

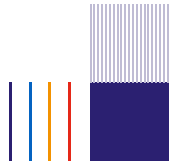


From microstructure to fracture toughness

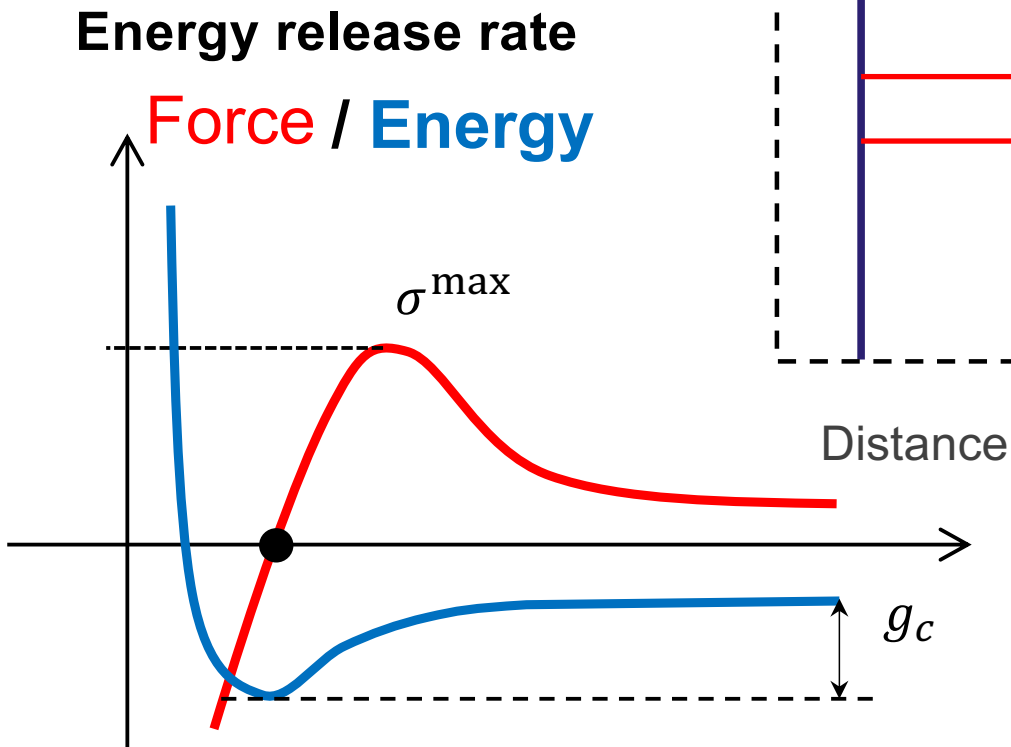
Gergely Molnár

COMPLAS 2023, Barcelona

05/09/2023

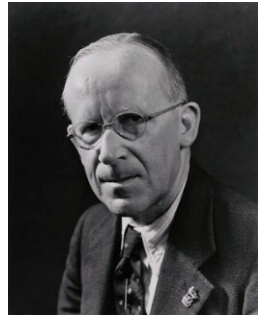
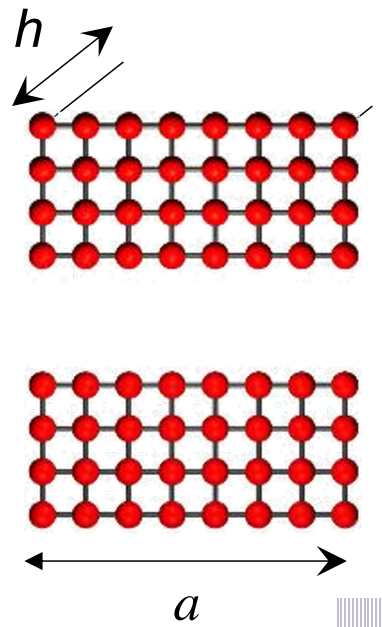
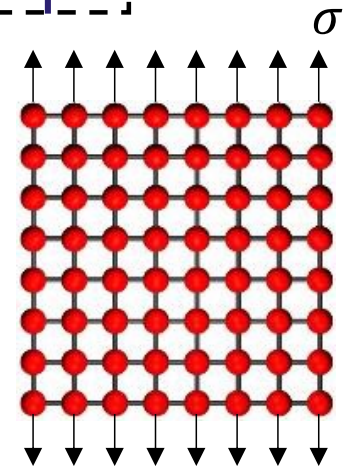
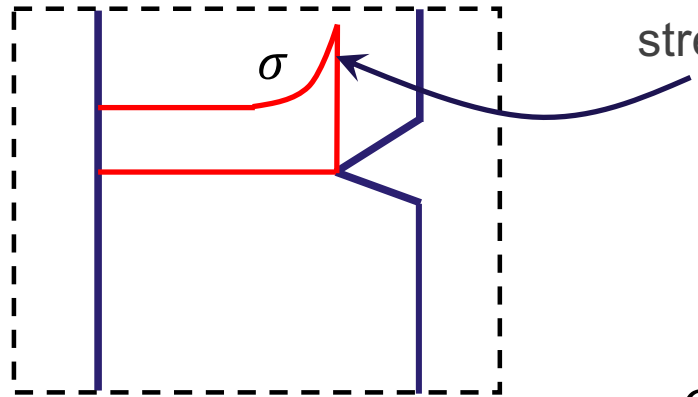


Motivation



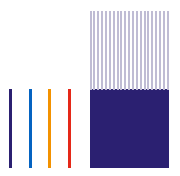
typical interatomic potential

$$S = 2g_c ha$$



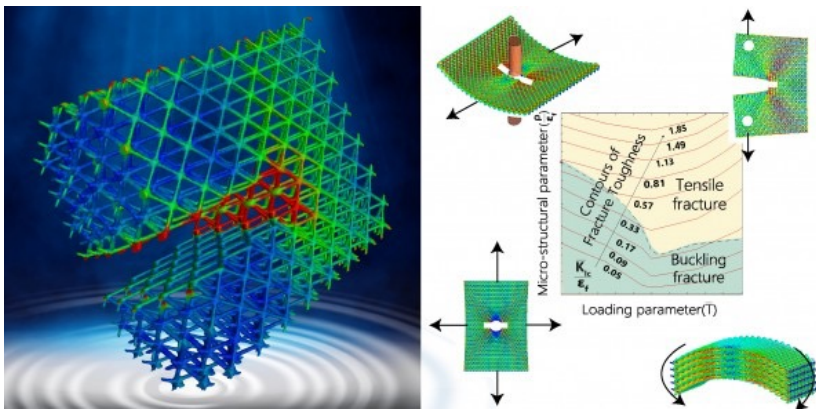
Griffith (1921, 1924)

