Construction of simplified models for crack propagation in random heterogeneous media Motivation

Conference Paper · July 2018

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WCCM 2018

Construction of simplified models for crack propagation in random heterogeneous media

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July 25 2018

World Congress in Computational Mechanics (WCCMXIII)
New-York, USA

Motivation

Macroscale perspective : need to 'break down' the symmetry

Microscale perspective : satisfactory for some configurations

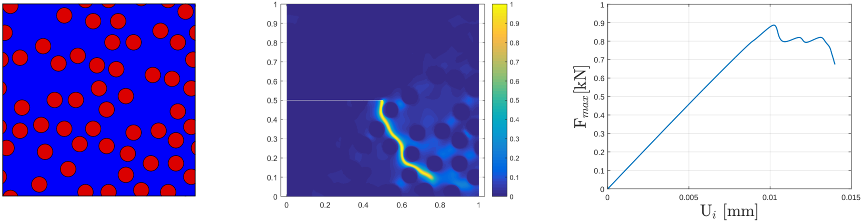

FIGURE 1 – Random microstructure with monodisperse spheres (left), simulated crack path (middle) and estimated mechanical response (right)

Can we envision a **mesoscale point of view** ?

This talk is focused on

- defining the mesostructure (elasticity, toughness) ; and
- assessing the impact on the mechanical response

Outline

Outline

Background

Variational energy minimization framework for brittle fracture ; see, *e.g.*,

- Marigo and collaborators, since 1998 (seminal theoretical works)
- Miehe *et al.*, 2010 (numerical aspects)

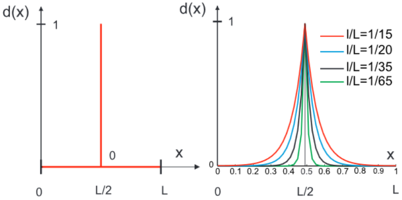

FIGURE 2 – Diffused representation of damage in the phase-field approach

The coupled elasticity-phase-field problem is given by

$$\begin{cases} \boldsymbol{\nabla} \cdot [\sigma(\boldsymbol{u}, d)] = \mathbf{0} \,, \\ \dfrac{g_c}{\ell}(d - \ell^2 \Delta d) - 2(1-d)\mathcal{H}(\boldsymbol{u}) = 0 \end{cases} , \quad \mathcal{H}(\boldsymbol{u}) = \max_t \Psi^+(\boldsymbol{u}) \tag{1}$$

in Ω, with $\boldsymbol{u} = \boldsymbol{u}_D$ on $\partial\Omega_D$, $[\sigma]\boldsymbol{n} = \boldsymbol{t}_N$ on $\partial\Omega_N$ and $\boldsymbol{\nabla} d \cdot \mathbf{n} = 0$ on $\partial\Omega$

Background

Stress tensor for the damaged material :

$$[\sigma(\boldsymbol{u}, d)] = (\mathcal{D}(d) + \eta)\frac{\partial\Psi^+([\epsilon(\boldsymbol{u})])}{\partial[\epsilon(\boldsymbol{u})]} + \frac{\partial\Psi^-([\epsilon(\boldsymbol{u})])}{\partial[\epsilon(\boldsymbol{u})]} \ , \tag{2}$$

where $\mathcal{D}(d) = (1-d)^2$, $0 < \eta \ll 1$ and

$$\Psi([\epsilon]) = \Psi^+([\epsilon]) + \Psi^-([\epsilon]) \ , \quad \Psi^{\pm}([\epsilon]) = [\epsilon^{\pm}] : [\![C]\!] : [\epsilon^{\pm}] \ , \tag{3}$$

with

$$[\epsilon^{\pm}] = \sum_{i=1}^{m} < \lambda_i >^{\pm} \boldsymbol{\varphi}^{(i)} \otimes \boldsymbol{\varphi}^{(i)} \tag{4}$$

and

$$< z >^{\pm} = \frac{1}{2}(z \pm |z|) \ , \quad \forall z \in \mathbb{R}$$

Example in 2D

Consider a homogeneous matrix, reinforced with monodisperse spheres :

- $\lambda_m = 121.6$ [GPa] and $\mu_m = 80.77$ [GPa]
- Contrast set to 10, ℓ and g_c constant in each phase
- Incremental shear displacement is prescribed

