Optimisation topologique des microstructures pour maximiser la résistance à la rupture des composites bi-phasique

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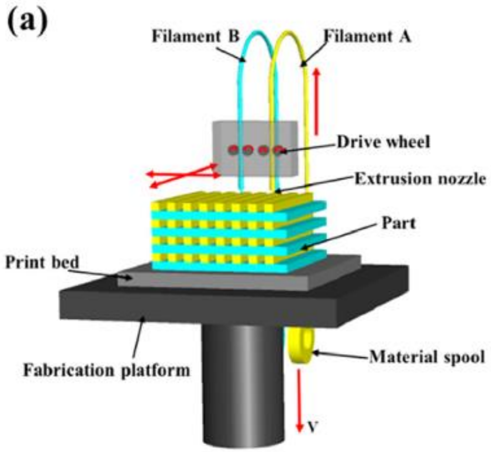
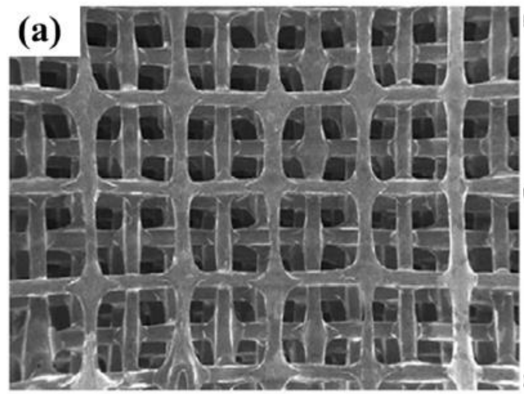
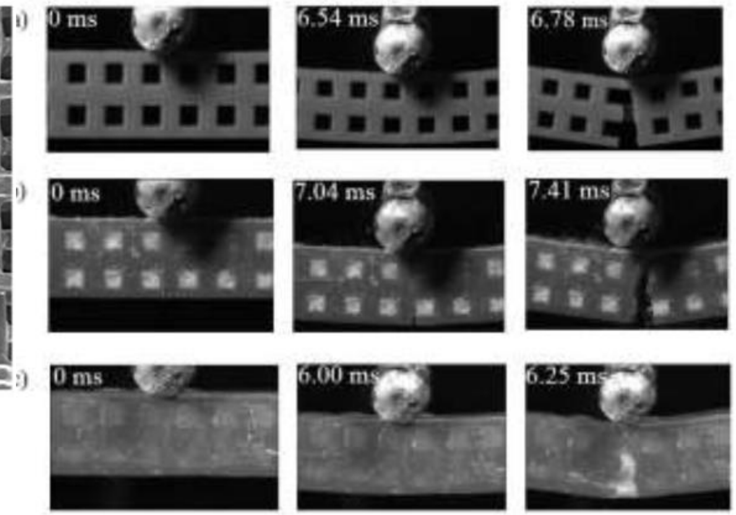
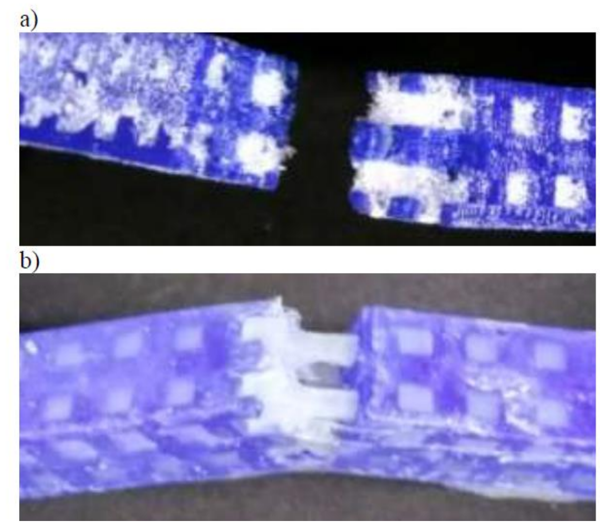
Motivations and context: new opportunities of 3D printing for designing materials with improved fracture resistance



Bi-materials 3D printing [Wang et al. Compos. Part B 2017]

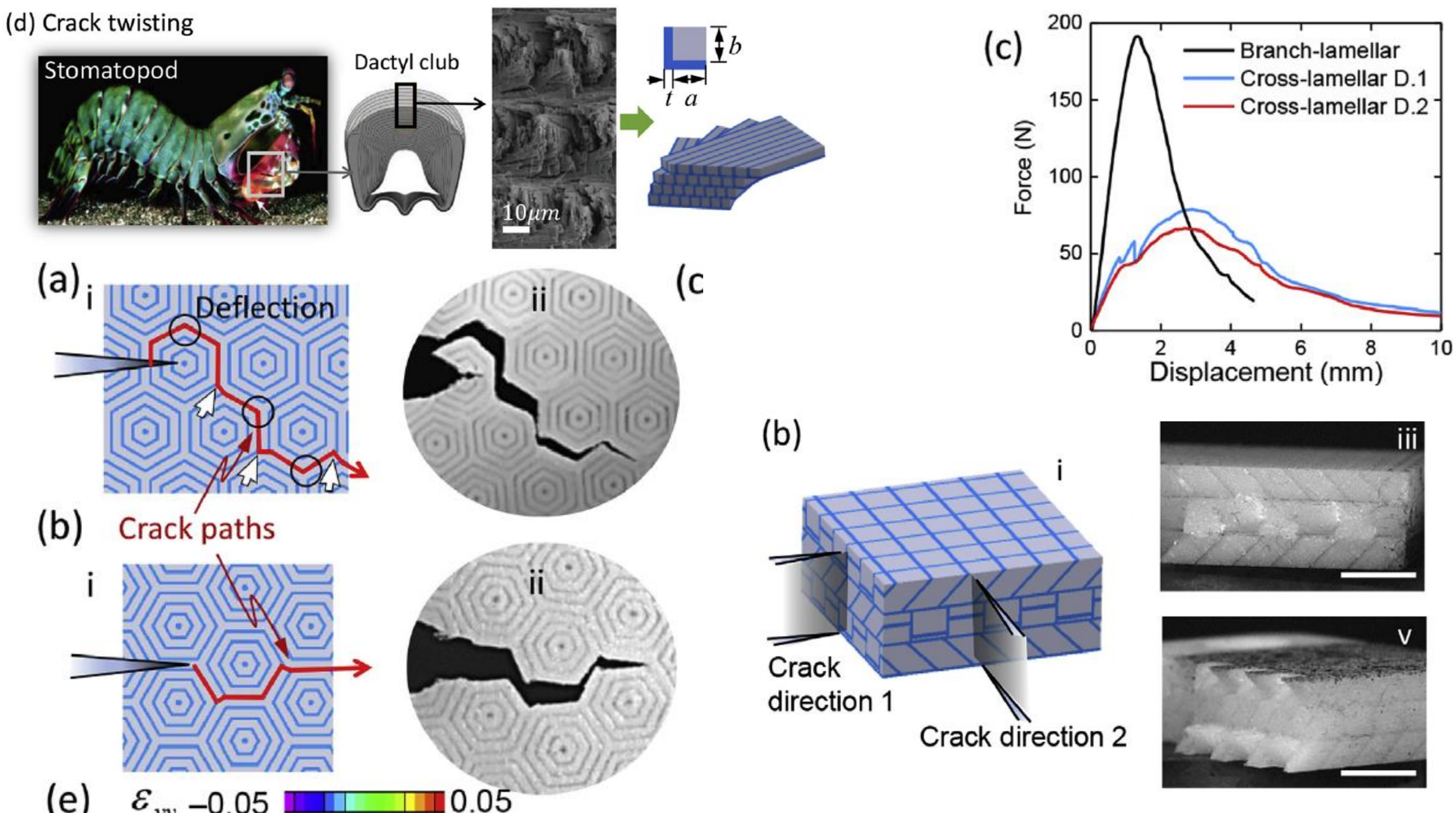






Fracture in 3D printed bi-materials [Kao et al. Proc. ASME MSEC 2016]

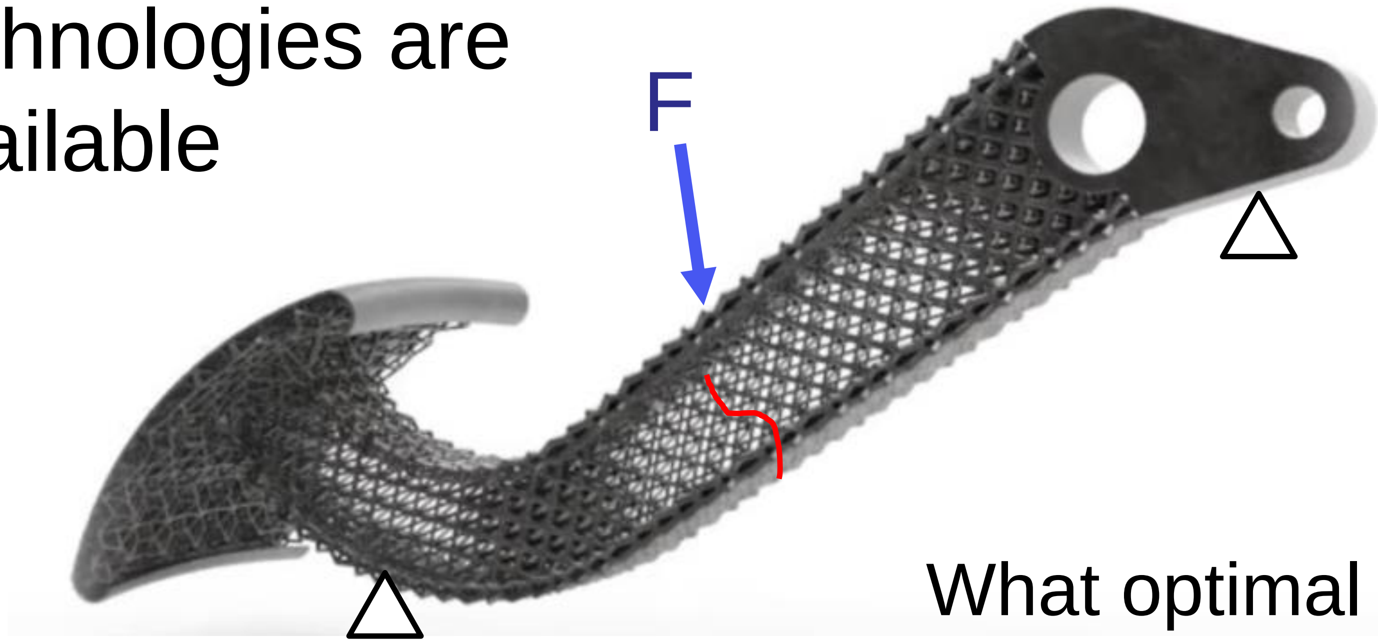
Motivations and context: new opportunities of 3D printing for designing materials with improved fracture resistance



Bio-inspired 3D printed materials [Jia and Wand Act. Mater. 2019]

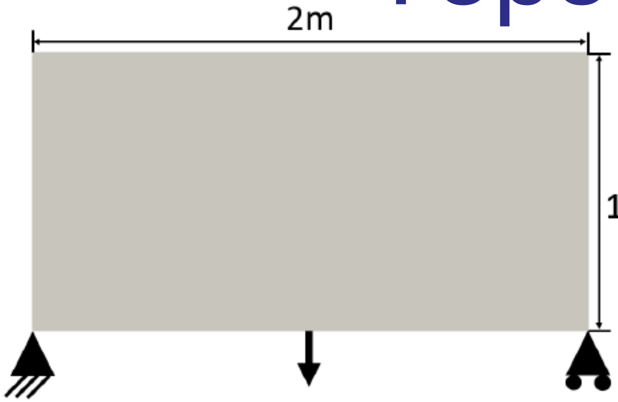
Motivations and context: new opportunities of 3D printing for designing materials with improved fracture resistance

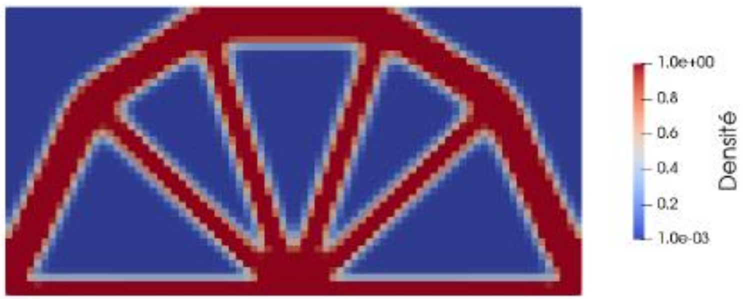
3D printing technologies are available

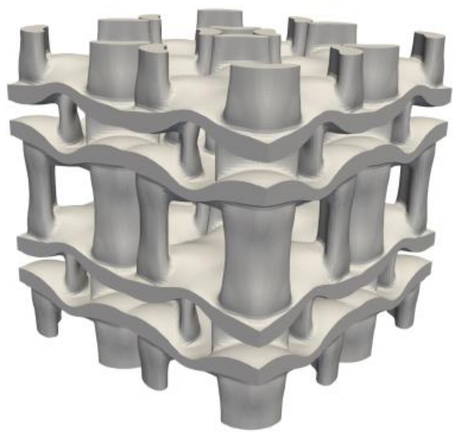


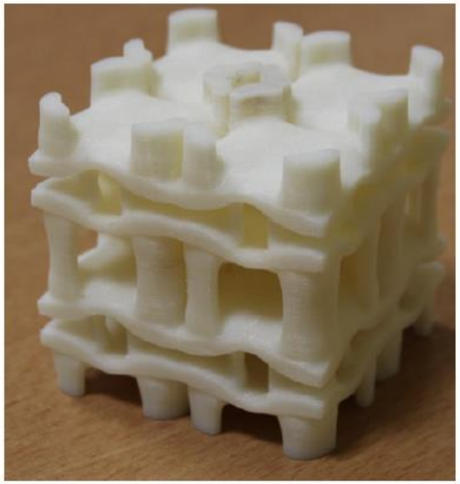
What optimal microstructural geometry?

