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

J. Yvonnet \(^{(1)}\), P. Li\(^{(1)}\), D. Da\(^{(2)}\), L. Xia\(^{(3)}\), Y. Wu\(^{(4)}\)

\(^{(1)}\) Université Gustave Eiffel, MSME, 5 bd Descartes, F-77454 Marne-la-Vallée, France.

\(^{(2)}\) Northwestern University, USA

\(^{(3)}\) Huazhong University of Science and Technology, Wuhan, China

\(^{(4)}\) State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, Hunan University, Changsha, 410082, China
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

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

3D printing technologies are available

What optimal microstructural geometry?
Maximizing the stiffness with respect to weight

\[
\begin{align*}
\min_{\rho_e} \quad & J(\rho_e), \quad 1 \leq e \leq N_e \\
\text{t.q.} \quad & Ku = F \\
& 0.001 \leq \rho_e \leq 1 \\
& \sum_e \rho_e < V_{\text{max}}
\end{align*}
\]

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

\[
\begin{align*}
\max_{\Omega} \quad & J(\Omega, u) = \sum_{ijkl} \eta_{ijkl} C^H_{ijkl} + \sum_{ij} \lambda_{ij} \alpha^H_{ij} \\
\text{t.q.} \quad & Ku^{ij} = f^{ij} \\
& K\chi^{a} = f^{a}
\end{align*}
\]

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 initiation/proagation 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]

\[ E = \int_{\Omega} \Psi (\varepsilon (u), \Gamma) + \int_{\Gamma} G_{c} dS \]

Griffith energy functional

\[ u^{n+1}, \Gamma^{n+1} = \text{Argmin}_{\begin{array}{c} u \in \mathcal{K}_{A} \\ \Gamma^{n} \leq \Gamma^{n+1} \end{array}} E \]

Free-discontinuity problem [Ambrosio et al. 2000]

Sharp description of interfaces
Continuous description of cracks: variational principle to damage

\[ E = \int_{\Omega} \Psi (\varepsilon (\mathbf{u}), d) \, d\Omega + \int_{\Omega} \omega (d) \, dS \]

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

\[ \mathbf{u}^{n+1}, d^{n+1} = \text{Argmin}_{\mathbf{u} \in \mathcal{K}_A} \quad E \quad \text{subject to} \quad 0 \leq d^n \leq d^{n+1} \leq 1 \]
Continuous description of cracks: variational principle to damage

Mechanical problem

\[ D_\delta u E = 0 \quad \text{Weak form} \quad \int_\Omega \frac{\partial \Psi}{\partial \varepsilon} (\varepsilon (u), d) : \varepsilon (\delta u) d\Omega = 0 \]

\[ \sigma = \frac{\partial \Psi}{\partial \varepsilon} (\varepsilon (u), d) \]

Strong form (Euler-Lagrange equations)

\[ \nabla \cdot \sigma = 0, \quad \sigma n = F \text{ on } \partial \Omega_F, \quad u = \bar{u} \text{ on } \partial \Omega_u \]

Phase field problem

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

Strong form (Euler-Lagrange equations)

\[ \frac{\partial \Psi}{\partial d} (\varepsilon (u), d) + \frac{\partial \omega (d)}{\partial d} = 0, \quad \nabla d \cdot n = 0 \text{ on } \partial \Omega_Q, \quad d = 1 \text{ on } \partial \Omega_d \]

Local relationship \( \rightarrow \) Lack of convergence, mesh-dependency issues
Continuous description of cracks with regularization by gradient of damage [Ambrosio and Tortorelli 1992, Bourdin et al. 2000]

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

Phase field problem  \[ D_{\delta d} E = 0, \quad \dot{d} \geq 0 \quad \text{Regularization term} \]

Weak form

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

Strong form (Euler-Lagrange equations)

\[ \frac{\partial \Psi}{\partial d} \left( \varepsilon \left( \mathbf{u} \right), d \right) + \frac{\partial \omega}{\partial d} - c_1 \ell^2 \Delta d = 0, \quad \nabla d \cdot \mathbf{n} = 0 \text{ on } \partial \Omega_Q, \quad d = 1 \text{ on } \partial \Omega_d \]
Example [Miehe et al. 2010]

\[ \omega(d) = \frac{G_c}{2\ell} d^2 \quad c_1 = \frac{G_c}{\ell} \]

\[ \Psi(\varepsilon(u)) = \left( (1 - d)^2 + k \right) \Psi^+ (\varepsilon(u)) + \Psi^- (\varepsilon(u)) \]

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

Other possible choices [Amor et al. 2009], [Borden, Hughes 2014], [He and Shao 2019]…
Example [Miehe et al. 2010]

Mechanical problem

\[ D_{\delta u} E = 0 \]  
Weak form

\[ \int_{\Omega} \sigma (\varepsilon(u), d) : \varepsilon(\delta u) d\Omega = 0 \]

Strong form (Euler-Lagrange equations)

\[ \nabla \cdot \sigma = 0, \quad \sigma n = F \text{ on } \partial \Omega_F, \quad u = \bar{u} \text{ on } \partial \Omega_u \]

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

\[ + \lambda \langle Tr \varepsilon(u) \rangle_- 1 + 2\mu \varepsilon(u)^- \]

\[ D_{\delta d} E = 0, \quad \dot{d} \geq 0 \]  
Phase field problem: weak form

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

Strong form (Euler-Lagrange equations)

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

Continuous 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

- Cement paste
- Pores
- Sand
Traction

Compression

(30 M elements FEM model)