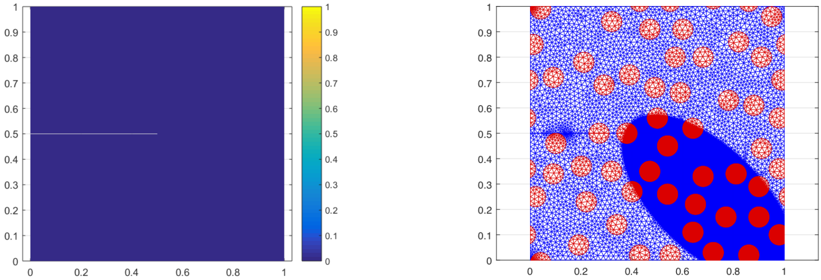

FIGURE 3 – Initial damage field and mesh of the microstructure

Example in 2D

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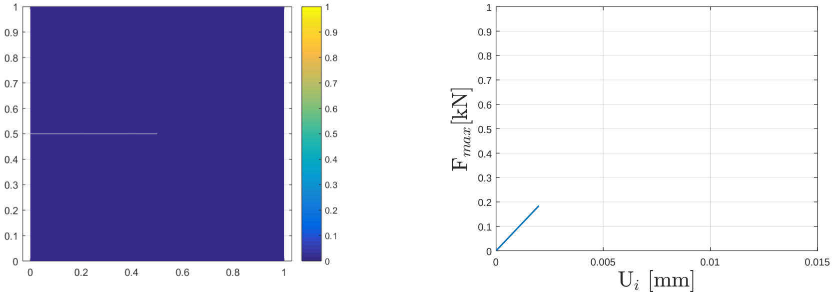

FIGURE 4 – Linear response

Example in 2D

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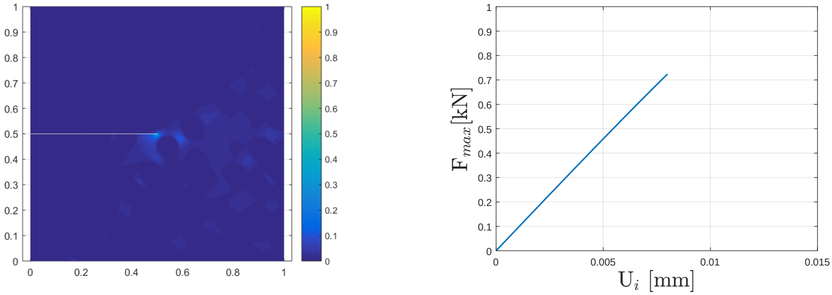

FIGURE 5 – Linear response

Example in 2D

Consider a homogeneous matrix, reinforced with monodisperse spheres :

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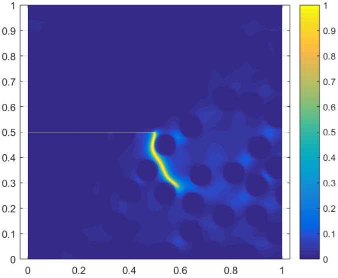

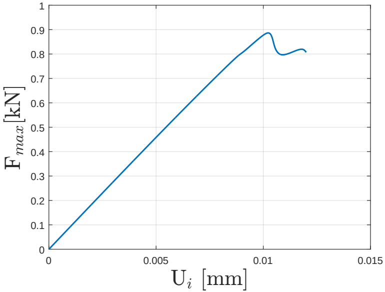

FIGURE 6 – Non-linear response and crack propagation

Example in 2D

Consider a homogeneous matrix, reinforced with monodisperse spheres :

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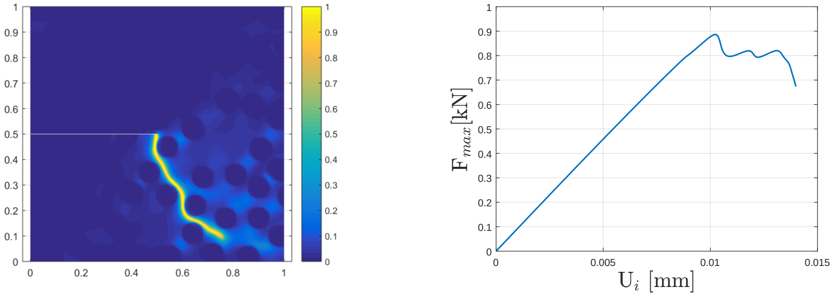