Topology optimization









Targetting Effective properties with given volume fraction [Djourakovitch, 2020]

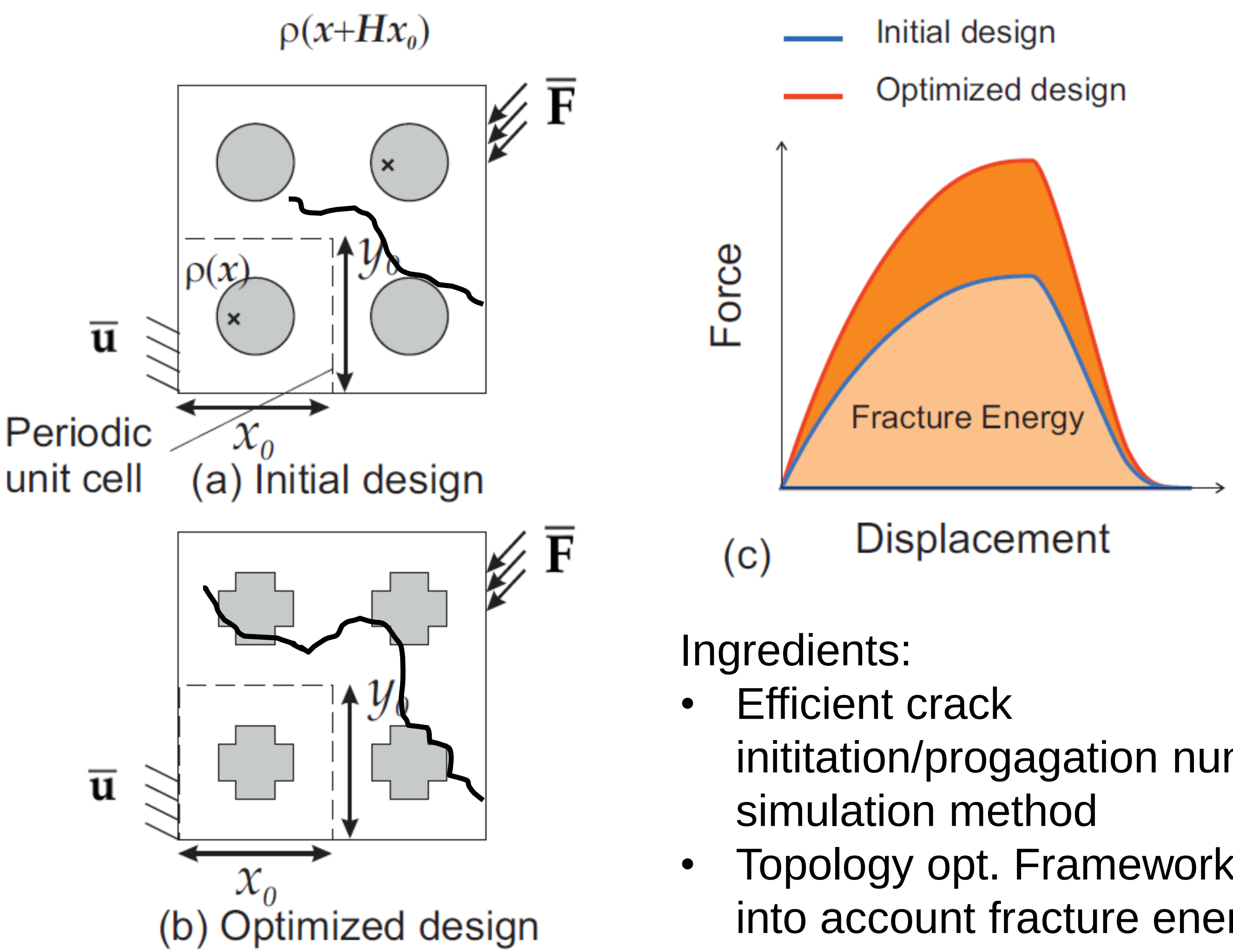
Maximizing the stiffness with respect to weight

$$\min_{\rho_e} \quad J(\rho_e), \quad 1 \leq e \leq N_e$$
$$t.q.$$
$$\mathbf{K}\boldsymbol{u} = \boldsymbol{F}$$
$$0.001 \leq \rho_e \leq 1$$
$$\sum_e \rho_e < V_{max}$$

$$\max_{\Omega} \quad J(\Omega, \boldsymbol{u}) = \sum_{ijkl} \eta_{ijkl} C^H_{ijkl} + \sum_{ij} \lambda_{ij} \alpha^H_{ij}$$
$$t.q.$$
$$\mathbf{K}\boldsymbol{u}^{ij} = \boldsymbol{f}^{ij}$$
$$\mathbf{K}\chi^{\alpha} = \boldsymbol{f}^{\alpha}$$

SIMP [Bendsoe, Sigmund 99], **Level-set** [Allaire et al. 04], **ESO** [Xie & Steven 93]

Topology optimization for fracture resistance of bi-materials structures



Ingredients:

- Efficient crack inititation/progagation numerical simulation method
- Topology opt. Framework taking into account fracture energy
- Interfacial damage

Variational approach to fracture/phase field method

[Francfort and Marigo, JMPS 1998], [Bourdin et al. JMPS 2000] [Mumford and Shah, CPAM 1989] [Kuhn and Müller 2010] [Miehe et al. 2010]

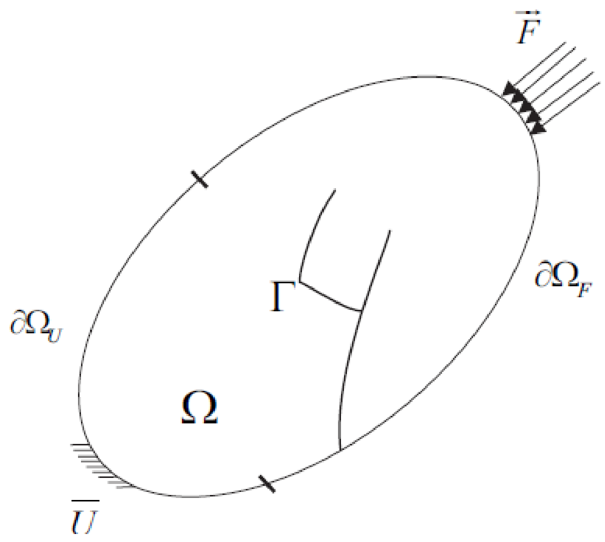
Variational principle for fracture [Francfort and Marigo 1998]

$$E = \int_{\Omega} \Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), \Gamma\right) + \int_{\Gamma} G_c dS$$

Griffith energy functional

$$\mathbf{u}^{n+1}, \Gamma^{n+1} = \underset{\substack{\mathbf{u} \in \mathcal{K}_A \\ \Gamma^n \leq \Gamma^{n+1}}}{\text{Argmin}} \quad E$$

Free-discontinuity problem **[Ambrosio et al. 2000]**



Sharp description of interfaces

Continuous description of cracks: variational principle to damage

$$E = \int_{\Omega} \Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) d\Omega + \int_{\Omega} \omega\left(d\right) dS$$

$$E = \int_{\Omega} \left[\Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) + \omega\left(d\right)\right] d\Omega$$

$$\mathbf{u}^{n+1}, d^{n+1} = \underset{\substack{\mathbf{u}\in\mathcal{K}_A \\ 0\leq d^n \leq d^{n+1} \leq 1}}{\text{Argmin}} \quad E$$

Continuous description of cracks: variational principle to damage

Mechanical problem

$$D_{\delta \mathbf{u}} E = 0$$ Weak form $$\int_{\Omega} \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} \left(\boldsymbol{\varepsilon} \left(\mathbf{u} \right), d \right) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) d\Omega = 0$$

$$\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} \left(\boldsymbol{\varepsilon} \left(\mathbf{u} \right), d \right)$$

Strong form (Euler-Lagrange equations)

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma} \mathbf{n} = \overline{F} \text{ on } \partial\Omega_F, \quad \mathbf{u} = \overline{\mathbf{u}} \text{ on } \partial\Omega_u$$

Phase field problem

$$D_{\delta d} E = 0, \ \dot{d} \geq 0$$ Weak form $$\int_{\Omega} \left[\frac{\partial \Psi}{\partial d} \left(\boldsymbol{\varepsilon} \left(\mathbf{u} \right), d \right) + \frac{\partial \omega \left(d \right)}{\partial d} \right] \delta d d\Omega = 0$$

Strong form (Euler-Lagrange equations)

$$\frac{\partial \Psi}{\partial d} \left(\boldsymbol{\varepsilon} \left(\mathbf{u} \right), d \right) + \frac{\partial \omega \left(d \right)}{\partial d} = 0, \quad \nabla d \cdot \mathbf{n} = 0 \text{ on } \partial\Omega_Q, \quad d = 1 \text{ on } \partial\Omega_d$$

Local relationship → Lack of convergence, mesh-dependency issues

Continuous description of cracks with regularization by gradient of damage [Ambrosio and Tortorelli 1992, Bourdin et al. 2000]

$$E = \int_\Omega \left[\Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) + \omega\left(d\right) + \underbrace{\frac{c_1 \ell^2}{2} \nabla d \cdot \nabla d}_{\text{Regularization term}} \right] d\Omega$$

Phase field problem $D_{\delta d} E = 0, \;\; \dot{d} \geq 0$ Regularization term

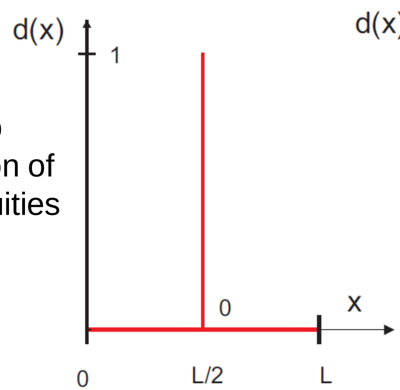
Weak form

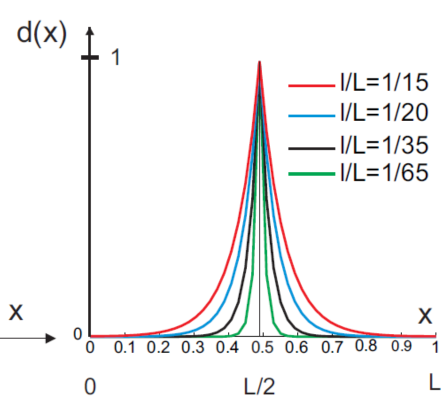
$$\int_\Omega \left[\frac{\partial \Psi}{\partial d}\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) + \frac{\partial \omega\left(d\right)}{\partial d} \right] \delta d + \frac{c_1 \ell^2}{2} \nabla d \cdot \nabla \delta d d\Omega = 0$$

Strong form (Euler-Lagrange equations)

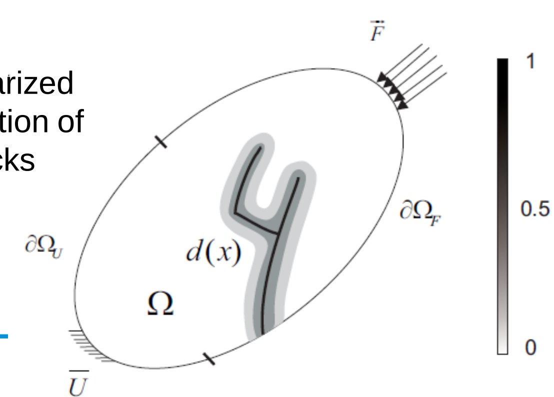
$$\frac{\partial \Psi}{\partial d}\left(\varepsilon\left(\mathbf{u}\right), d\right) + \frac{\partial \omega\left(d\right)}{\partial d} - c_1 \ell^2 \Delta d = 0, \;\; \nabla d \cdot \mathbf{n} = 0 \text{ on } \partial\Omega_Q, \;\; d = 1 \text{ on } \partial\Omega_d$$

Sharp description of discontinuities





Regularized description of cracks



Example [Miehe et al. 2010]

$$\omega(d) = \frac{G_c}{2\ell} d^2 \qquad c_1 = \frac{G_c}{\ell}$$

$$\Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\right) = \left(\left(1-d\right)^2 + k\right)\Psi^+\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\right) + \Psi^-\left(\varepsilon\left(\mathbf{u}\right)\right)$$

$$\Psi^{\pm}(\boldsymbol{\varepsilon}\left(\mathbf{u}\right)) = \frac{\lambda}{2}\left(\langle Tr(\boldsymbol{\varepsilon}\left(\mathbf{u}\right))\rangle_{\pm}\right)^2 + \mu Tr\left\{\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right)^{\pm}\right)^2\right\}$$

Other possible choices **[Amor et al. 2009], [Borden, Hughes 2014], [He and Shao 2019]…**

Example [Miehe et al. 2010]

Mechanical problem

$$D_{\delta \mathbf{u}} E = 0$$ Weak form $$\int_\Omega \boldsymbol{\sigma}\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) d\Omega = 0$$

Strong form (Euler-Lagrange equations)

$$\nabla \cdot \boldsymbol{\sigma} = 0, \quad \boldsymbol{\sigma}\mathbf{n} = \overline{F} \text{ on } \partial\Omega_F, \quad \mathbf{u} = \overline{\mathbf{u}} \text{ on } \partial\Omega_u$$

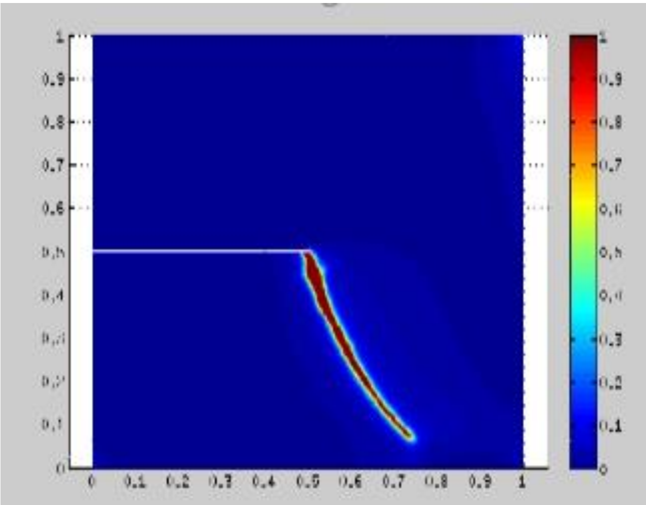
$$\boldsymbol{\sigma} = \left((1-d)^2 + k\right)\left\{\lambda \left\langle Tr\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\right\rangle_+ \mathbf{1} + 2\mu\boldsymbol{\varepsilon}\left(\mathbf{u}\right)^+\right\}$$
$$+\lambda \left\langle Tr\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\right\rangle_- \mathbf{1} + 2\mu\boldsymbol{\varepsilon}\left(\mathbf{u}\right)^-$$

$$D_{\delta d} E = 0, \; \dot{d} \geq 0$$ Phase field problem: weak form

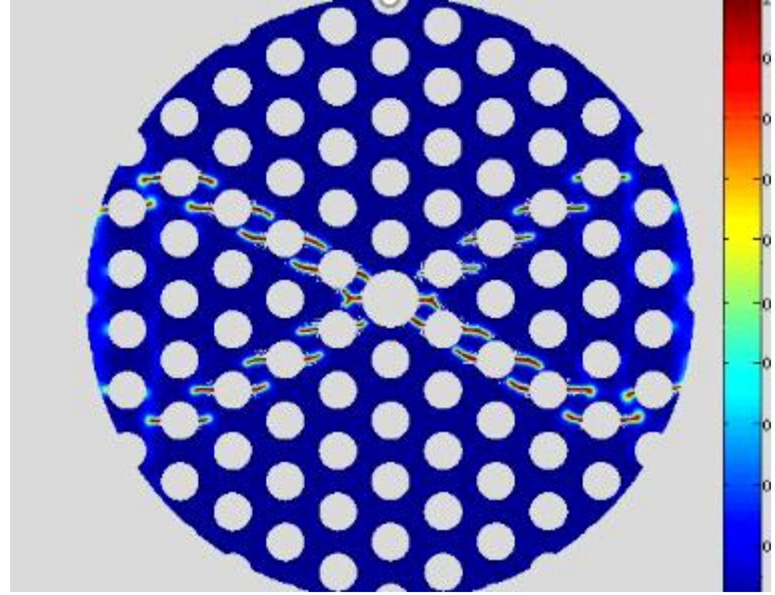
$$\int_\Omega \left(2\Psi^+\left(\mathbf{u}\right) + \frac{G_c}{\ell}\right) d\delta d + G_c \ell \nabla d \cdot \nabla(\delta d) d\Omega = \int_\Omega 2\Psi^+\left(\mathbf{u}\right)\delta d d\Omega$$

Strong form (Euler-Lagrange equations)