Microcracks orientation
Convergence with respect to RVE size

Maximum tensile stress

$\sigma_{\text{max}}$ [GPa]

$1/h_e$ [mm$^{-1}$]

Comparisons experimental in situ testing and simulations

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

Projet ANR MMELED – MSME/Navier/Univ Lorraine/WeAre
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

Load [kN]

Displacement [mm]

z-direction
y-direction
x-direction

whole sample and crack
fiber, particles and crack
particles and crack

(a)

(b)

(c)
Taking into account interfacial damage

Field related to interfaces

\[
\begin{align*}
\beta(x) - l_\beta^2(x) \Delta \beta(x) &= 0 \quad &\text{in } \Omega \\
\beta(x) &= 1 \quad &\text{on } \Gamma^I, \\
\nabla \beta(x) \cdot n &= 0 \quad &\text{on } \partial \Omega,
\end{align*}
\]

Voxel-based model

\[
\beta(x) = \text{Arg} \left\{ \inf_{\beta \in S_\beta} \Gamma_\beta(\beta) \right\}
\]
Energy functional for interfacial damage

\[ E = \int_\Omega \Psi (\varepsilon (u), d) + \omega (d) + \frac{c_1 \ell^2}{2} \nabla d \cdot \nabla d + \beta_1 \Psi^{I1} ([u], d) + \beta_2 \Psi^{I2} (\varepsilon^s (u), d) \, d\Omega \]

Cohesive interface energy density

Thin interphase energy density

Crack

Thin material interphase

Cohesive interface
Smeared displacement jump approximation

\[
\begin{cases}
  \phi(x) > 0 & \text{for } x \in \Omega^i \\
  \phi(x) < 0 & \text{for } x \in \Omega \setminus \Omega^i \\
  \phi(x) = 0 & \text{for } x \in \Gamma^I
\end{cases}
\]

Level-set function describing the interfaces

Using Taylor expansion around \( x \in \Gamma^I \)

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

\[
= h \nabla u(x) \frac{\nabla \phi(x)}{\| \nabla \phi(x) \|}
\]
Randomly distributed inclusions
Interactions between bulk and interfacial damage
Topology optimization problem for fracture resistance of periodic composites

Maximize: \( J(\rho, \mathbf{u}, d) \)

\[ \rho(x) \]
\[ \mathbf{u}(t) \in \mathcal{S}_u \]
\[ d(t) \in \mathcal{S}_d \]

subject: \( \mathcal{R}_1(\rho, \mathbf{u}(t), d(t)) = 0, \ t \in [0, t^{\text{max}}] \)
\[ \mathcal{R}_2(\rho, \mathbf{u}(t), d(t)) = 0, \ t \in [0, t^{\text{max}}] \]

\[ \bar{f} = \frac{\text{Vol}(\Omega^i)}{\text{Vol}(\Omega)} = \frac{\int_{\Omega} \rho(x) d\Omega}{\text{Vol}(\Omega)} \]
\[ \rho(x) = \rho(x + Hx_0) \]

\[ J = \int_0^{t^{\text{max}}} f^{\text{ext}}(t) \cdot \ddot{U}(t) dt \]
### Sensitivity analysis (SIMP)

\[ J = \int_0^{t_{\text{max}}} \mathbf{F}_{\text{ext}}(t) \cdot \mathbf{u}(t) dt \]

\[
\left\{
\begin{align*}
  E(x) &= (\rho(x))^p E_{\text{inc}} + (1 - (\rho(x))^p) E_{\text{mat}}, \\
  \psi_c(x) &= (\rho(x))^p \psi_{c,\text{inc}} + (1 - (\rho(x))^p) \psi_{c,\text{mat}}
\end{align*}
\right.
\]

\[
\frac{\partial J}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{\text{load}}} \left\{ (\lambda_1^n)^T \frac{\partial \mathbf{K}_u^n}{\partial \rho_e} \mathbf{u}^n + \left( \mathbf{K}_{u,\text{FE}}^n \lambda_{1,E}^n + \mathbf{K}_{u,\text{FF}}^n \lambda_{1,F}^n \right)^T \frac{\partial \mathbf{u}_F^n}{\partial \rho_e} \right. \\
  & \quad \quad \left. + (\lambda_2^n)^T \frac{\partial \mathbf{K}^{n-1}}{\partial \rho_e} \mathbf{u}^{n-1} + \left( \mathbf{K}_{u,\text{FE}}^{n-1} \lambda_{2,E}^n + \mathbf{K}_{u,\text{FF}}^{n-1} \lambda_{2,F}^n \right)^T \frac{\partial \mathbf{u}_F^{n-1}}{\partial \rho_e} \right\}
\]

\[
\lambda_{1,F}^n = \left( \mathbf{K}_{u,\text{FF}}^n \right)^{-1} \mathbf{K}_{u,\text{FE}}^n \Delta \mathbf{u}_E^n \quad \text{and} \quad \lambda_{2,F}^n = \left( \mathbf{K}_{u,\text{FF}}^{n-1} \right)^{-1} \mathbf{K}_{u,\text{FE}}^{n-1} \Delta \mathbf{u}_E^n
\]
Numerical example: periodic composite structure subjected to symmetric 3-point bending
Initial design

Optimized design

Load [kN] vs. displacement [mm]

124% increase
Size effects

Gain in fracture resistance when using the same optimized microstructure w.r. 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) Optimized with respect to loads 1 and 2

(b) Optimized with respect to loads 1, 2 and 3
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
References


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