G. Molnár et al.



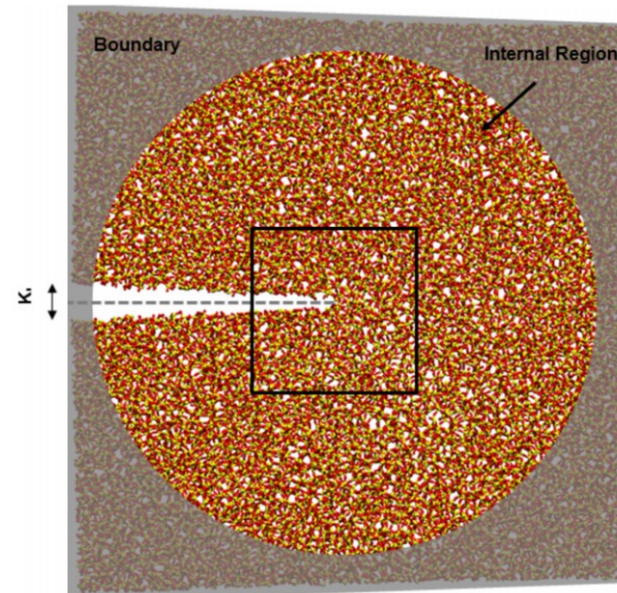
Motivation

Toughness of metamaterials



Shaikkea et al. (2022), Nature Materials

Toughness of amorphous matter



J integral

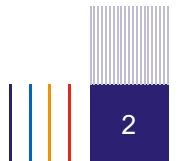
$$J_I = \int_S \left(\Pi_\varepsilon n_x - \mathbf{t} \frac{\partial \mathbf{u}}{\partial x} \right) dS$$

Asymptotic analysis:

$$\tilde{\sigma}_{ij} \equiv \frac{\sigma_{ij}}{\sigma_f} = \bar{K}_I \left[\bar{r}^{-\frac{1}{2}} f_{ij}^I + \bar{T}_{11} \delta_{1i} \delta_{1j} + \bar{T}_{33} \delta_{3i} \delta_{3j} + \bar{T}_{13} \delta_{1i} \delta_{3j} + \mathcal{O}(\bar{r}^{\frac{1}{2}}) + \mathcal{O}(\bar{r}) + \dots \right]$$

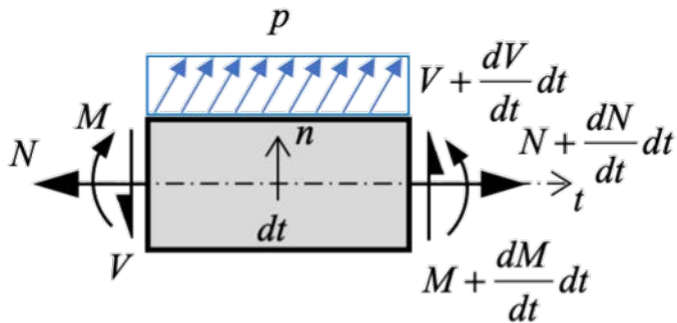
QUESTION:
Can we calculate toughness based on an RVE?

G. Molnár et al.

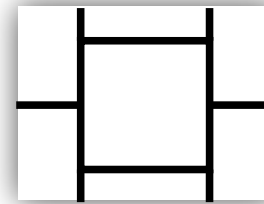


Euler-Bernoulli beams

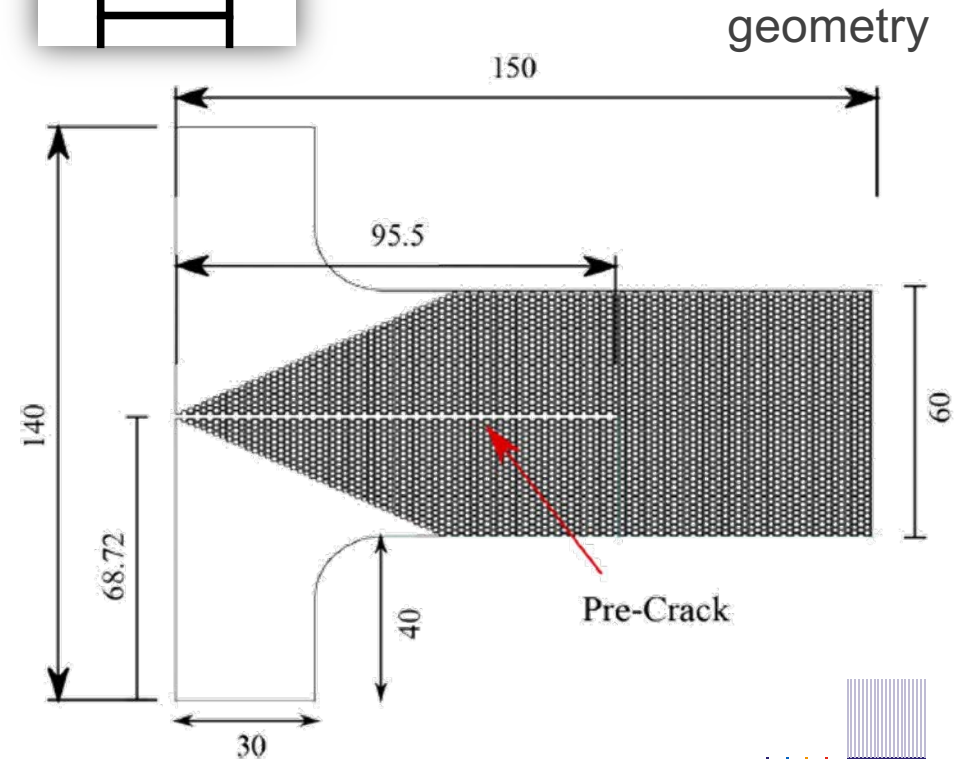
Modelling assumptions



- beams are flawless
- no stress concentration at joints
- $\sigma_t < \sigma_{c,m}$



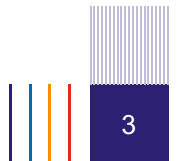
microstructure



geometry

Nguyen et al. (2017)