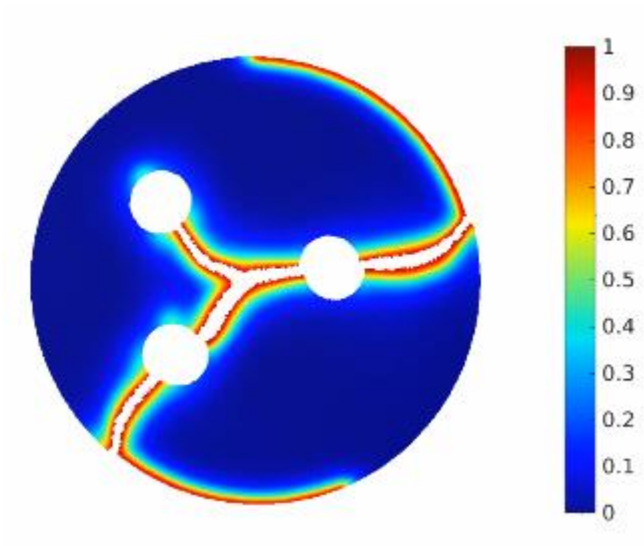
$$\left(2\Psi^+\left(\mathbf{u}\right) + \frac{G_c}{\ell}\right) d - \ell G_c \Delta d = 2\left[\Psi^+\left(\mathbf{u}\right)\right]$$



Curved cracks



Multiple cracks



Initiation
Branching
Cracks merging

Advantages of phase field for heterogeneous materials

Damage model with regularization (damage gradient)

→

- **Crack initiation** naturally handled
- **Arbitrary geometrical configurations** of microcrack networks (**3D**, **branching**, **merging**, **multiple cracks**)
- **Mesh-independent** (convergent, not dependent to mesh orientation)
- Can be used in regular/structured meshes

Variational framework

- Can be easily extended (**plasticity**, **interfaces**, **anisotropy**…)
- Consistent with discrete fracture mechanics (Γ-convergence)

Continuuous approximation of damage

- **Numerically simple** : classical FEM (no additional dof nor embedded discontinuities)

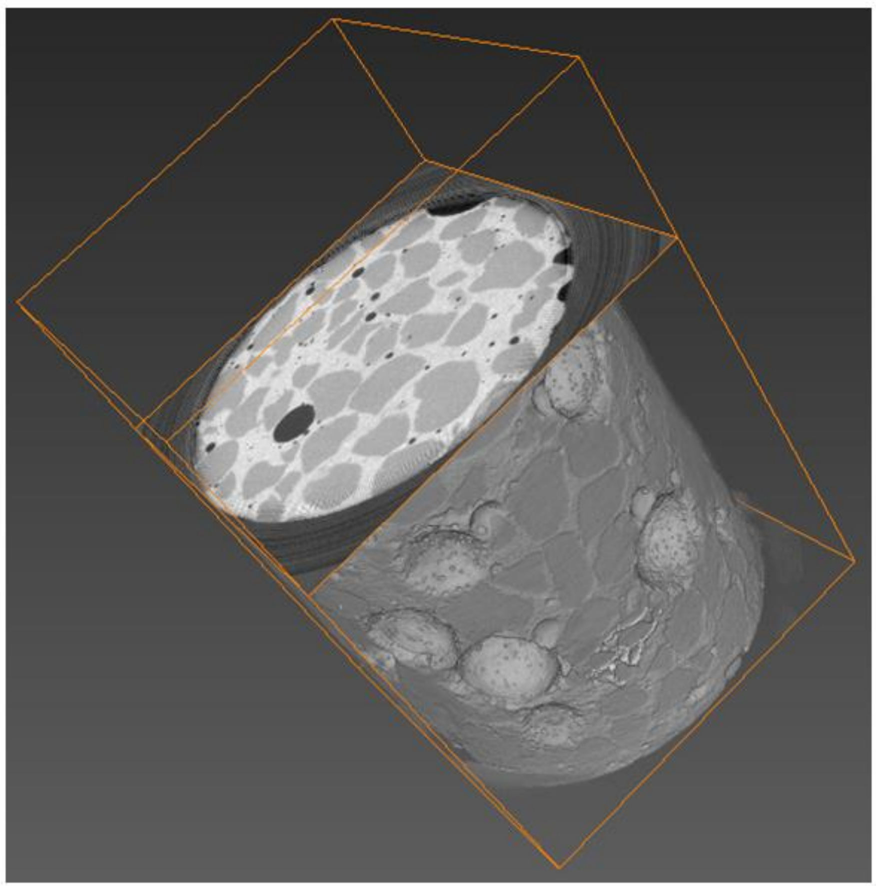
Drawback

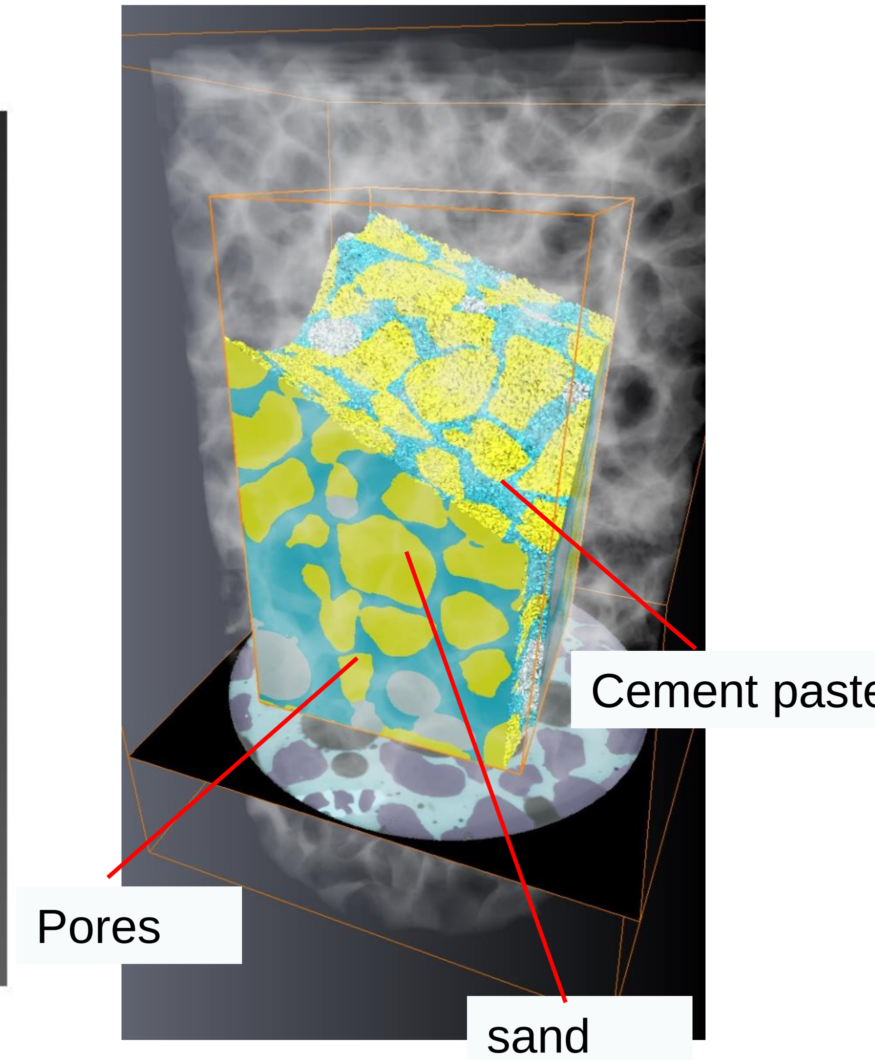
- **A fine mesh is required related to the regularization length: heavy computations for large 3D volumes**

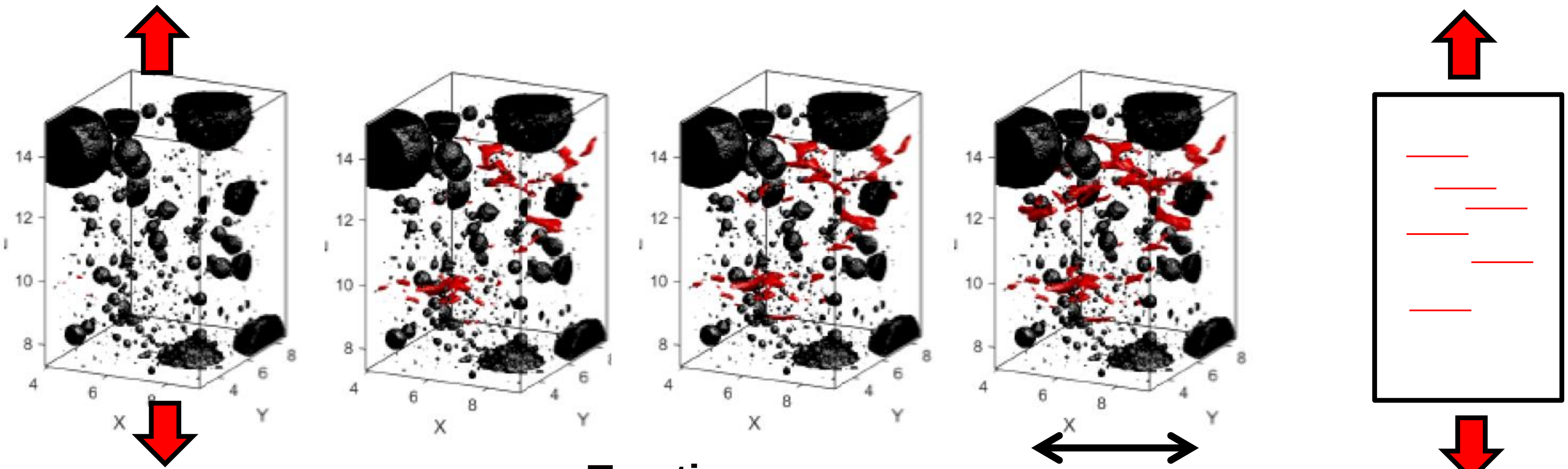
Examples of phase field simulations for microcracking in heterogeneous materials

Large-scale simulations of microcracking in material models obtained from micro tomography

Lightweight concrete sample

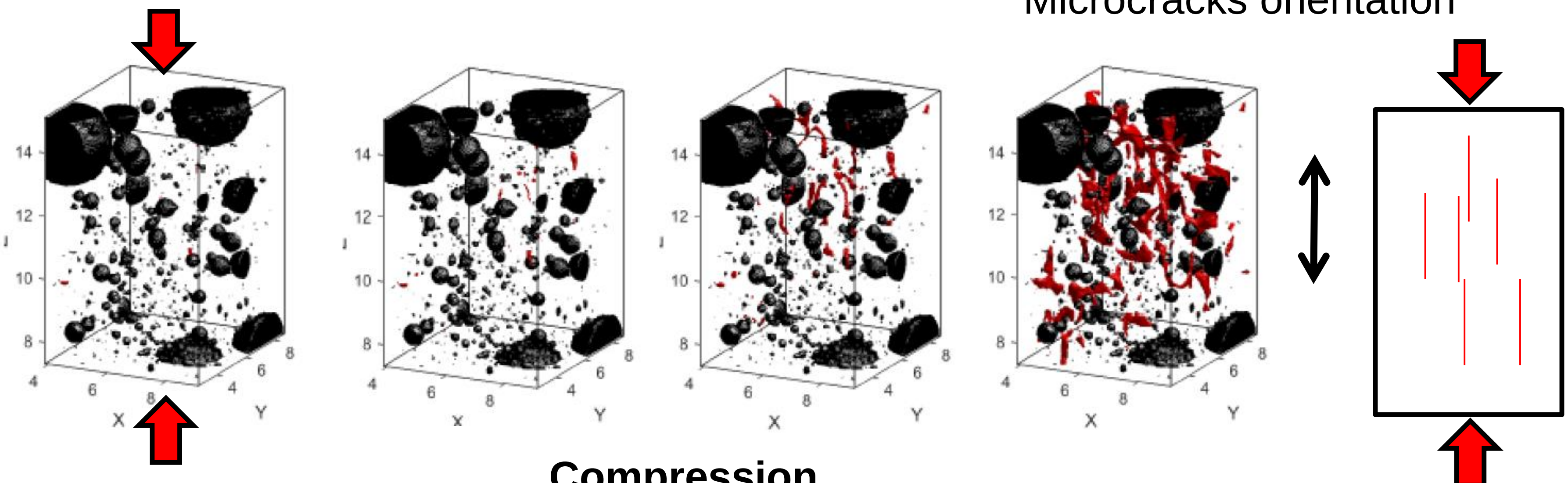






Traction

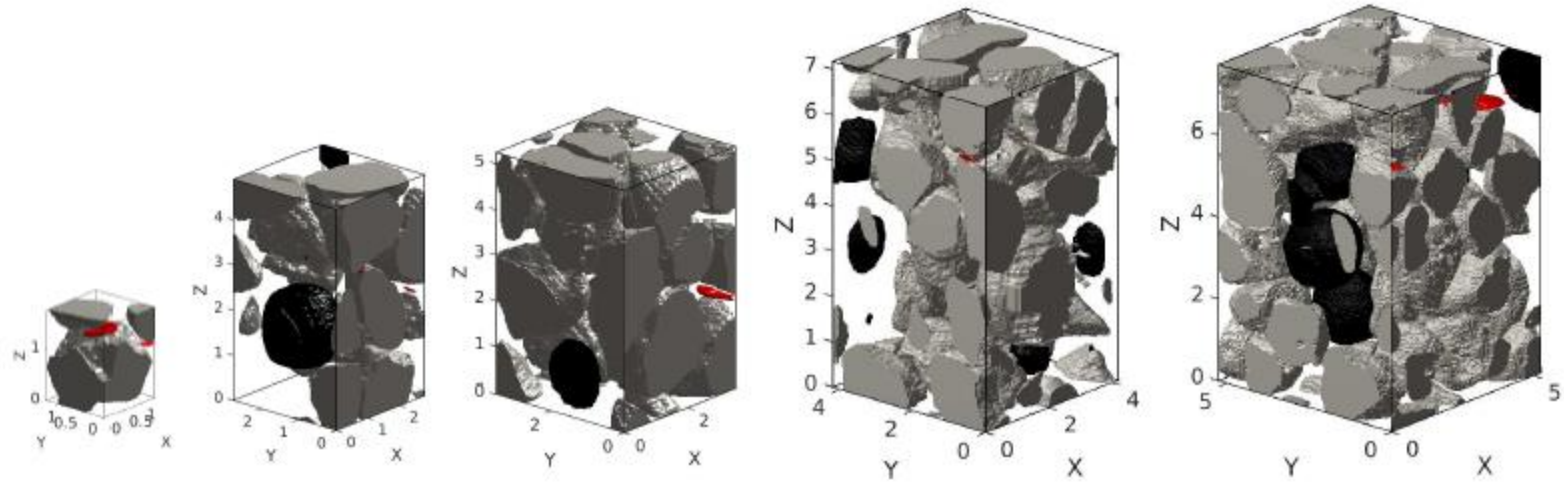
Microcracks orientation



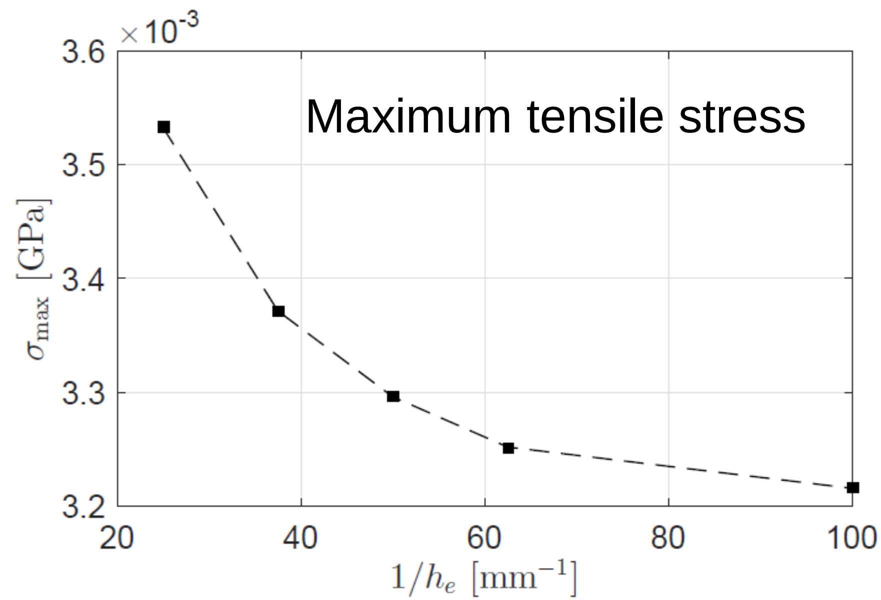
Compression

(30 M elements FEM model)

