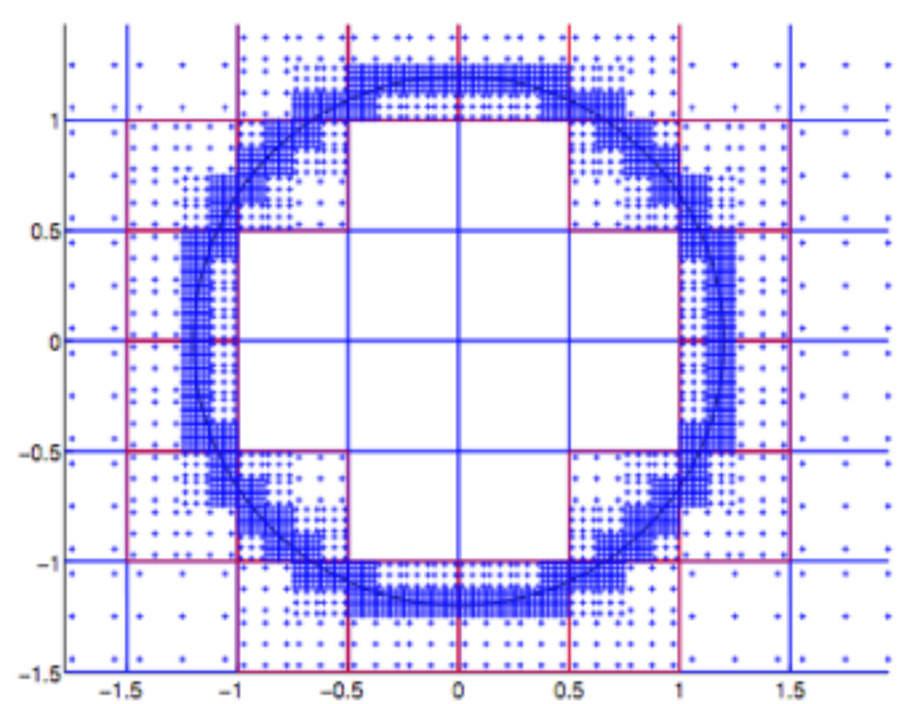


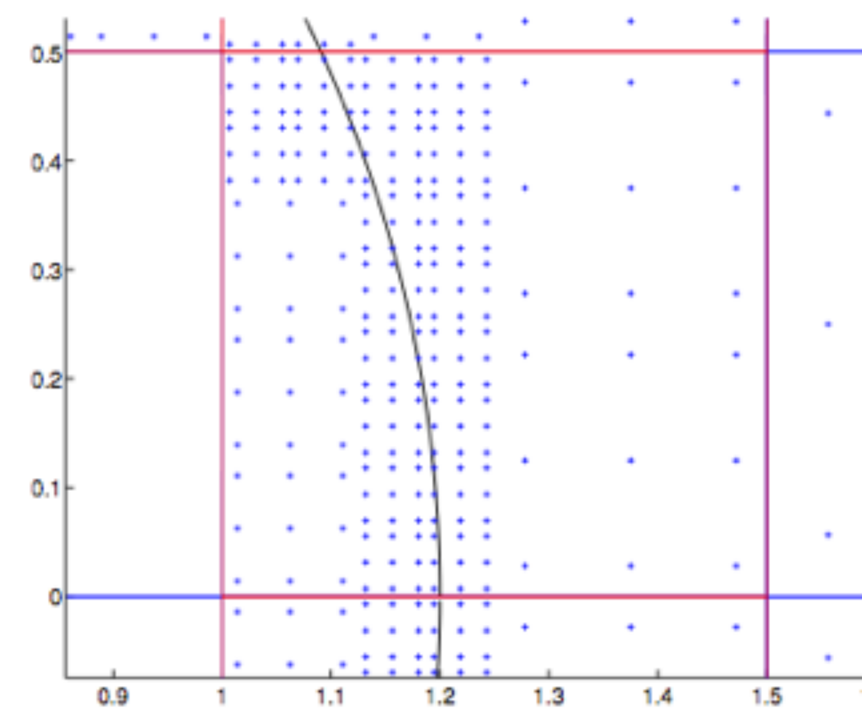


Finite Cell Method (FCM)

(Fictitious Domain Methods)







Tools

Matlab is not enough. Consider Fortran, C++, **Python**.