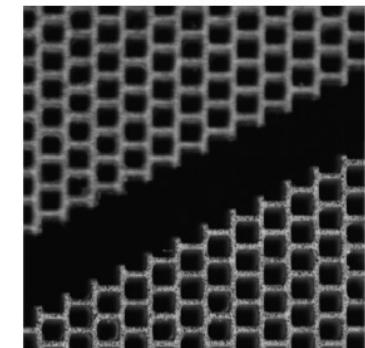
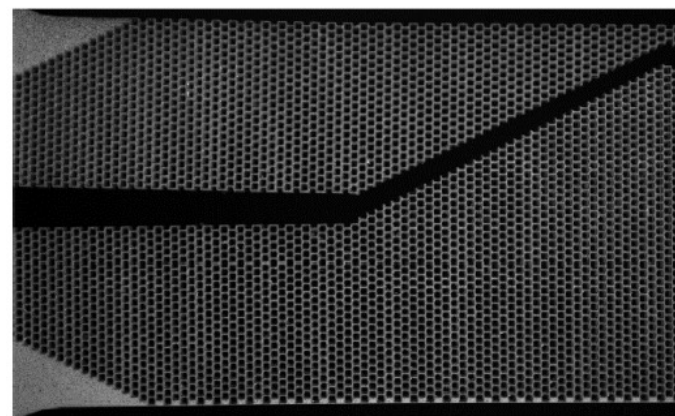
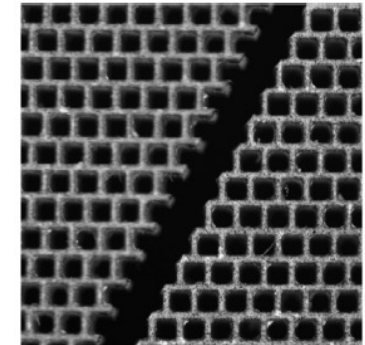
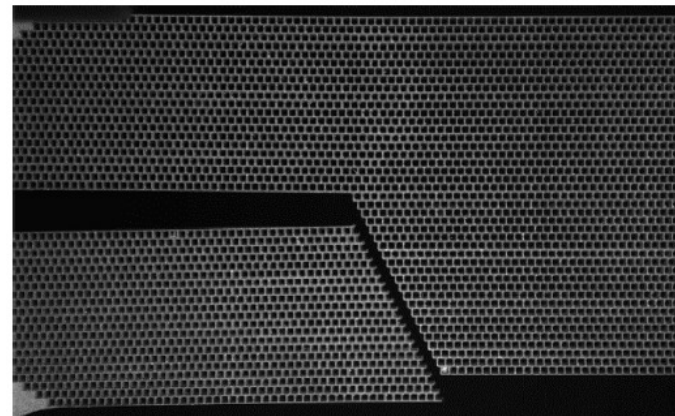
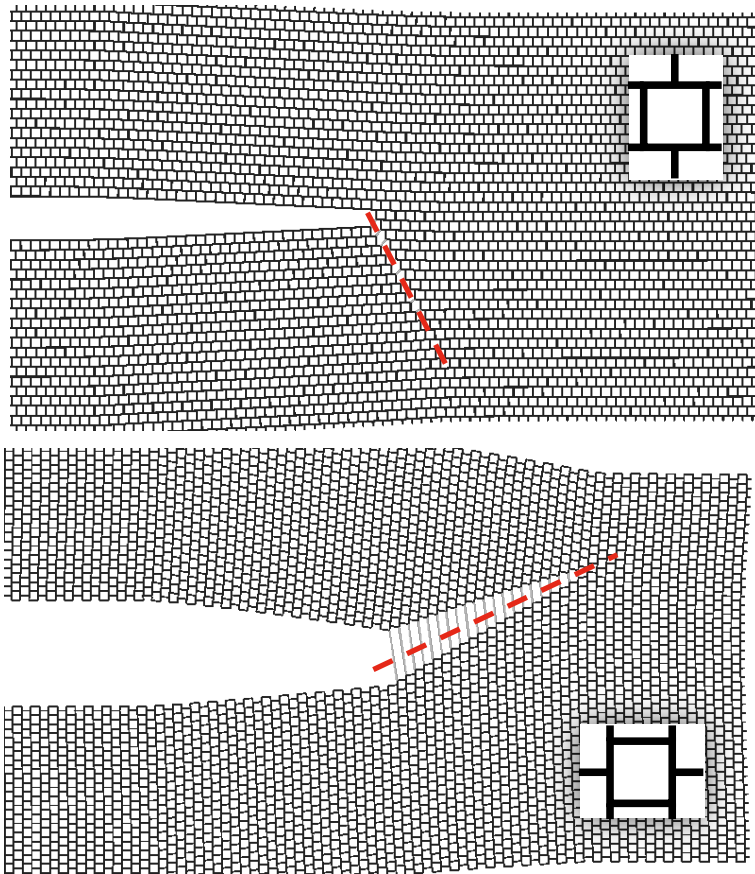
G. Molnár et al.



Nguyen et al. (2017)

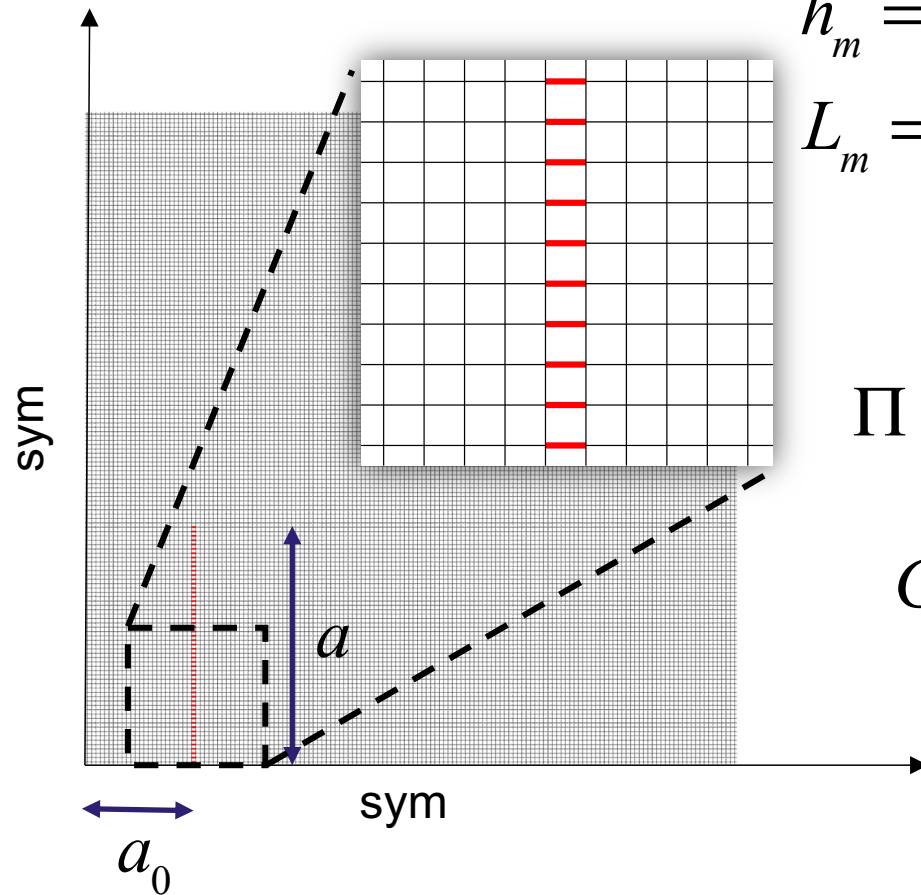
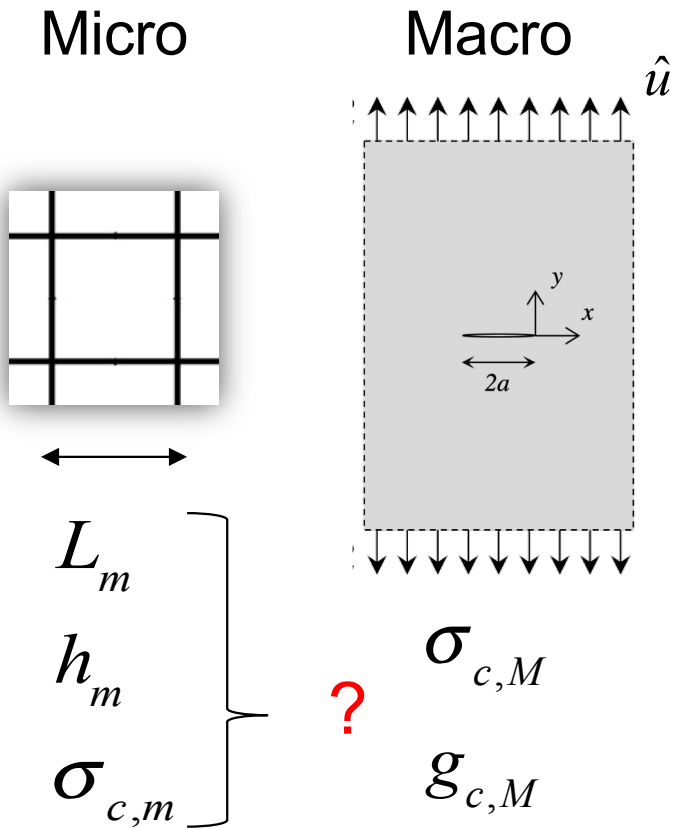
Euler-Bernoulli beams