Convergence with respect to RVE size

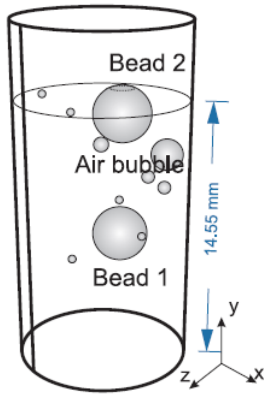


0.5M_STRUCT 5M_STRUCT 9M_STRUCT 17M_STRUCT 30M_STRUCT

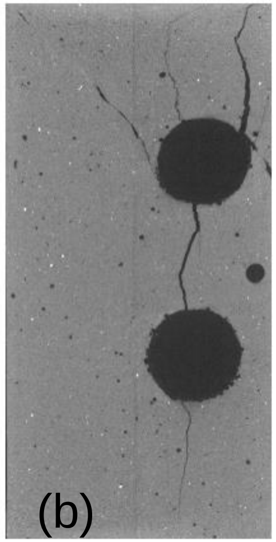


[TT Nguyen, J. Yvonnet, M. Bornert, et al. Extr. Mech. Lett. 2017]

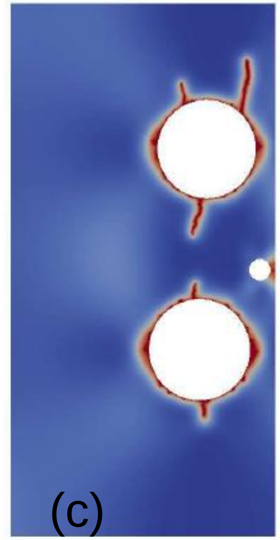
Comparisons experimental in situ testing and simulations



(a)



(b)



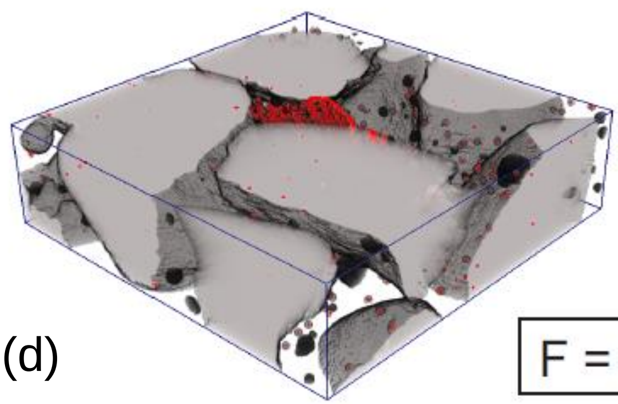
(c)

[TT Nguyen, J. Yvonnet, M. Bornert, C. Chateau, J.Mech. Phys. Solids, 2016]

Experiments

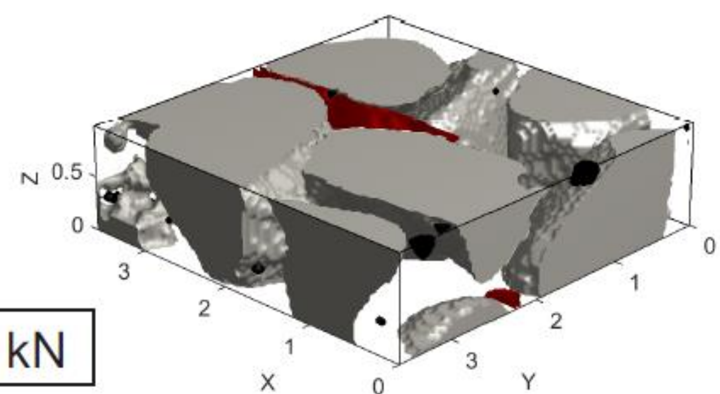
Simulations

(b)



(d)

F = 1.800 kN

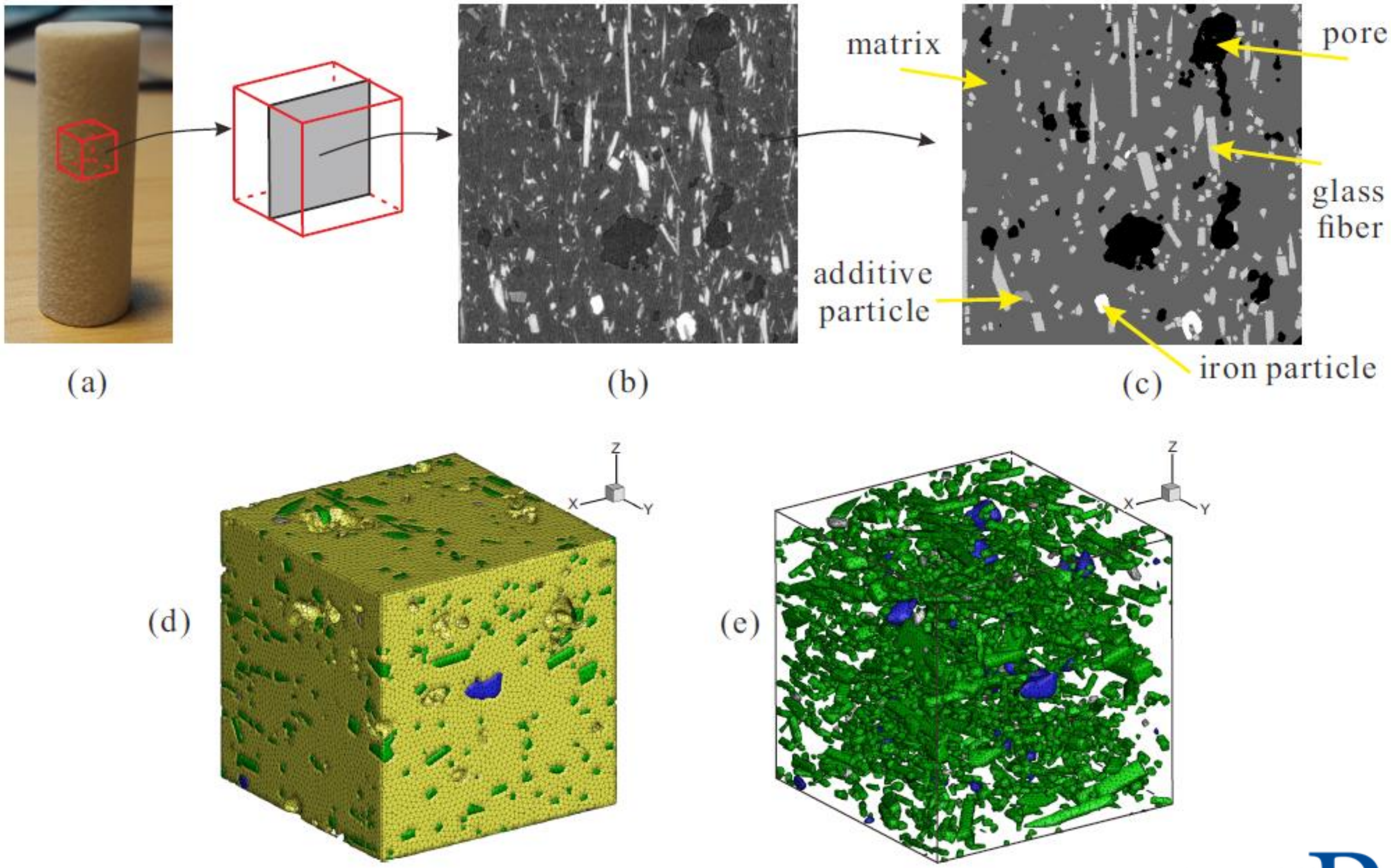


(e)

Experimental

Simulation

Simulation de micro fissuration dans les matériaux complexes (composite imprimé en 3D)



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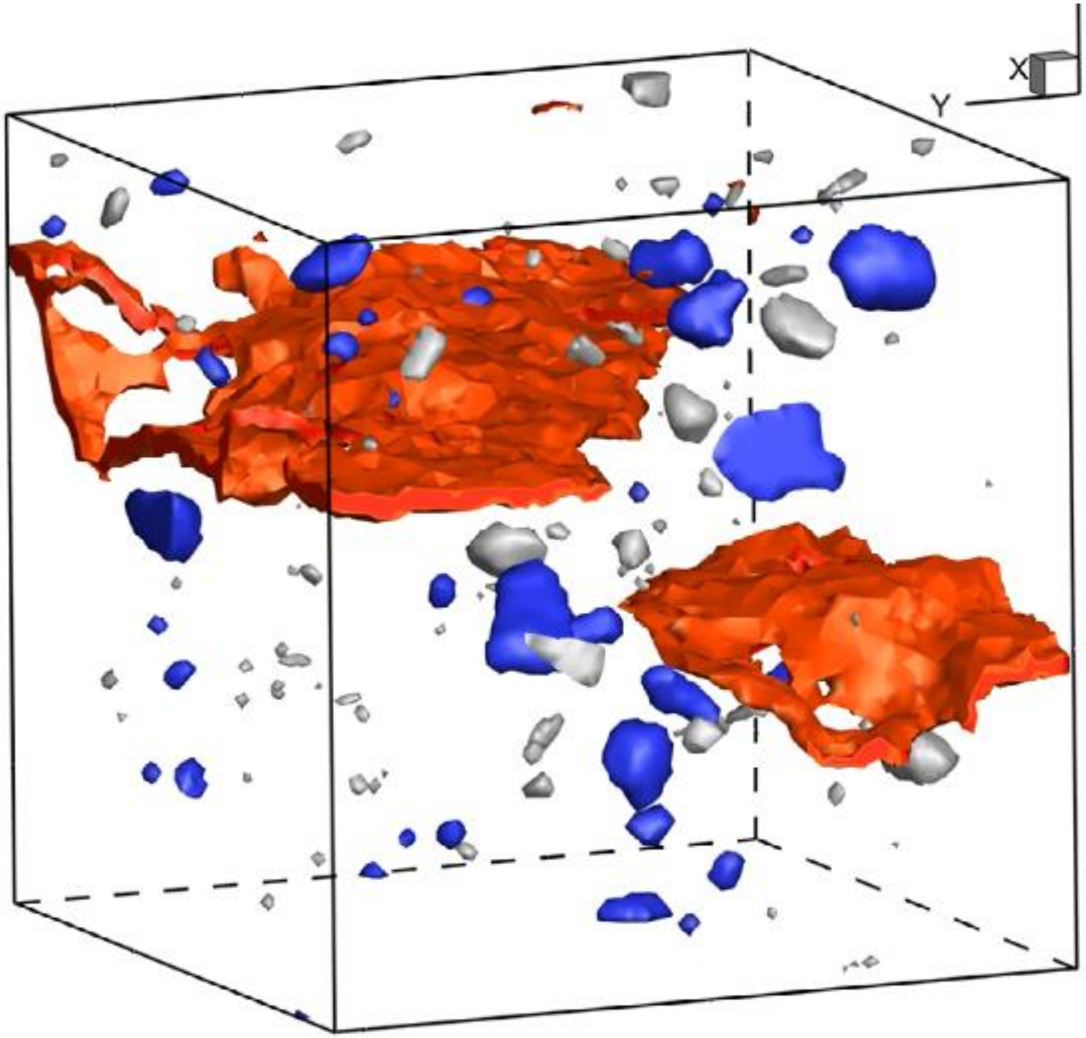
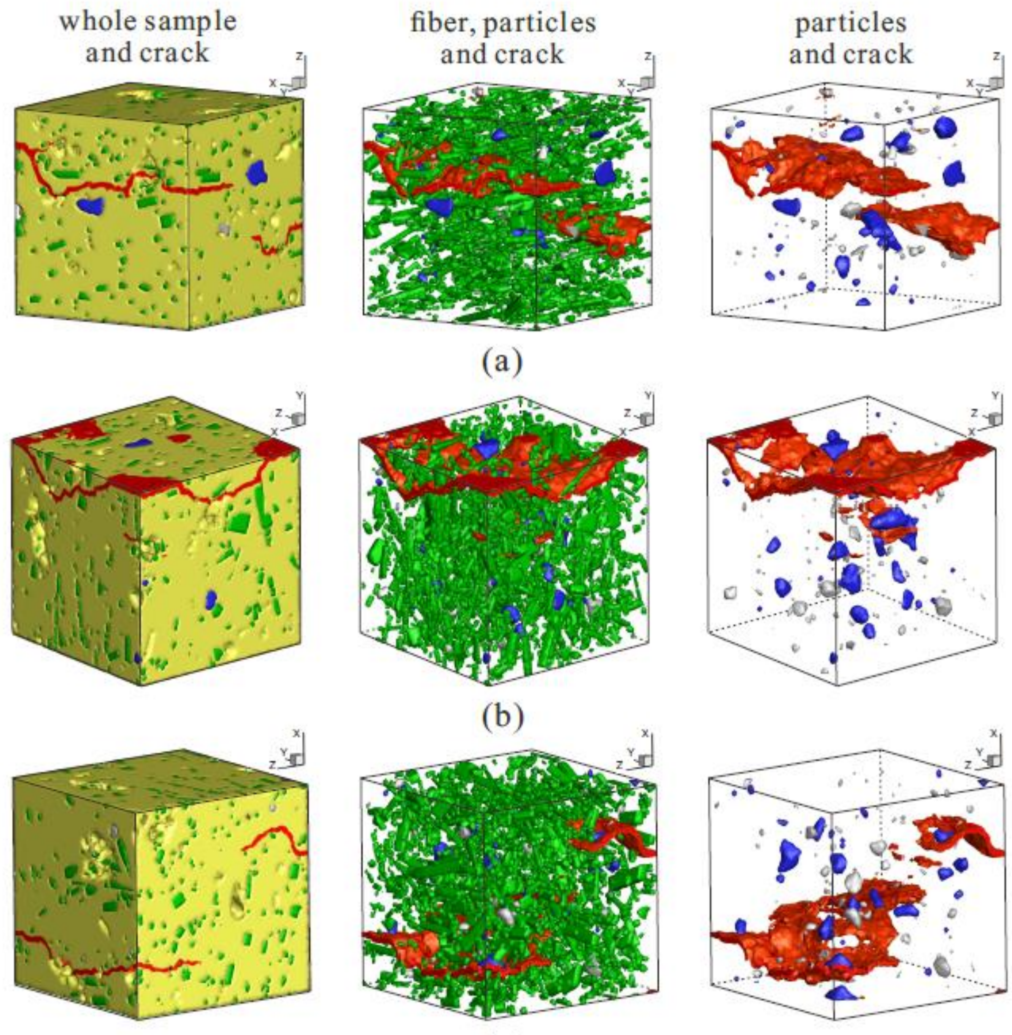
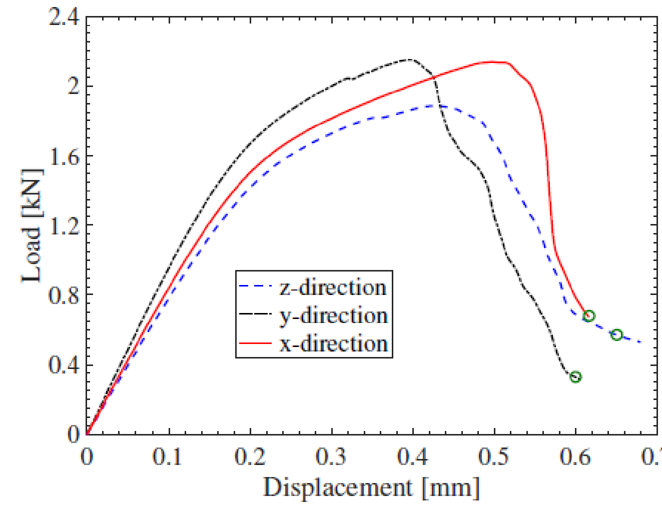
Simulation de micro fissuration dans les matériaux complexes (composite imprimé en 3D)