FIGURE 7 – Non-linear response and crack propagation

Example in 2D

Solving the coupled problem for a set of microstructural samples :

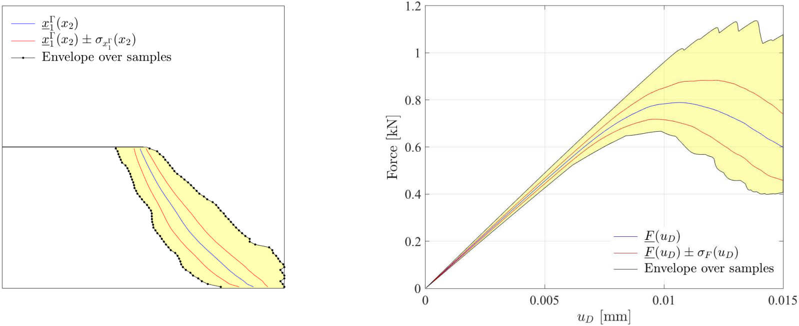

FIGURE 8 – Statistics and envelope on the crack path and the macroscopic response

Outline

Overview

Two-step approach :

- Obtain samples of elasticity fields through local upscaling (under KUBC and SUBC), and project them into the set of isotropic tensors
- Derive a stochastic model to sample these fields with no need to solve the homogenization problems (especially, in the damaged region)

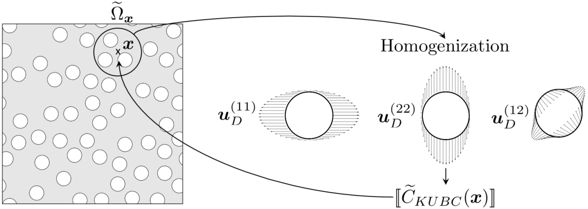

FIGURE 9 – Defining the field of mesoscale elasticity (KUBC)

Impact of the resolution, for $\delta = \widetilde{R}/_{R}$:

- For $\delta \to 0^+$, microscopic fields are recovered
- For $\delta \to +\infty$, the effective properties are obtained

Looking at the projection

The isotropic approximation is defined by the moduli

$$(\widetilde{k}_{BC}(\boldsymbol{x}), \widetilde{\mu}_{BC}(\boldsymbol{x})) = \underset{k>0,\, \mu>0}{\operatorname{argmin}} \; \|[\widetilde{C}_{BC}(\boldsymbol{x})] - 2k[J] - 2\mu[K]\|_F \tag{5}$$

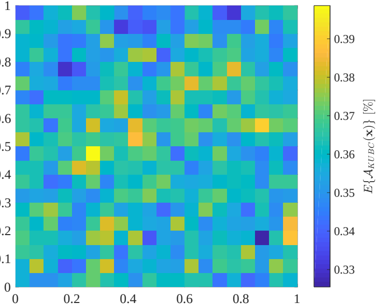

FIGURE 10 – Mean relative errors between the apparent tensor and its isotropic approximation for KUBC (left) and SUBC (right)

Application to the prototypical microstructure

Impact of the resolution for the isotropic approximation (KUBC) :

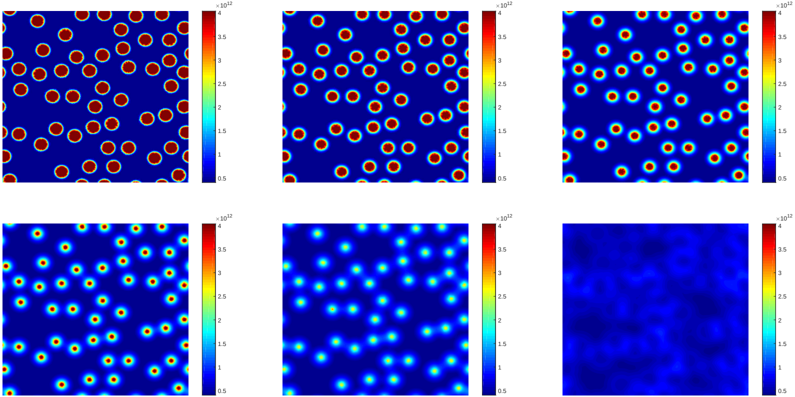

FIGURE 11 – Realization $\boldsymbol{x} \mapsto \|[C(\boldsymbol{x})]\|_F$ for $\delta \in \{0.2, 0.4, 0.6, 0.8, 1, 2\}$