Move to **Ubuntu Linux** to make your programming life much easier.

- Preprocessing: GMSH, GID, *ANSYS*, *ABAQUS*

- Solvers:

trilinos.sandia.gov

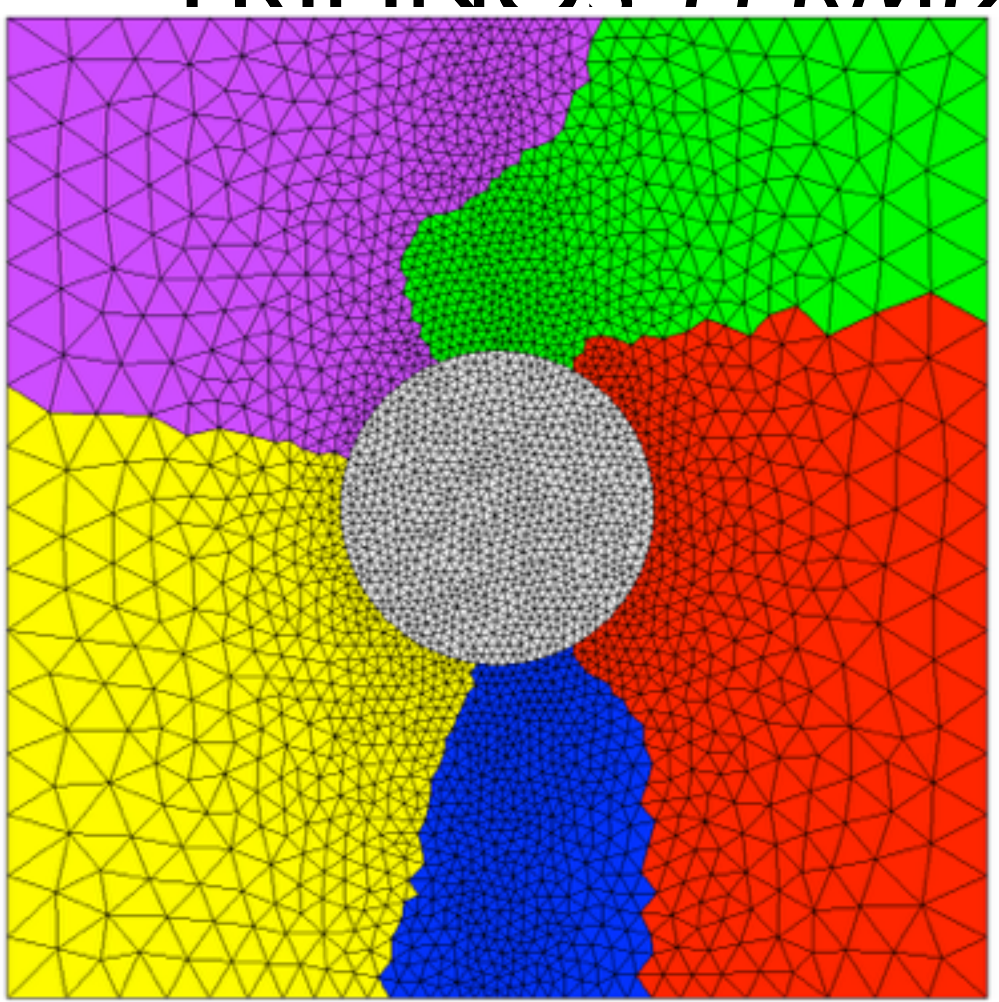
- FEM: FEAP, OOFEM, libMesh, KRATOS, Code Aster, TRILINOS, *PERMIX*, OpenSees (earthquake, structures)

RATOS, YADE…

, KRATOS…

SH, PARAVIEW, *MATLAB*, *TECPLOT*

OpenMPI
ParMETIS



domain decomposition

Prof. S. Bordas

Dr. O. Lloberas Valls

Prof. L.J. Sluys

A. Karamnejad

Dr. E. Lingen

Dr. M. Stroeven

Habanera develops jem/jive C++ library

Thank you for your attention