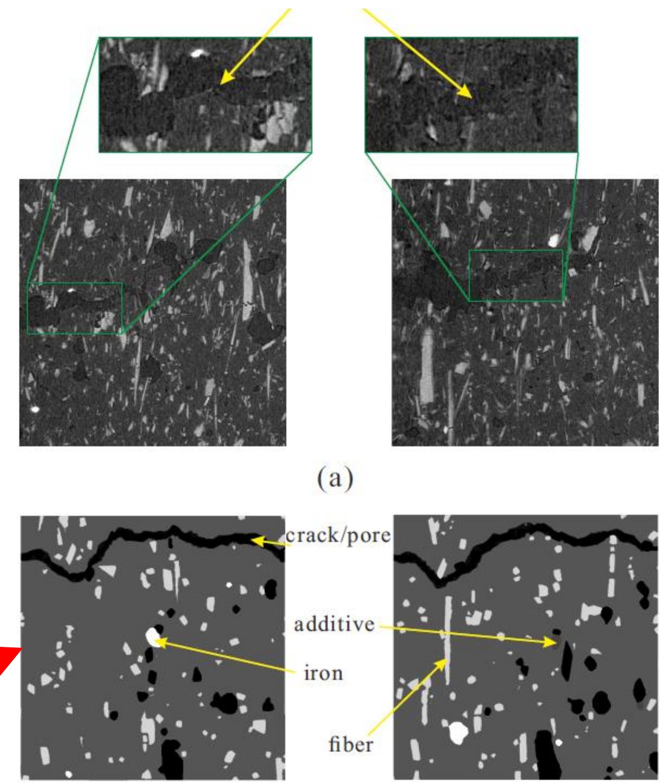


Elastoplastic fracture



Effects of anisotropy

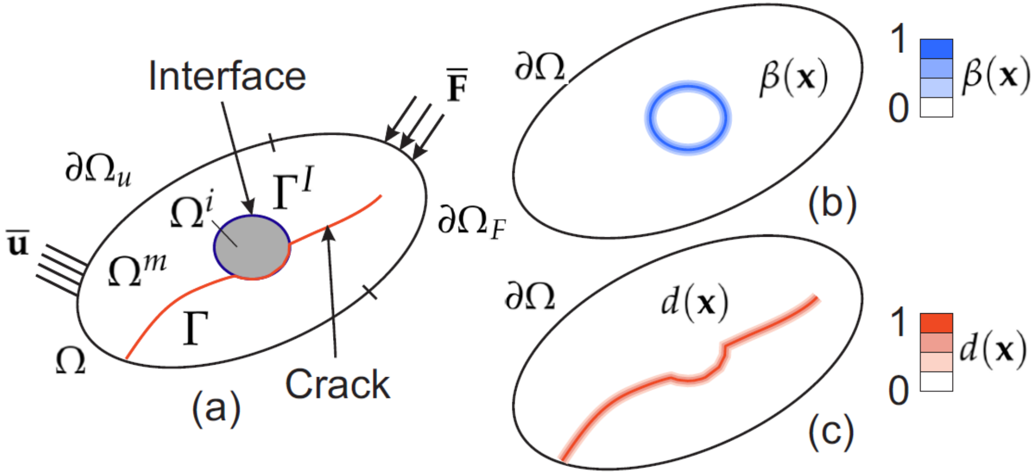


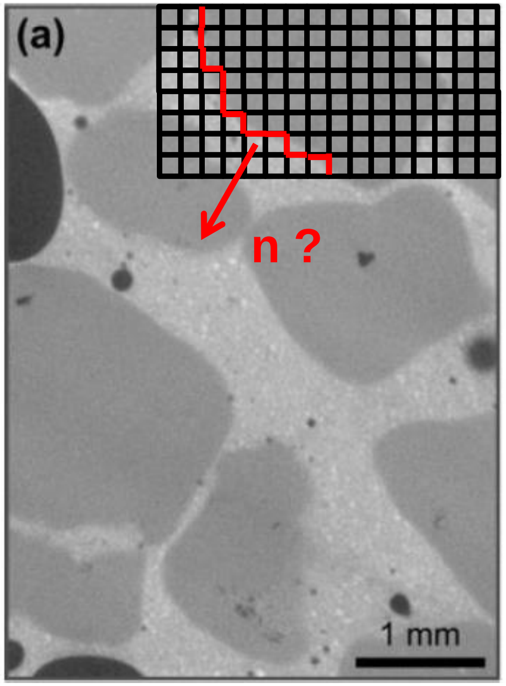


Travaux en cours post-doc Pengfei LI

Qualitative comparisons in-situ tests/simulations

Taking into account interfacial damage





Voxel-based model

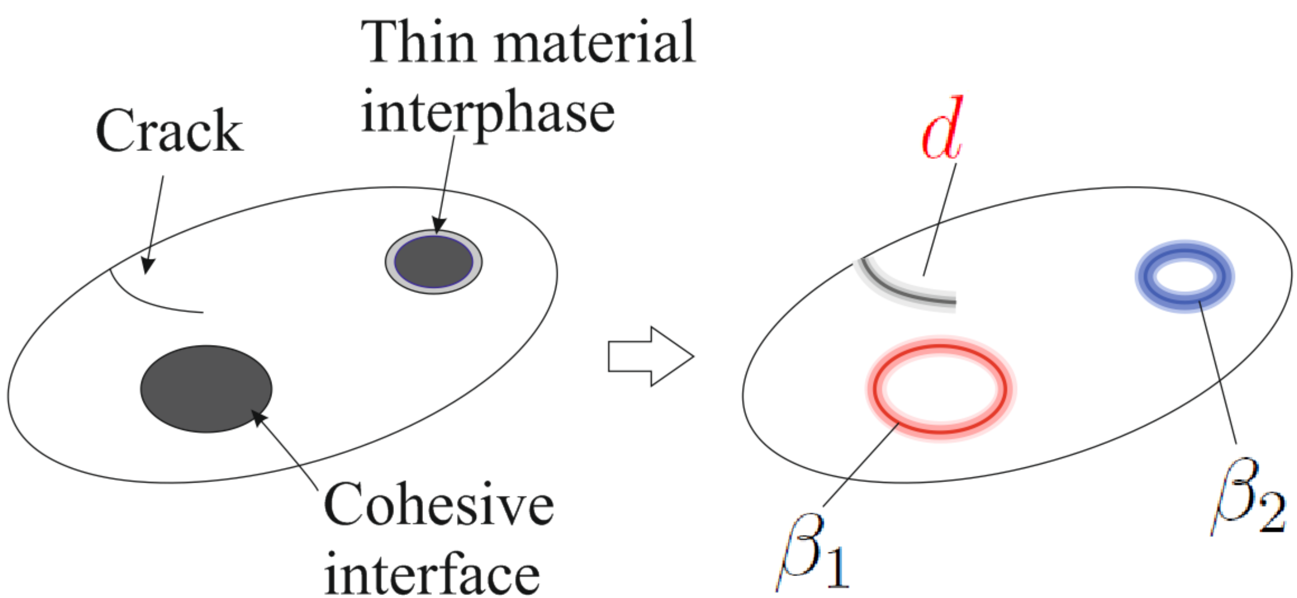
$$\begin{cases} \beta(\mathbf{x}) - l_\beta^2(\mathbf{x})\triangle\beta(\mathbf{x}) = 0 \quad \text{in } \Omega \\ \beta(\mathbf{x}) = 1 \quad \text{on } \Gamma^I, \\ \nabla\beta(\mathbf{x}) \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \end{cases}$$

Field related to interfaces

$$\beta(\mathbf{x}) = Arg\left\{ \inf_{\beta \in \mathcal{S}_\beta} \Gamma_\beta(\beta) \right\}$$

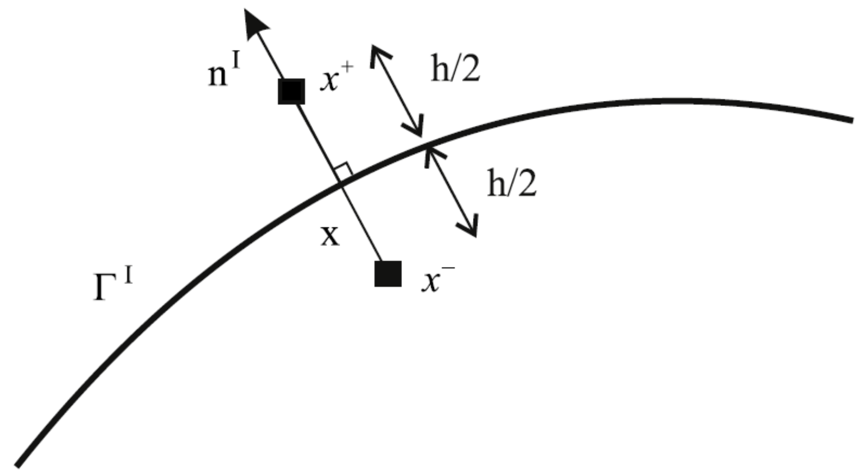
Energy functional for interfacial damage

$$E = \int_{\Omega} \Psi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right), d\right) + \omega\left(d\right) + \frac{c_1 \ell^2}{2} \nabla d \cdot \nabla d$$
$$+ \beta_1 \underbrace{\Psi^{I1}\left([[\mathbf{u}]], d\right)}_{\text{Cohesive interface energy density}} + \beta_2 \underbrace{\Psi^{I2}\left(\varepsilon^s(\mathbf{u}), d\right)}_{\text{Thin interphase energy density}} d\Omega$$



Smeared displacement jump approximation

$$\begin{cases} \phi(\mathbf{x}) > 0 & \text{for } \mathbf{x} \in \Omega^i \\ \phi(\mathbf{x}) < 0 & \text{for } \mathbf{x} \in \Omega / \Omega^i \\ \phi(\mathbf{x}) = 0 & \text{for } \mathbf{x} \in \Gamma^I \end{cases}$$



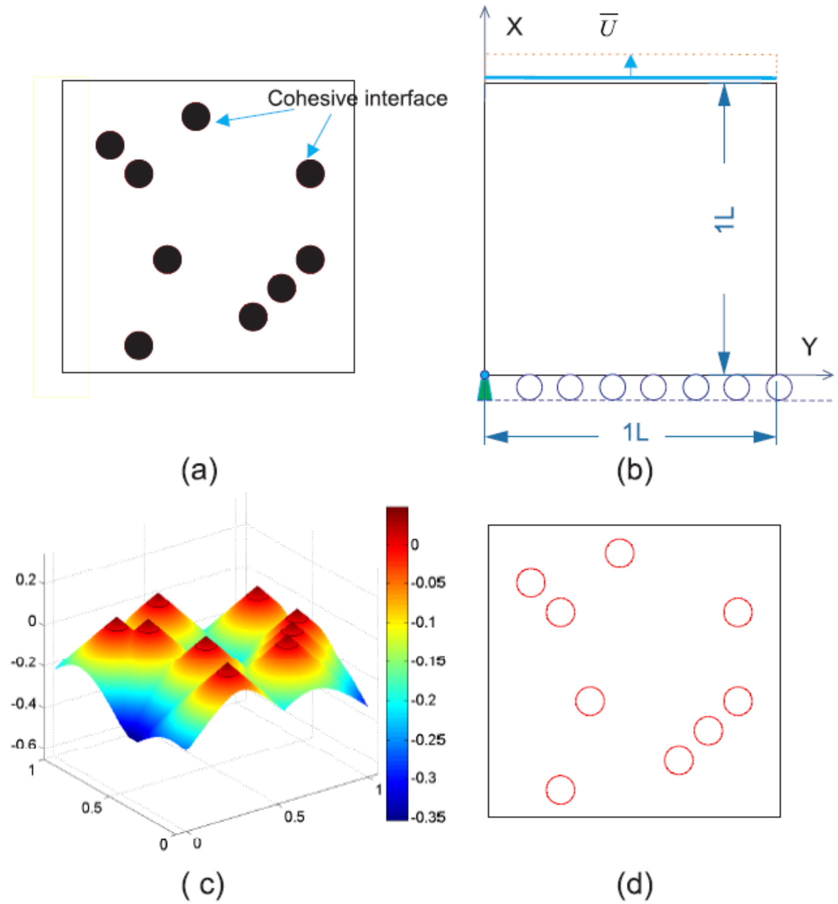
Level-set function describing the interfaces

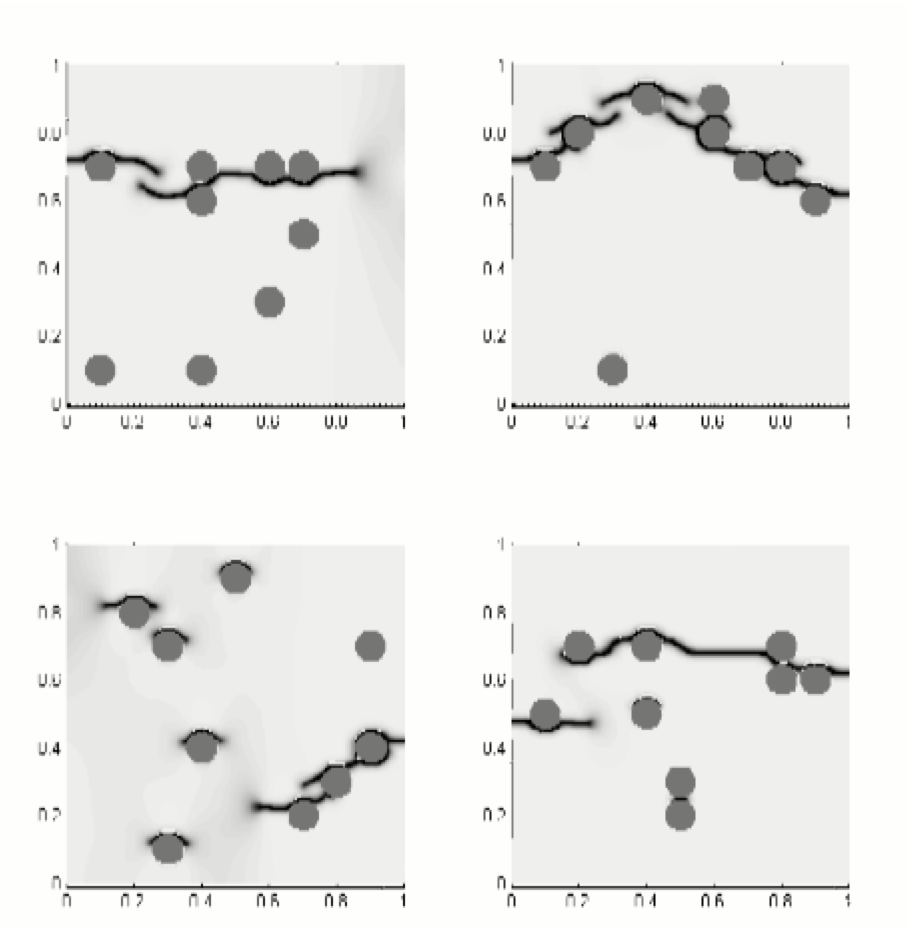
Using Taylor expansion around $\mathbf{x} \in \Gamma^I$

$$[\![\mathbf{u}(\mathbf{x})]\!] \simeq \mathbf{w}(\mathbf{x}) = \mathbf{u}\left(\mathbf{x} + \frac{h}{2}\mathbf{n}^I\right) - \mathbf{u}\left(\mathbf{x} - \frac{h}{2}\mathbf{n}^I\right)$$