Beam results



Model

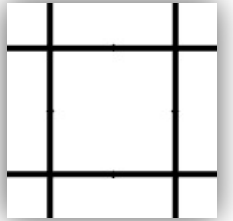
Toughness calculation



microstructure

$$h_m = 0.2$$

$$L_m = 1$$

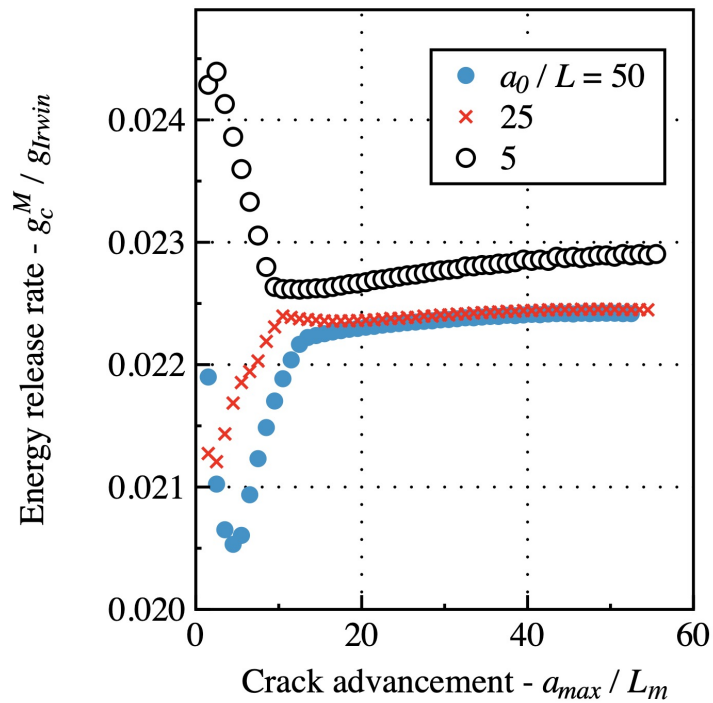


Π potential energy

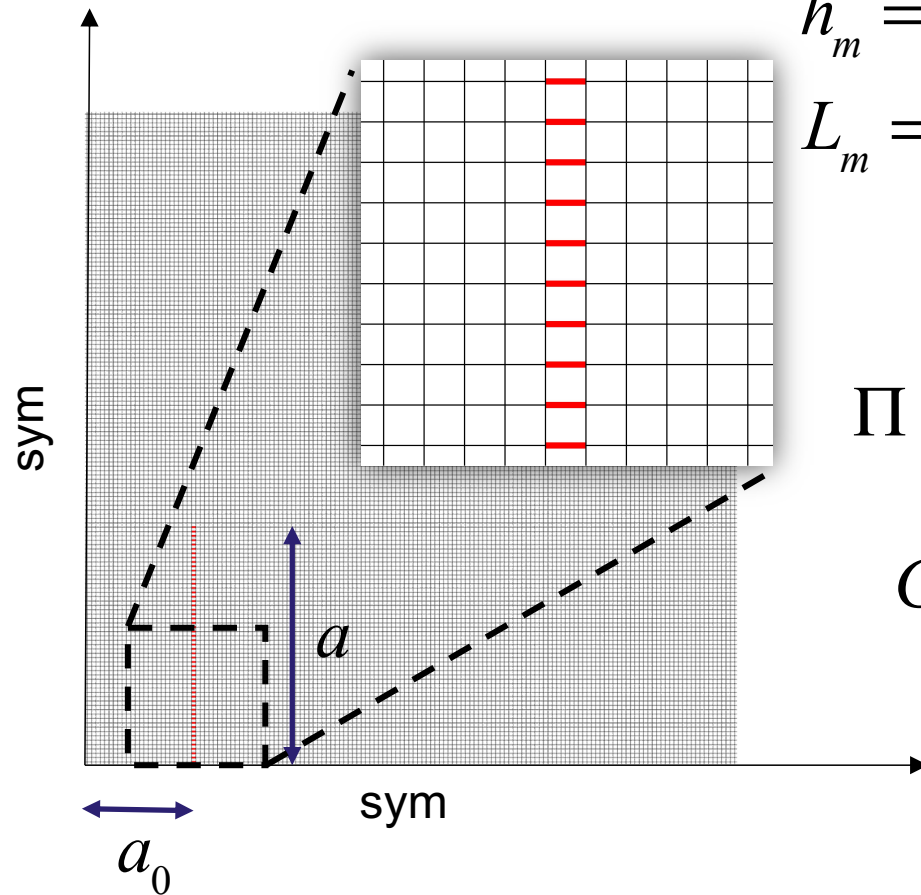
$$G = \frac{d\Pi}{da}$$

Macro-scale results

Toughness calculation



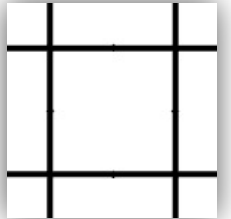
$$g_{Irwin} = \frac{L_m \sigma_{c,m}^2}{E_m}$$



microstructure

$$h_m = 0.2$$

$$L_m = 1$$



Π potential energy

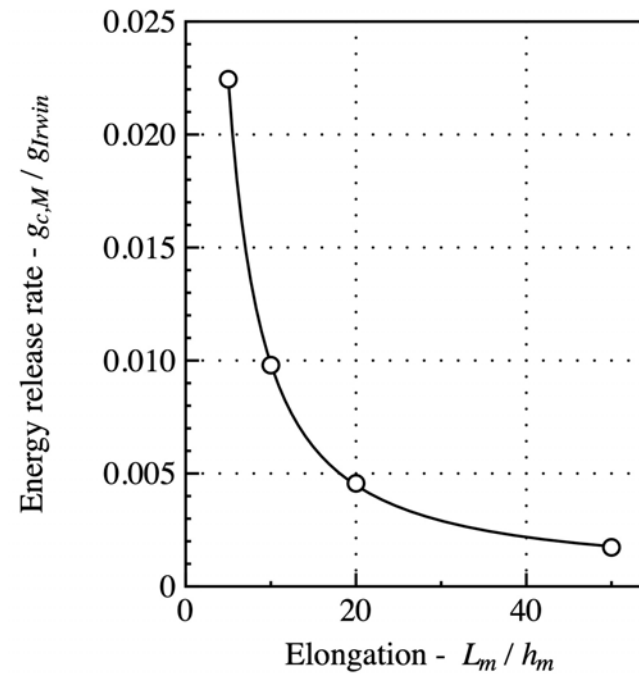
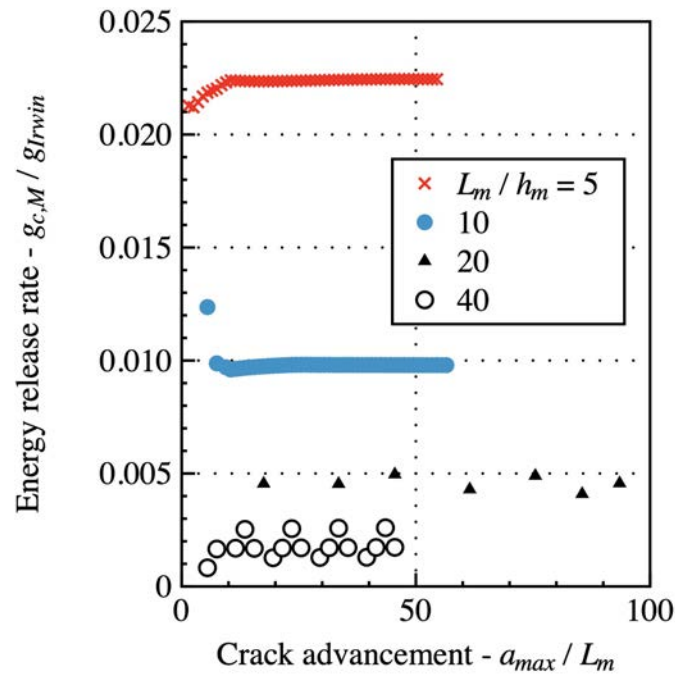
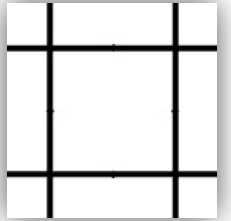
$$G = \frac{d\Pi}{da}$$