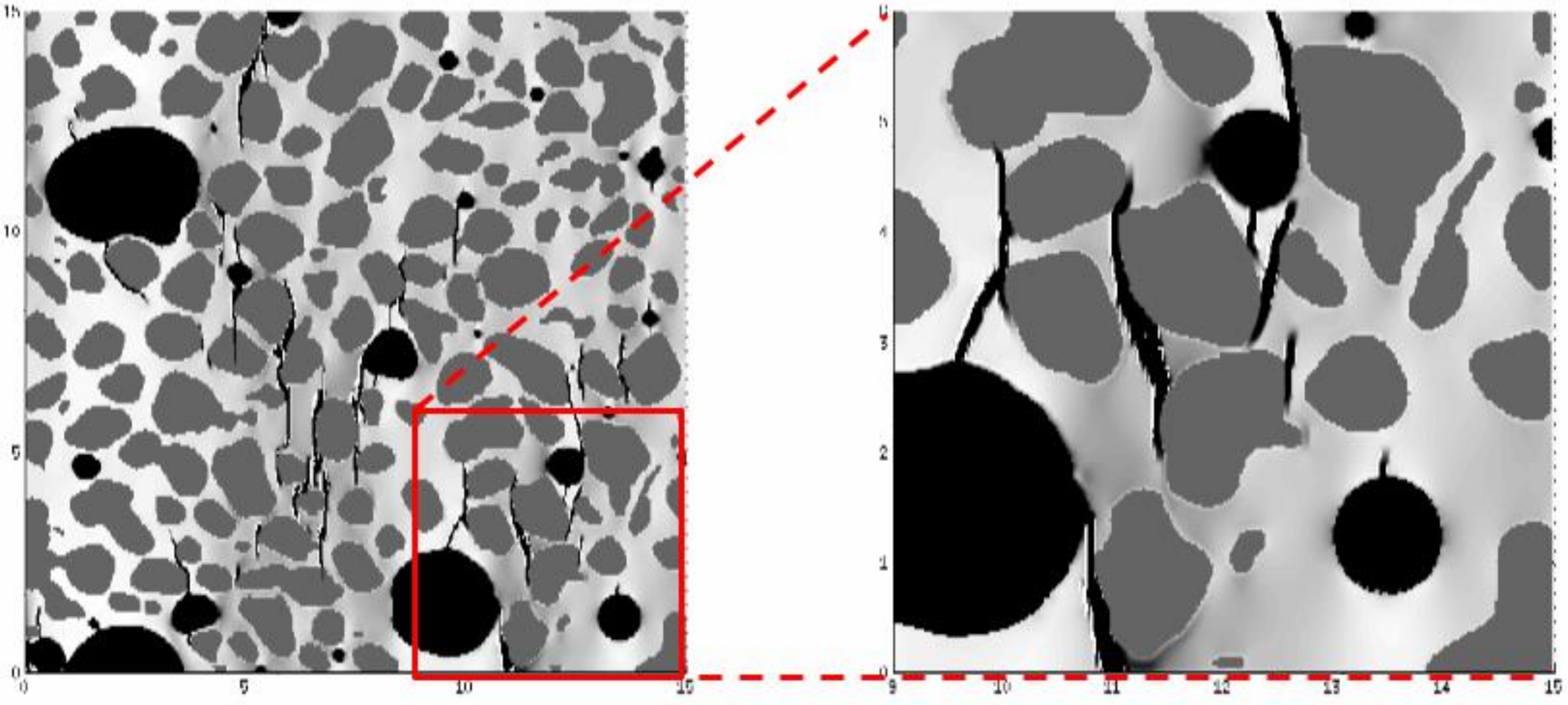
$$= h\nabla\mathbf{u}(\mathbf{x})\frac{\nabla\phi(\mathbf{x})}{\|\nabla\phi(\mathbf{x})\|}$$

Randomly distributed inclusions





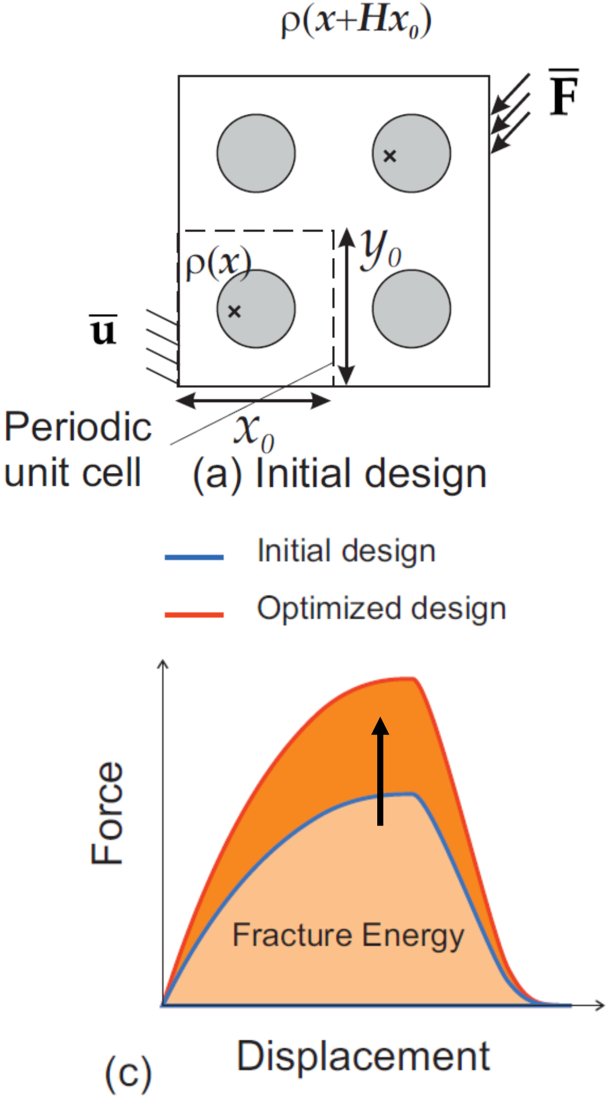
Interactions between bulk and interfacial damage



Topology optimization problem for fracture resistance of periodic composites

$$\text{Maximize}: J(\boldsymbol{\rho}, \mathbf{u}, d)$$
$$\rho(\mathbf{x})$$
$$\mathbf{u}(t) \in \mathcal{S}_u$$
$$d(t) \in \mathcal{S}_d$$
$$\text{subject}: \mathcal{R}_1(\rho, \mathbf{u}(t), d(t)) = 0,\ t \in [0, t^{max}]$$
$$\mathcal{R}_2(\rho, \mathbf{u}(t), d(t)) = 0,\ t \in [0, t^{max}]$$
$$\overline{f} = \frac{Vol(\Omega^i)}{Vol(\Omega)} = \frac{\int_\Omega \rho(\mathbf{x}) d\Omega}{Vol(\Omega)},$$
$$\rho(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{H}\mathbf{x}_0),$$

$$J = \int_0^{t^{max}} \mathbf{f}^{ext}(t) \cdot \bar{\mathbf{U}}(t) dt,$$



Sensitivity analysis (SIMP)

$$J = \int_0^{t^{max}} \mathbf{F}_{ext}(t) \cdot \overline{\mathbf{u}}(t) dt$$

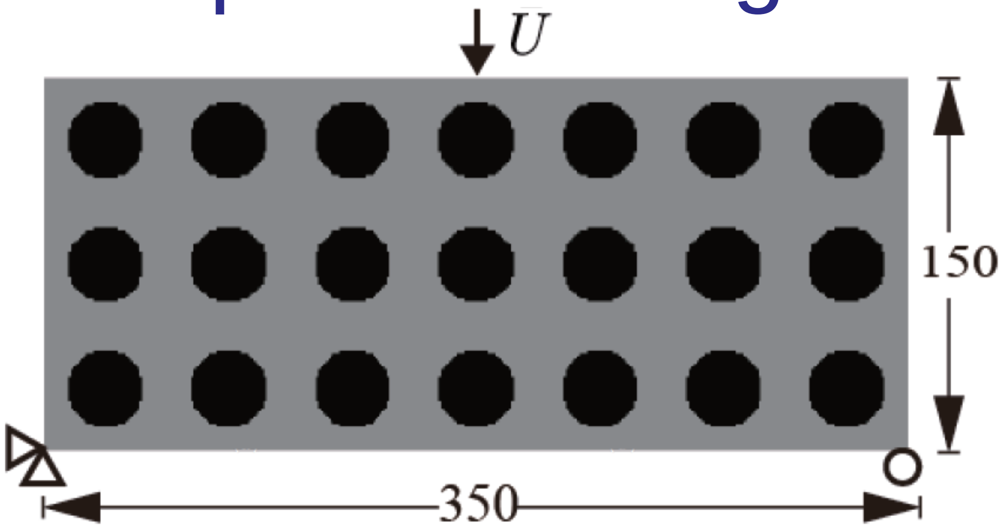
$$\begin{cases} E(\mathbf{x}) = (\rho(\mathbf{x}))^p \, E_{inc} + (1 - (\rho(\mathbf{x}))^p) \, E_{mat}, \\ \psi_c(\mathbf{x}) = (\rho(\mathbf{x}))^p \, \psi_{c,inc} + (1 - (\rho(\mathbf{x}))^p) \, \psi_{c,mat} \end{cases}$$

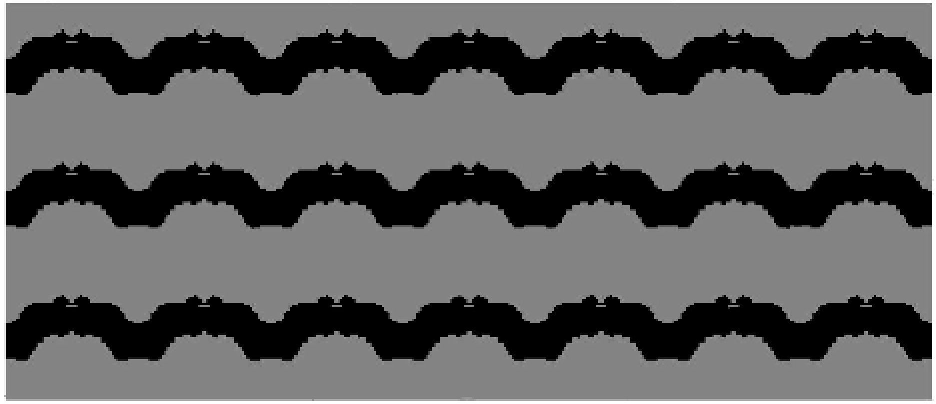
$$\frac{\partial \overline{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{load}} \Bigg\{ (\boldsymbol{\lambda}_1^n)^T \frac{\partial \mathbf{K}_u^n}{\partial \rho_e} \mathbf{u}^n + \left(\mathbf{K}_{u,\mathrm{FE}}^n \lambda_{1,\mathrm{E}}^n + \mathbf{K}_{u,\mathrm{FF}}^n \lambda_{1,\mathrm{F}}^n \right)^T \frac{\partial \mathbf{u}_\mathrm{F}^n}{\partial \rho_e}$$

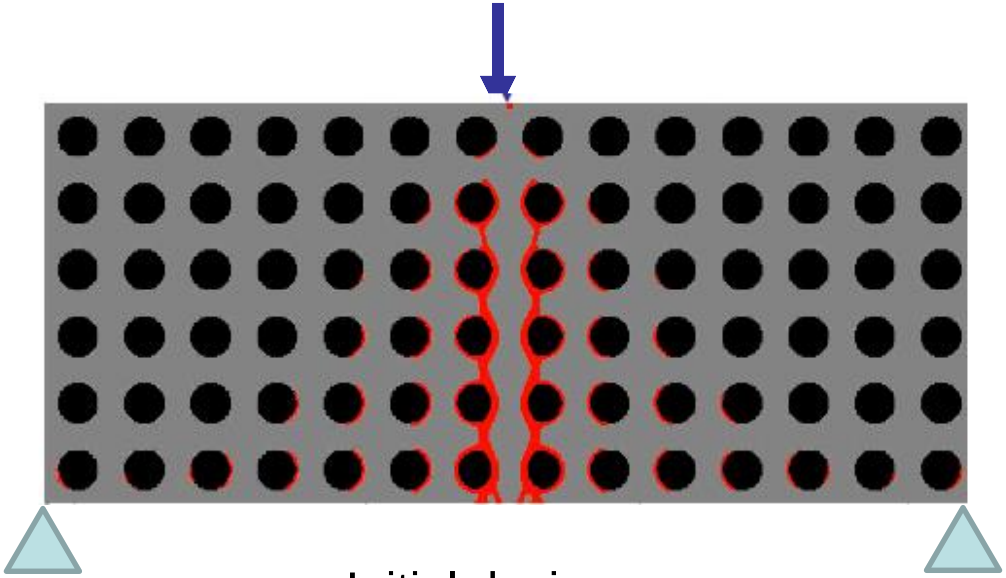
$$+ (\boldsymbol{\lambda}_2^n)^T \frac{\partial \mathbf{K}_u^{n-1}}{\partial \rho_e} \mathbf{u}^{n-1} + \left(\mathbf{K}_{u,\mathrm{FE}}^{n-1} \lambda_{2,\mathrm{E}}^n + \mathbf{K}_{u,\mathrm{FF}}^{n-1} \lambda_{2,\mathrm{F}}^n \right)^T \frac{\partial \mathbf{u}_\mathrm{F}^{n-1}}{\partial \rho_e} \Bigg\}$$

$$\boldsymbol{\lambda}_{1,\mathrm{F}}^n = \left(\mathbf{K}_{u,\mathrm{FF}}^n \right)^{-1} \mathbf{K}_{u,\mathrm{FE}}^n \Delta \mathbf{u}_\mathrm{E}^n \quad \text{and} \quad \boldsymbol{\lambda}_{2,\mathrm{F}}^n = \left(\mathbf{K}_{u,\mathrm{FF}}^{n-1} \right)^{-1} \mathbf{K}_{u,\mathrm{FE}}^{n-1} \Delta \mathbf{u}_\mathrm{E}^n$$

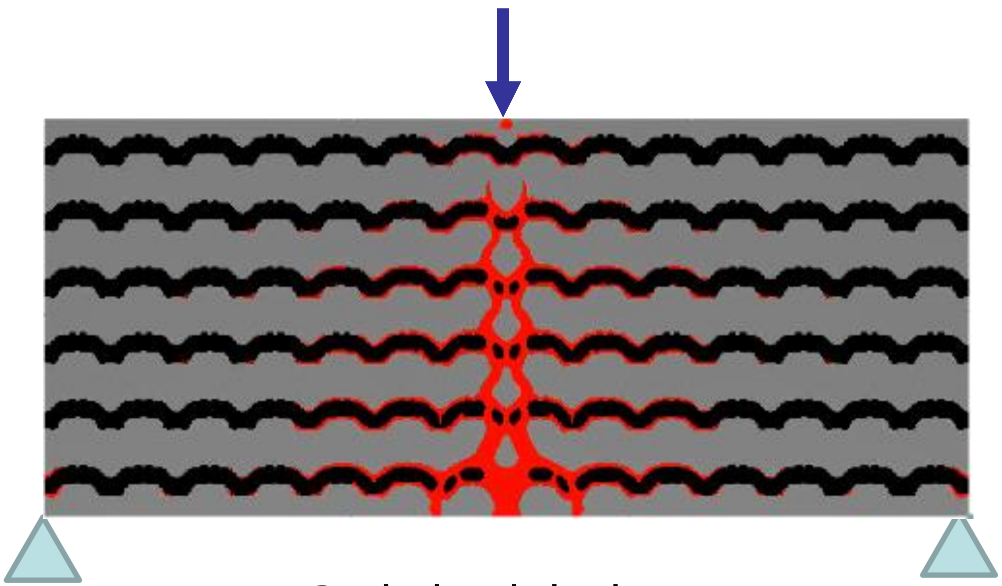
Numerical example: periodic composite structure subjected to symmetric 3-point bending