Macro-scale results

microstructure

Effect of elongation

$$a_0 / L_m = 25$$



Macro-scale results

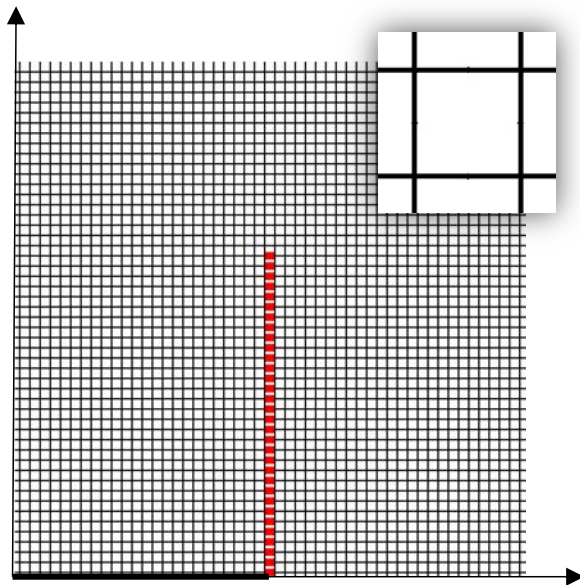
Effect of structure type



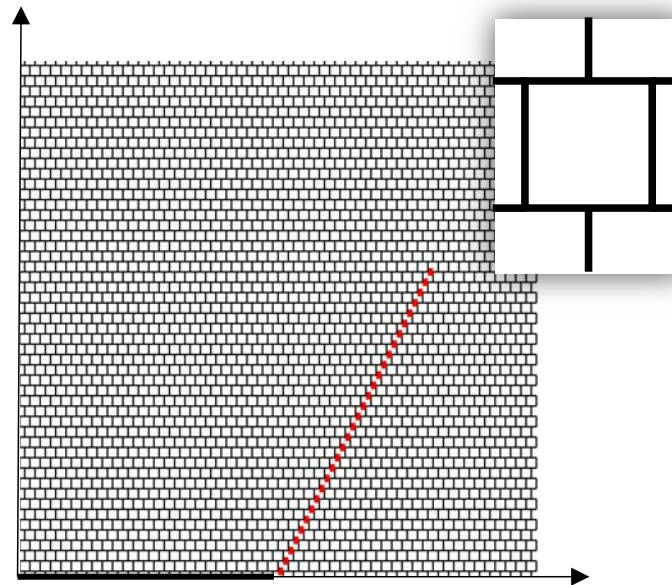
$$h_m = 0.1$$

$$a_0/L_m = 25 \quad L_m = 1$$

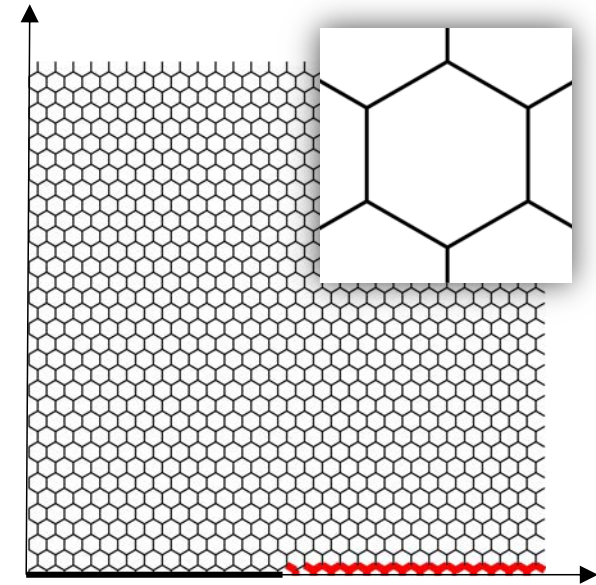
Square grid



Shifted square grid



Honeycomb grid

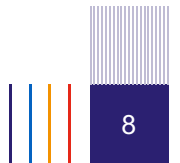


$$\frac{g_{c,M}}{g_{Irwin}} = 0.010$$

0.029

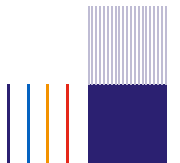
0.033

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Question

Can we calculate the fracture toughness based on the unit cell?

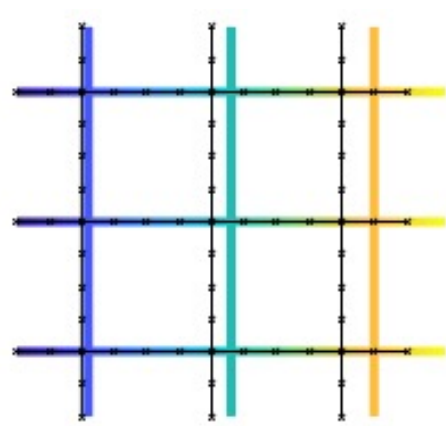


Continuum model

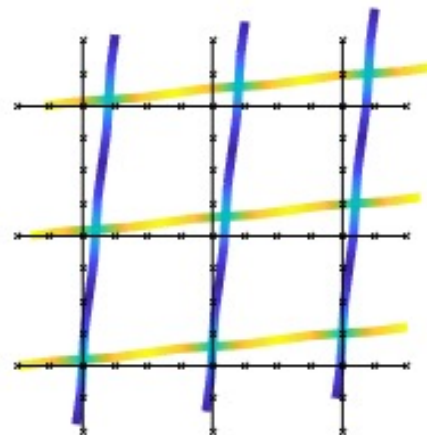
Phase-field theory + Cosserat continuum

Elastic energy $\Pi(\mathbf{u}, \phi, \mathbf{d}) = \int_{\Omega} g(\mathbf{d}) \psi(\varepsilon(\mathbf{u}, \phi)) d\Omega + W(\mathbf{d}, \nabla \mathbf{d})$

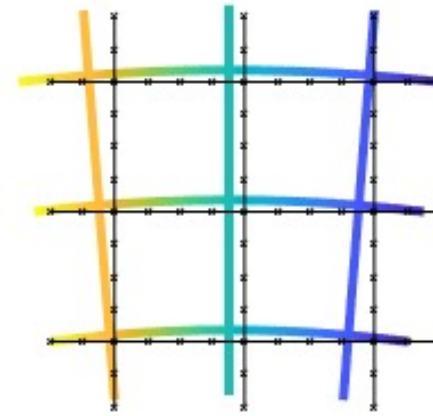
Deformations



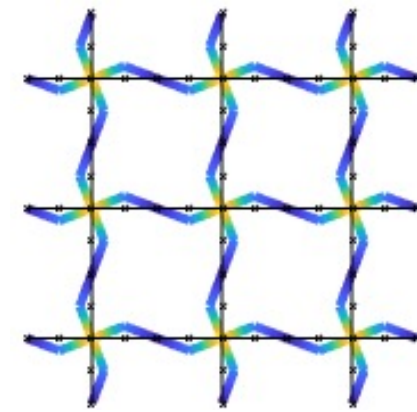
extension



shear



curvature



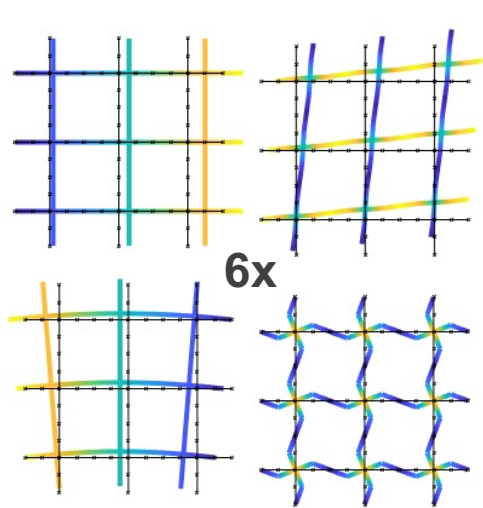
uniform rotation of joints

(Cosserat & Cosserat, 1909)

Parameter identification

Computational homogenization (elasticity)

Beam model



+
PBC

$$\left. \begin{array}{l} \sigma_M \\ \mathbf{m}_M \\ {}^3\mathbf{Q}_M \end{array} \right\}$$

36x

$$\begin{bmatrix} \sigma_{M,j} \\ \mathbf{m}_{M,j} \\ {}^3\mathbf{Q}_{M,j} \\ \dots \end{bmatrix}$$

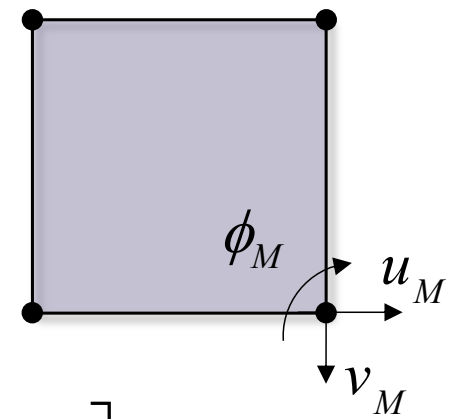
$$= \begin{bmatrix} \varepsilon_{x,j} & \varepsilon_{y,j} & \dots \\ 0 & 0 & 0 \\ \dots & \dots & \dots \end{bmatrix}$$

21x

$$\begin{bmatrix} C_{11} \\ C_{12} \\ \dots \end{bmatrix}$$

21x

Cosserat continuum



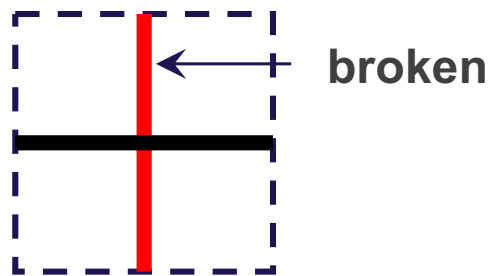
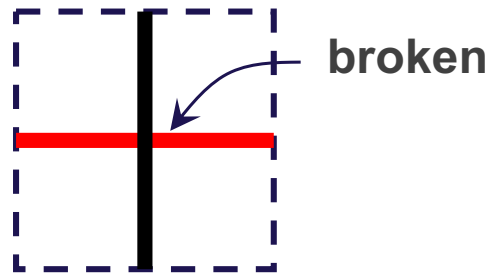
G. Molnár et al.

V. Kouznetsova et al. (2002)
S Liebenstein et al. (2018)

Parameter identification

Asymmetric elastic energy degradation

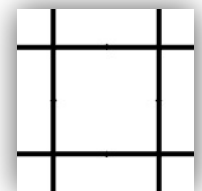
Beam model



$$\underline{\underline{C}}(d_1 = 1) = \begin{bmatrix} 0 & & & & & \\ & C_{22} & & & & \\ & & C_{33} & & & \\ & & & 0 & & \\ & \text{sym.} & & & 0 & \\ & & & & & C_{66} \end{bmatrix}$$

$$\underline{\underline{C}}(d_2 = 1) = \begin{bmatrix} C_{11} & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & C_{44} & & \\ & \text{sym.} & & & C_{55} & \\ & & & & & 0 \end{bmatrix}$$

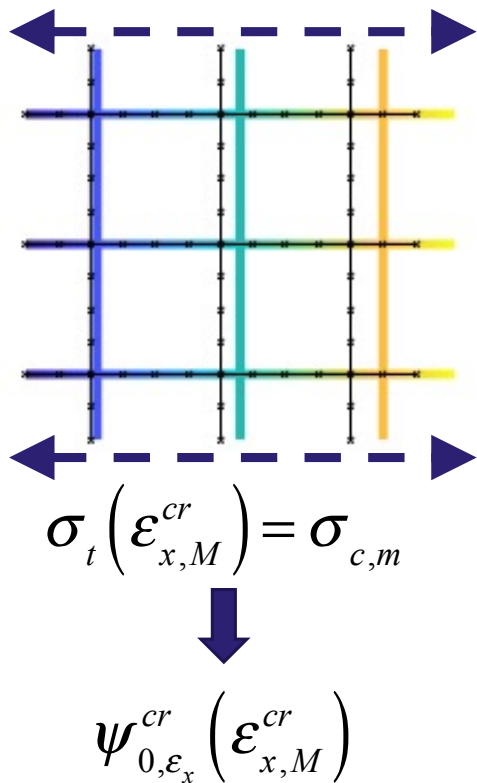
Cosserat continuum



Parameter identification

Localization coefficients (γ_{ij})

Beam model



Cosserat continuum

Homogeneous phase-field solution (AT1)