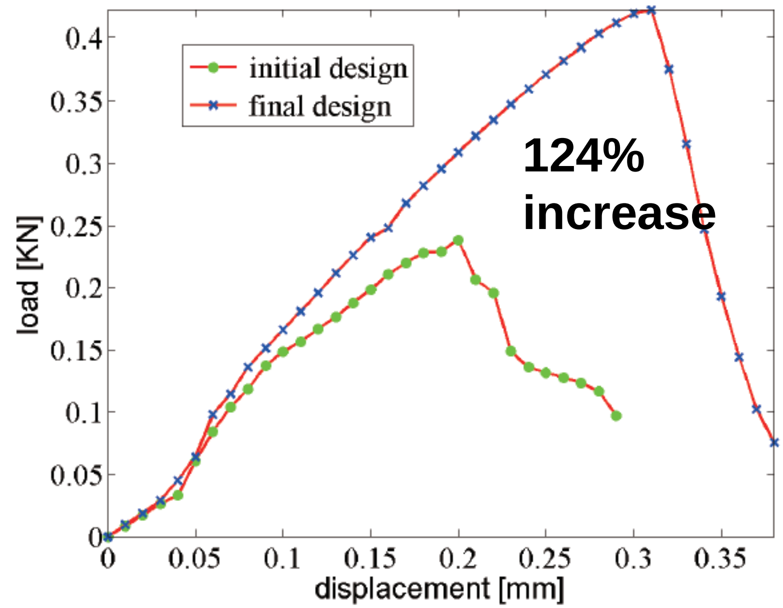




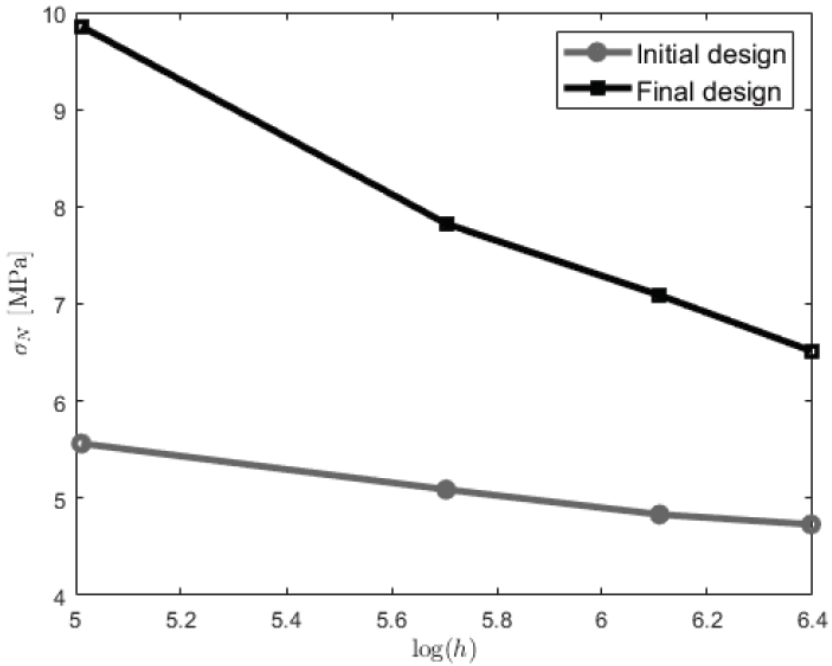
Initial design



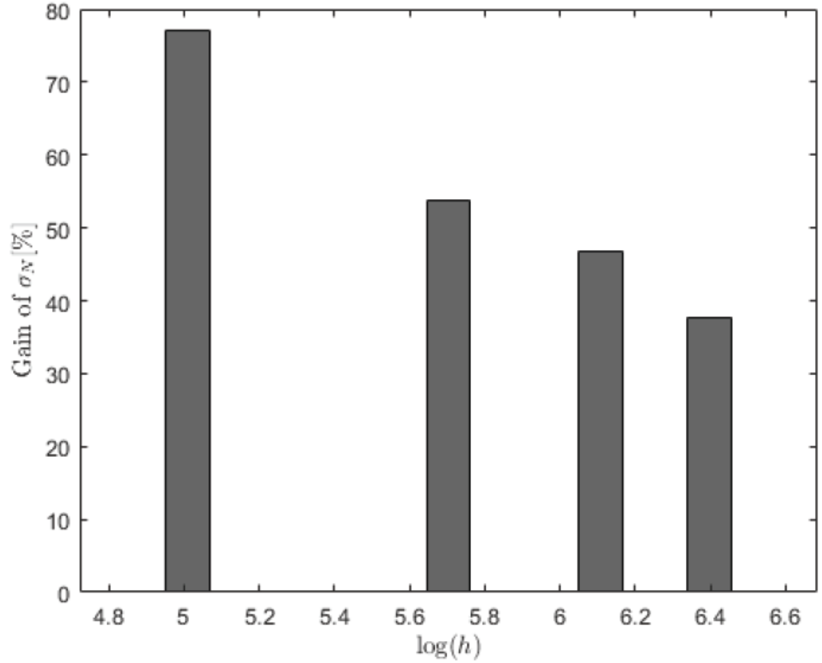
Optimized design



(a)

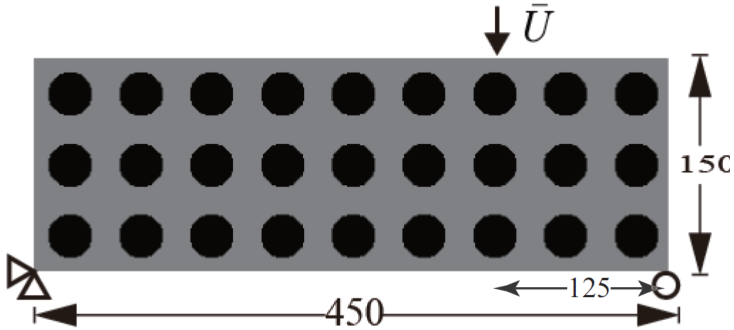


Size effects

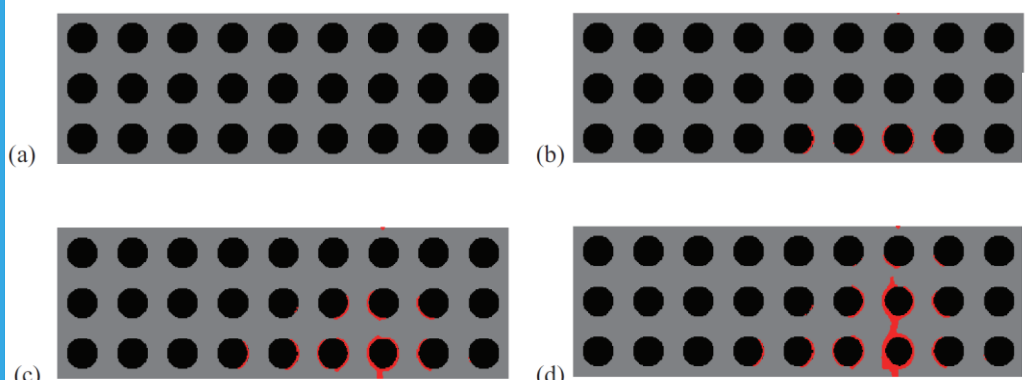


Gain in fracture resistance when using the same optimized microstructure w.r.t. to structure size

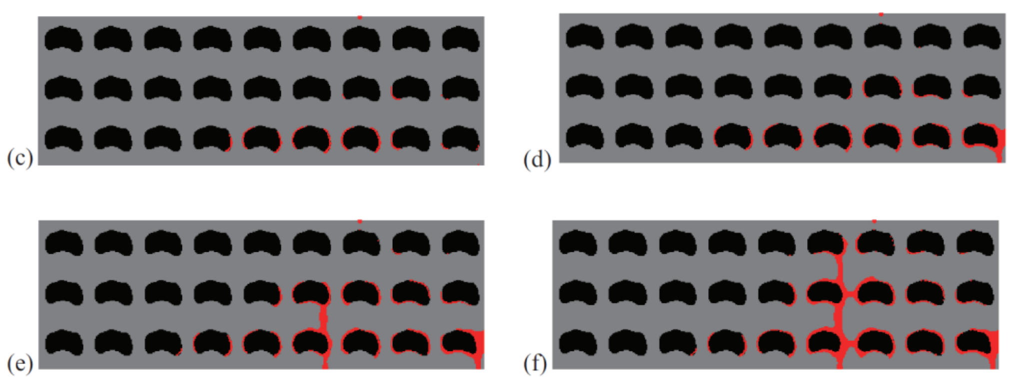
[Da and Yvonnet, Materials, 2020]



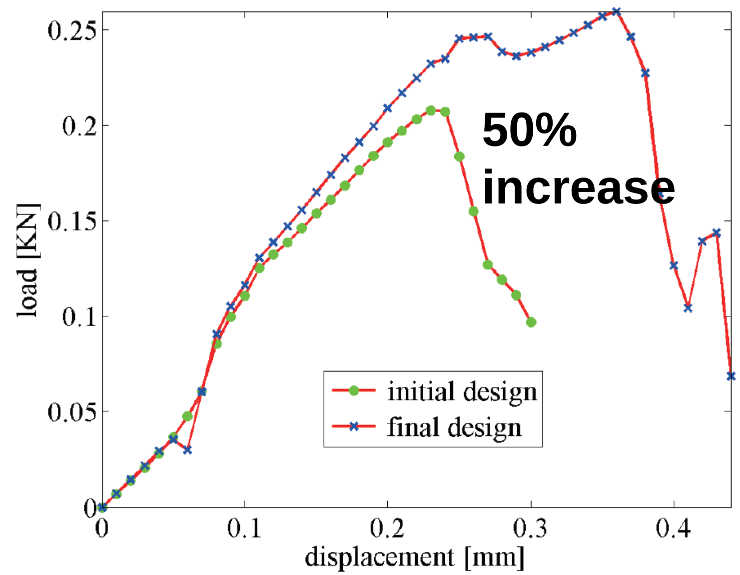
Unsymmetric 3-point bending



Initial design



Optimized design



3D reinforced structure

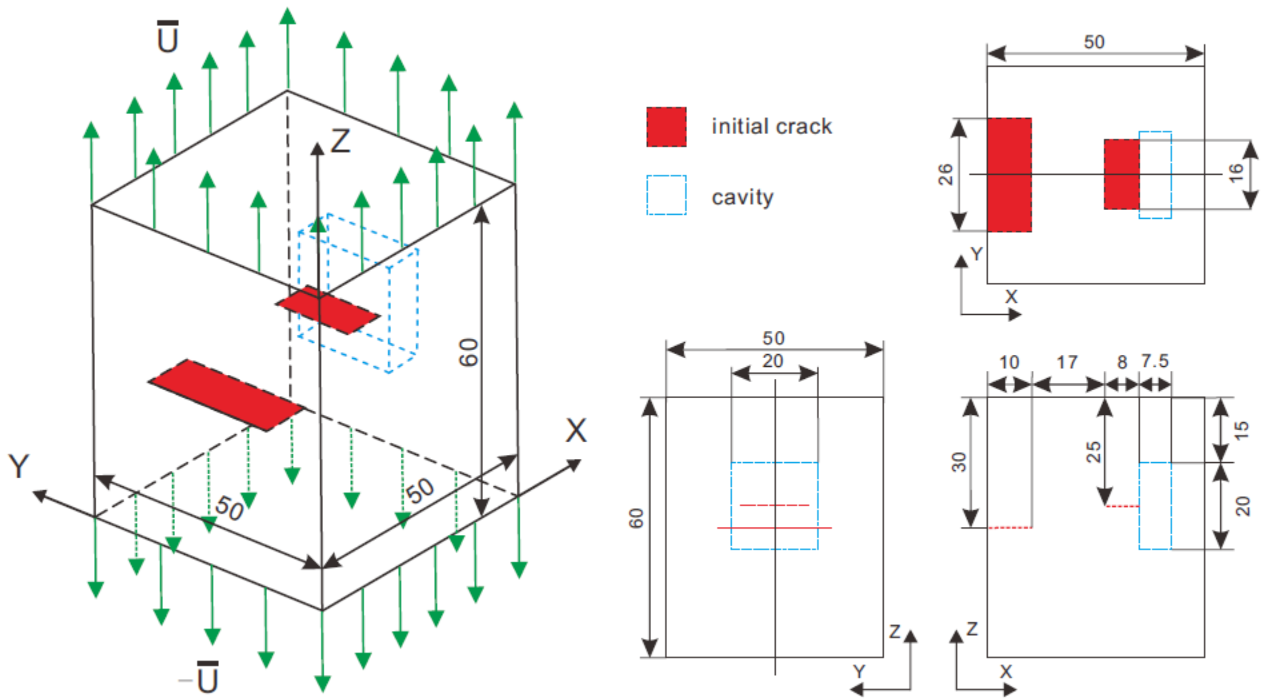
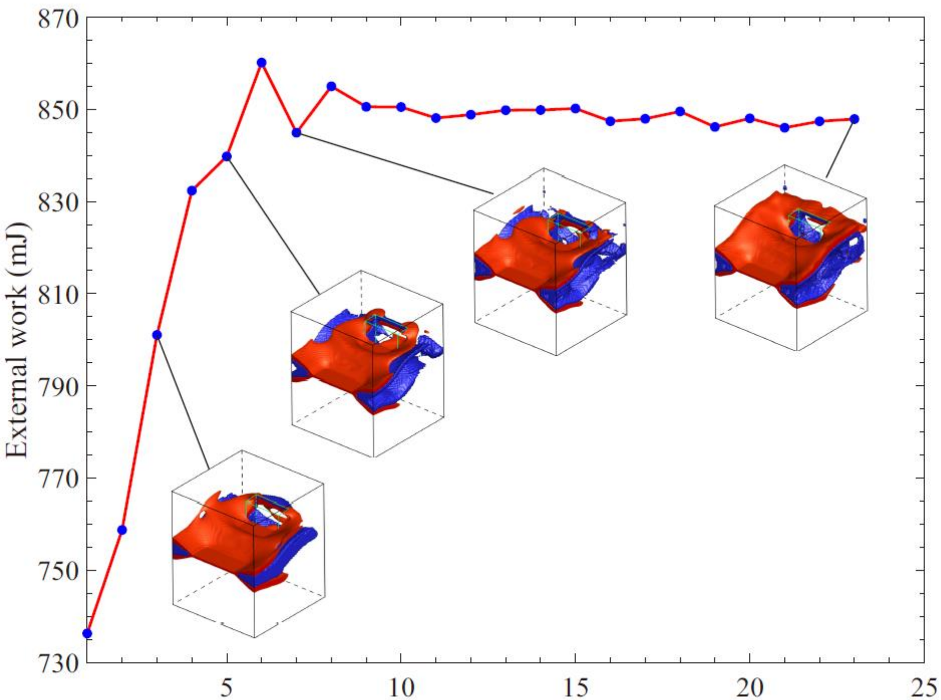
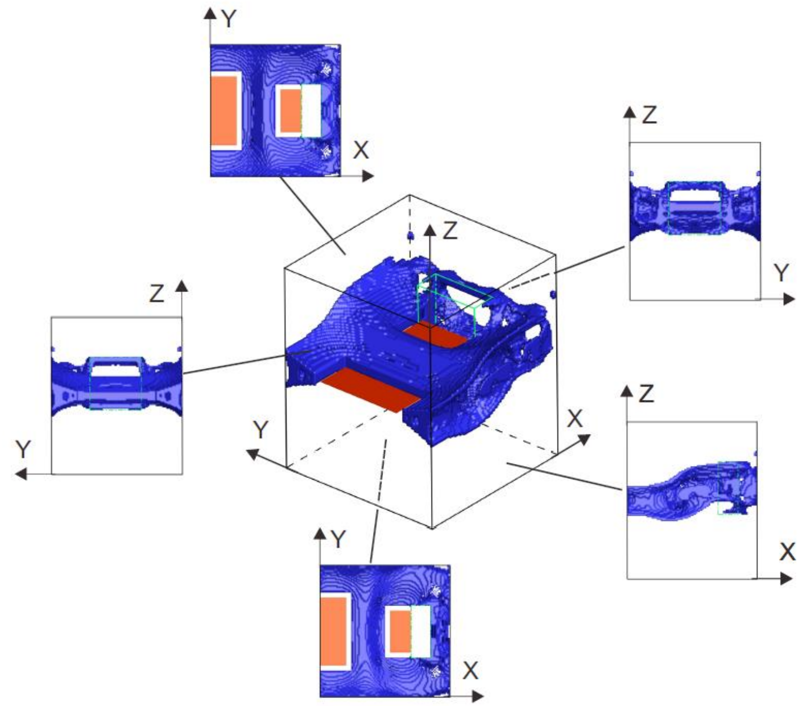


Fig. 17: 3D sample with two pre-existing cracks and including parallelepipedic cavity: (a) geometry and boundary conditions.