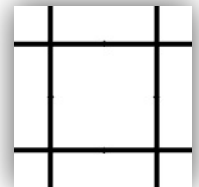
$$\frac{\partial \Pi}{\partial d_i} = \frac{\partial \Psi(\mathbf{u}, \phi, \mathbf{g}_{ij}(d_i))}{\partial d_i} + \frac{3g_{c,M,i}}{8l_{c,M,i}} = 0$$

$$\sigma_M^{\max} \rightarrow d = 0$$

$$\frac{\partial g(d=0, \gamma)}{\partial d} = -(1 + \gamma)$$

$$(1 + \gamma_{ij}) \psi_{0,j}^{cr} = \frac{3g_{c,M,i}}{8l_{c,M,i}}$$

microstructure

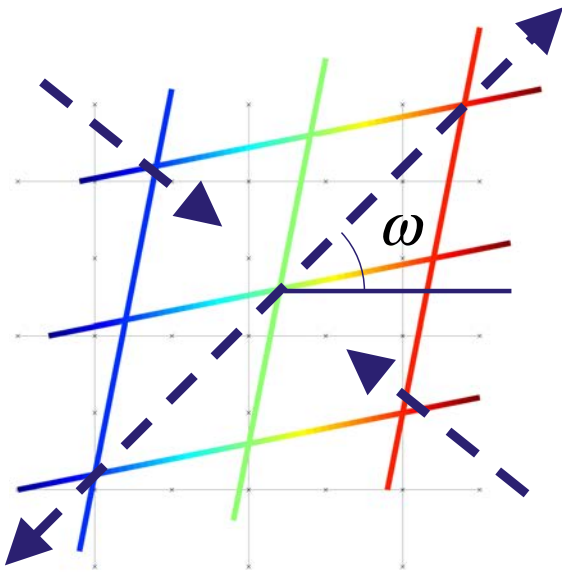


$$\gamma_{ij} = \begin{bmatrix} 0 & 0 & 0 & 8 & 2 & 0 \\ 0 & 0 & 8 & 0 & 0 & 2 \end{bmatrix}$$

Parameter identification

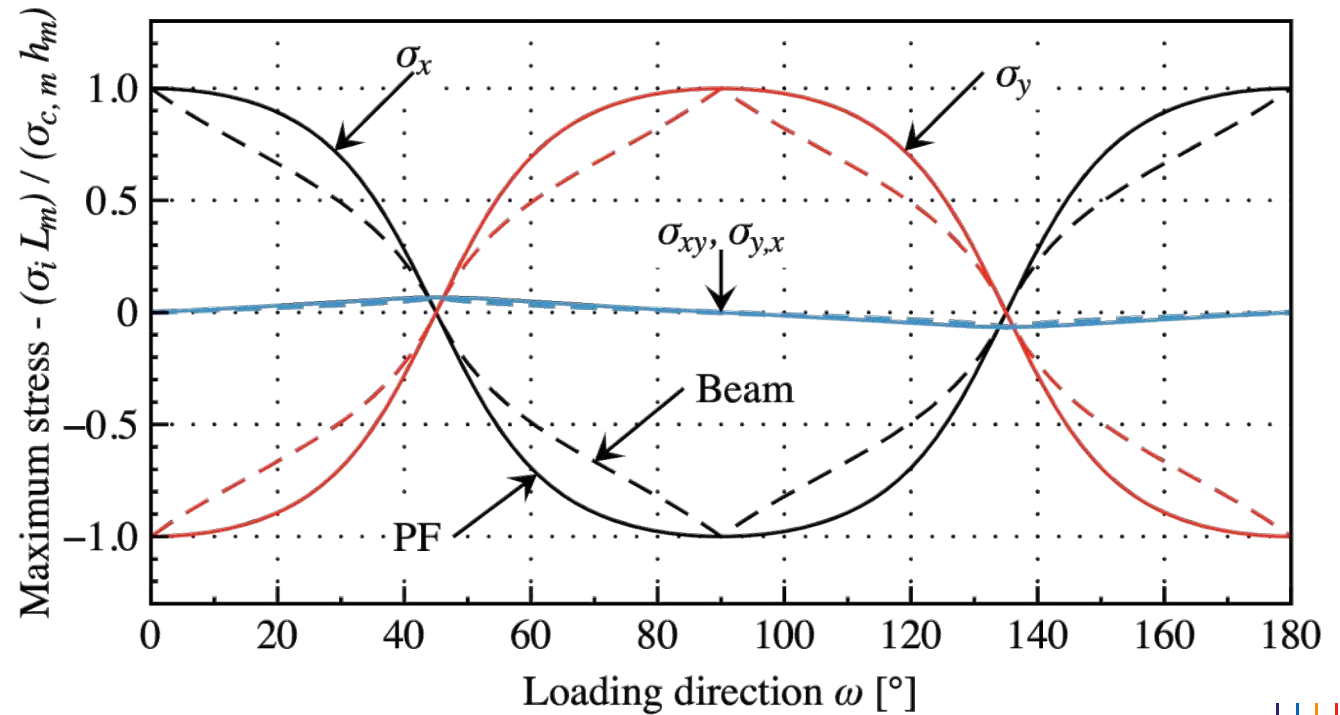
Localization coefficients (γ_{ij})

Beam model



Cosserat continuum

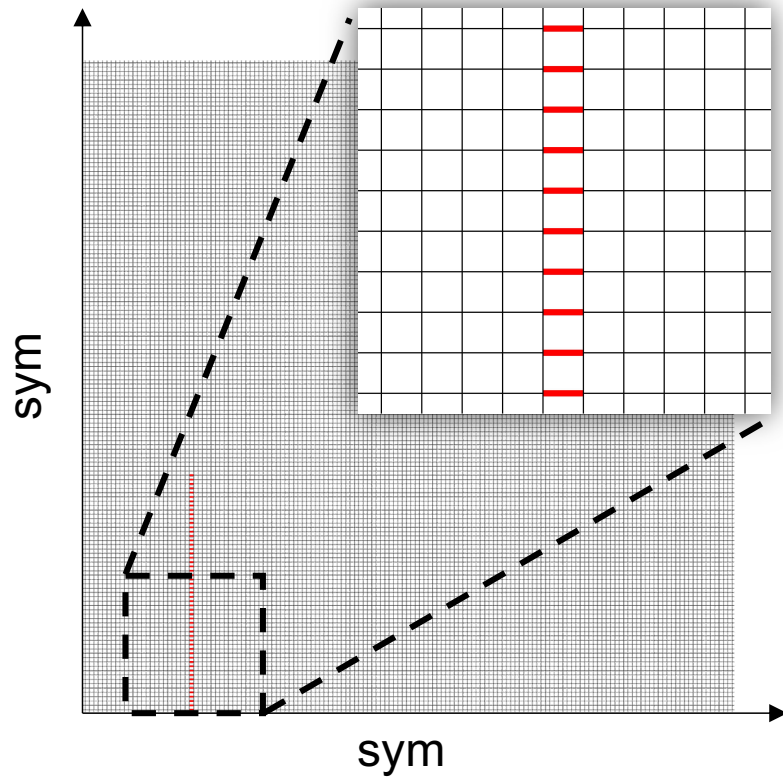
Homogeneous phase-field solution (AT1)



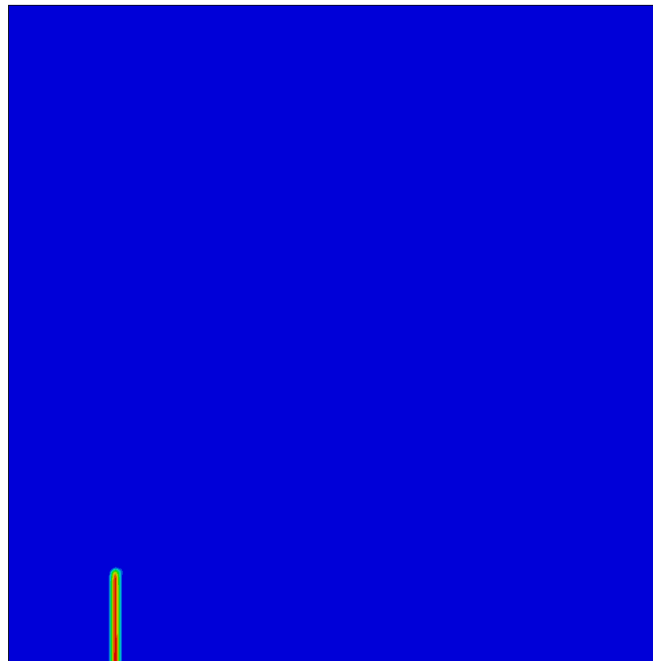
Macro-scale phase-field results

Square grid in tension (Mode I)

Beam model



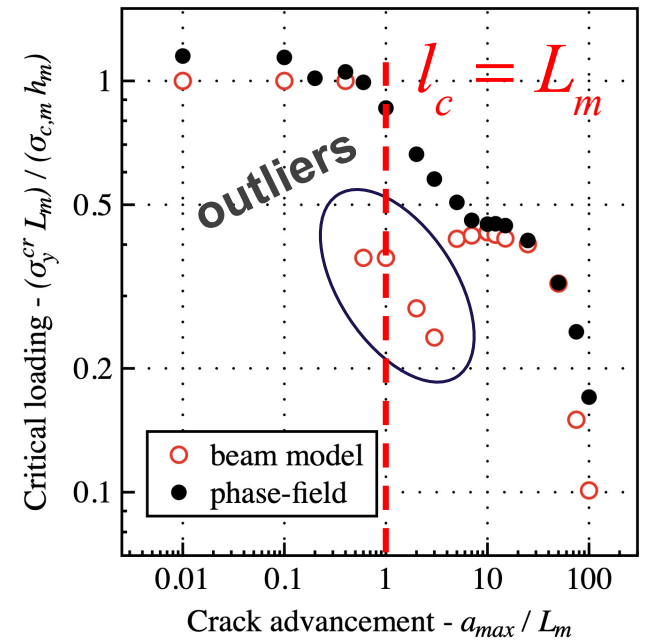
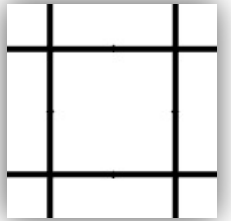
Phase-field



microstructure

$$h_m = 0.2$$

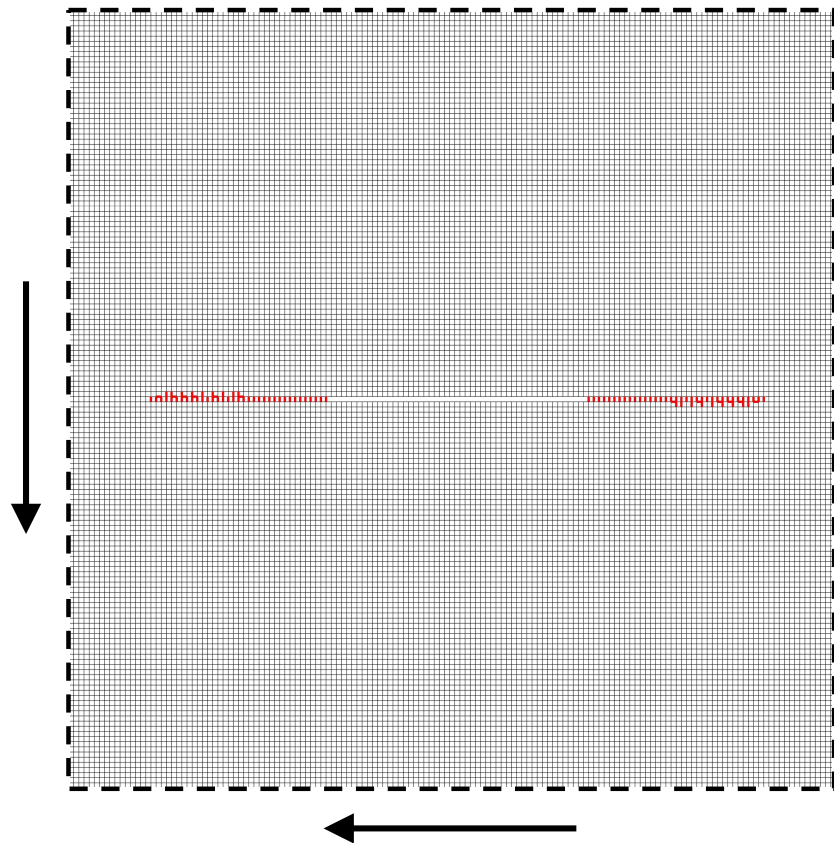
$$L_m = 1$$



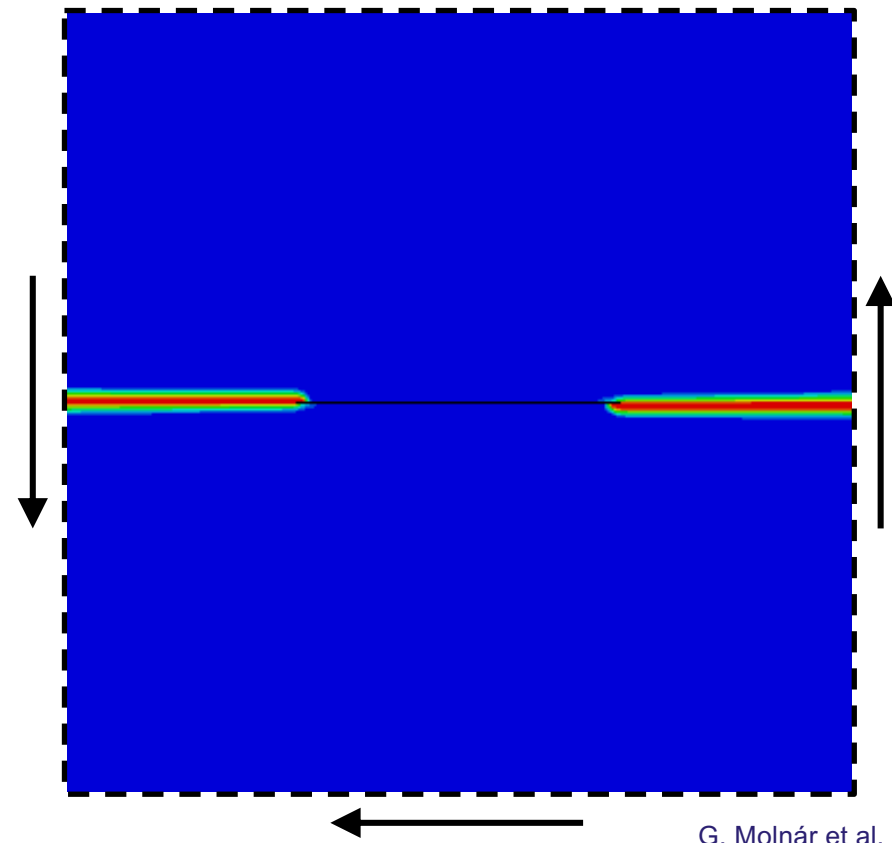
Macro-scale phase-field results

Square grid in shear (Mode II)

Beam model



Phase-field



Conclusion / Perspectives

Fracture in periodic beam lattices

- **Toughness** depends on:
 - micro-strength
 - cross section / elongation
 - structure type
- **Homogenization**
 - Cosserat continuum
 - Multiple damage variables
 - Anisotropic phase-field



Other lattice types, 3D, etc...