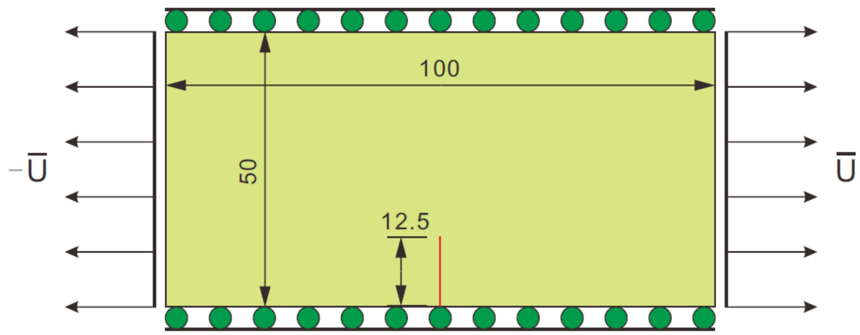
3D reinforced structure

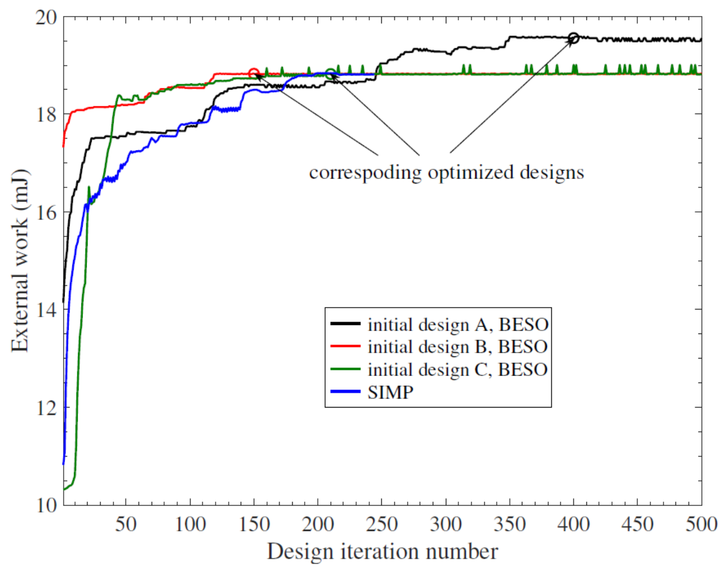


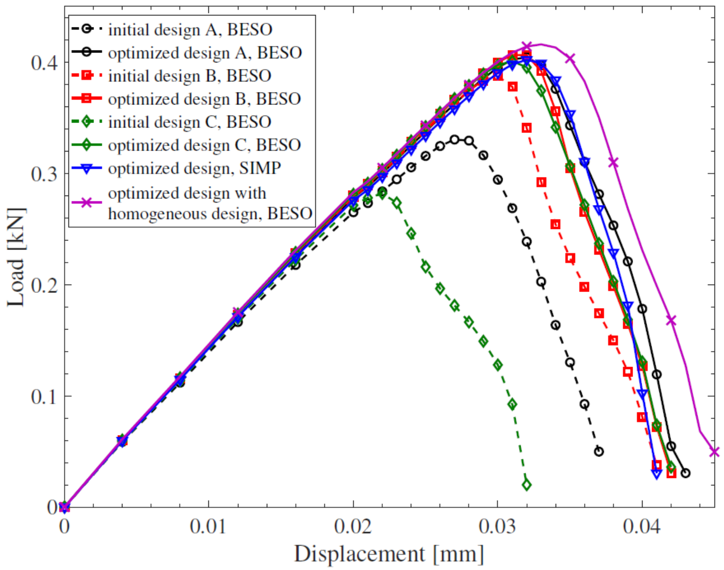


Optimized heterogeneous structure

Comparisons BESO/SIMP

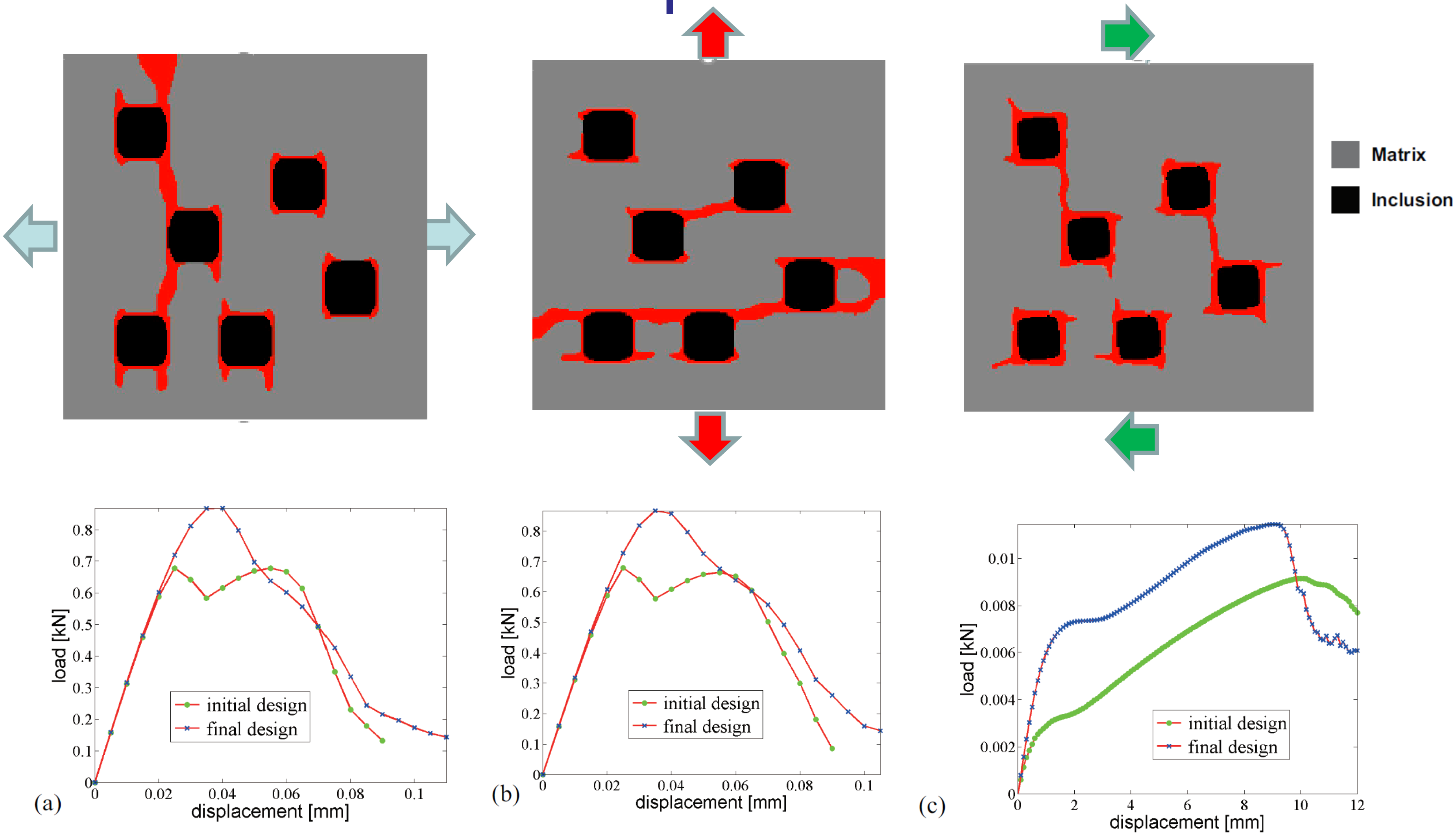


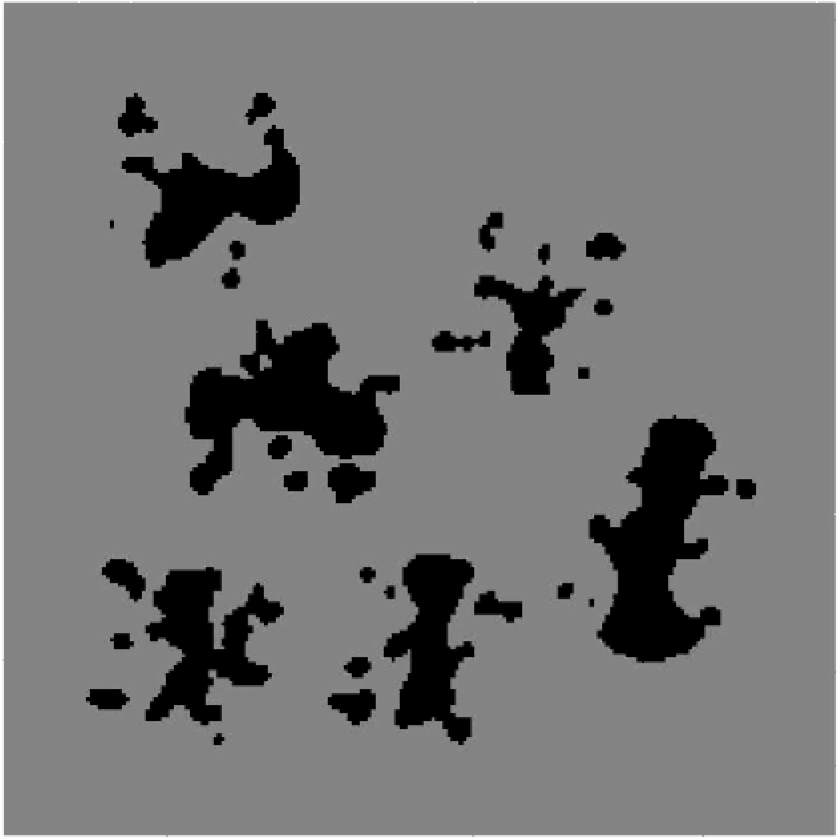




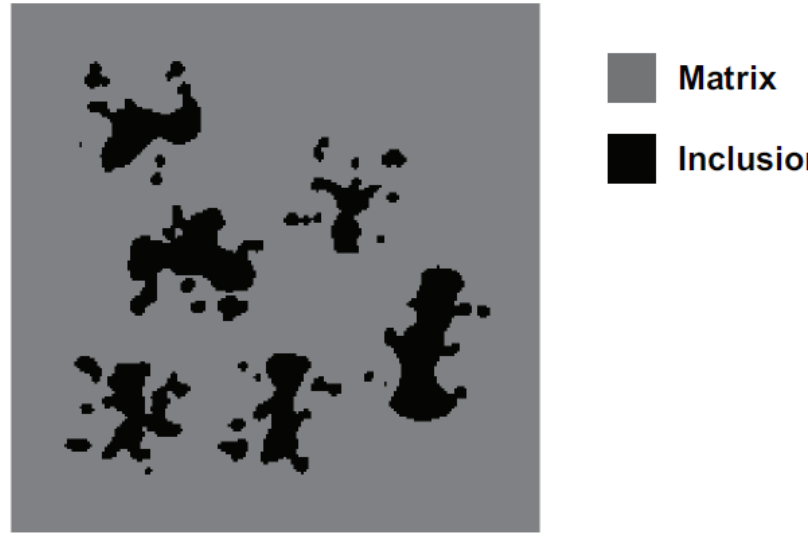
- Advantage of SIMP: possibility to start from homogeneous design with the target volume fraction; BESO: requires a guess initial design
- In the studied applications, comparable performances (iterations, optimal values for SIMP and BESO

Multi objective topology optimization : multiple loads



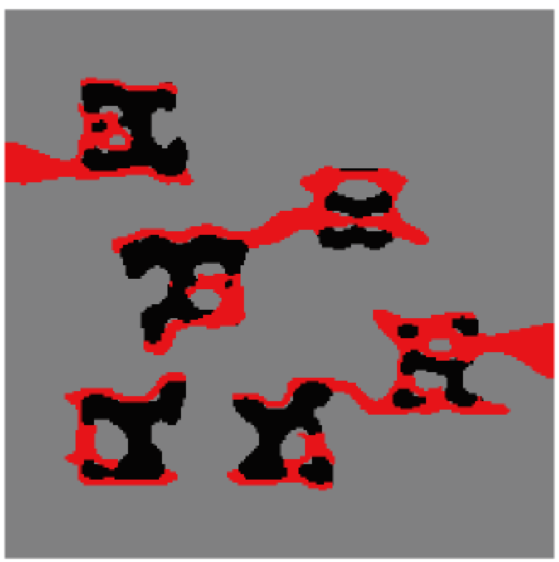


(a) 

(b) 

Optimized with respect to loads 1 and 2

Optimized with respect to loads 1, 2 and 3



(b) 

Conclusions

- Combining **Phase field fracture** and **topology optimization** for **maximizing the fracture resistance** of **composites** (bi-materials)
- Phase field formulation taking into account **interface failure**
- Formulation for **periodic composites**
- Formulation for multiple objectives: application to **resistance to multiple loads**
- **Comparisons SIMP/BESO**: similar performances/advantages
- Advanced 3D applications can be conducted

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- P. Li, Y. Wu, J. Yvonnet, A SIMP-Phase field topology optimization framework to maximize quasi-brittle fracture resistance of 2D and 3D composites, **Theoret. Appl. Fract. Mech**. accepted, 2021
- D. Da, J. Yvonnet, Topology Optimization for Maximizing the Fracture Resistance of Periodic Quasi-brittle Composites Structures, **Materials**, 13:3279, 2020.
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- L. Xia, D. Da, J. Yvonnet, Topology optimization for maximizing the fracture resistance of quasi-brittle composites, **Computer Methods in Applied Mechanics and Engineering**, 332:234-254,2018.

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