Computational aspects

So far, the strategy requires

- to generate and mesh the microstructure ; and
- to extract and mesh all subdomains, solve two homogenization problems and project the apparent tensors

For a given type of BC : $\approx 120,000$ homogenization problems

Next steps :

- Develop a model for the tensor-valued elasticity fields
- Sample the stochastic models on a coarser grid, and interpolate

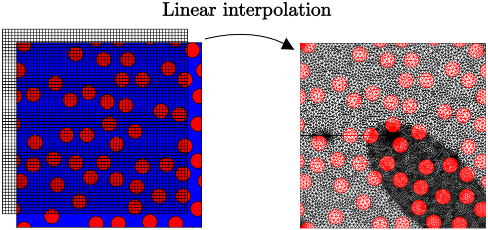

FIGURE 12 – Introducing a coarser grid to reduce computation time

Outline

Construction of the probabilistic model

Let $\{k(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$ and $\{\mu(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$ be the random fields of bulk and shear moduli, and let $\{\boldsymbol{\Xi}(\boldsymbol{x}), \boldsymbol{x} \in \Omega\}$ be a bivariate Gaussian field with independent normalized components

Define the non-Gaussian fields through the MaxEnt-consistent transformations

$$k(\boldsymbol{x}) = F^{-1}_{G(\alpha_k,\theta_k)}\left(F_{N(0,1)}(\Xi_1(\boldsymbol{x}))\right) \tag{6}$$

and

$$\mu(\boldsymbol{x}) = F^{-1}_{G(\alpha_\mu,\theta_\mu)}\left(F_{N(0,1)}(\rho\Xi_1(\boldsymbol{x}) + \sqrt{1-\rho^2}\,\Xi_2(\boldsymbol{x}))\right) \;, \tag{7}$$

where ρ is the correlation coefficient between $k(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$

It follows that

- the first-order marginal probability measure is a bivariate Gamma law ;
- the fields of stiffness and compliance tensors are of second-order

$$E\{\|\boldsymbol{C}(\boldsymbol{x})\|_F^2\} < +\infty \;, \quad E\{\|\boldsymbol{C}(\boldsymbol{x})^{-1}\|_F^2\} < +\infty$$

The SBVP is thus well posed

Identification

Identification strategy :

- Direct estimators for (α_k, θ_k) and (α_μ, θ_μ) and ρ
- Inverse problem for the correlation functions of the underlying Gaussian fields
- Inverse problem for the toughness g_c, using the mean peak force

Results for $\delta = 3$:

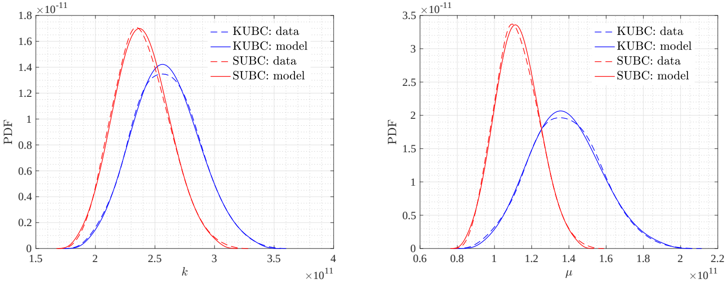

FIGURE 13 – Comparing of the first-order mPDFs for the bulk (left) and shear (right) moduli

Note the ordering with respect to the boundary conditions (well known)

Identification (KUBC)

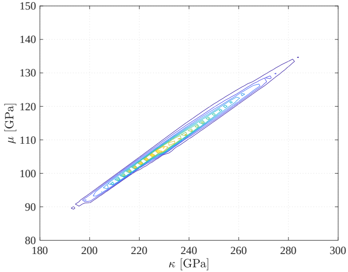

FIGURE 14 – Comparing the jPDFs : reference (left) and model-based (right) estimations

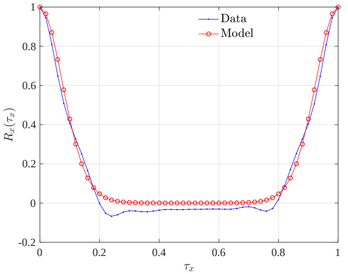

FIGURE 15 – Comparing of the correlation functions for the elastic moduli

Optimization problem

The toughness is identified by imposing a match in mean for the peak force

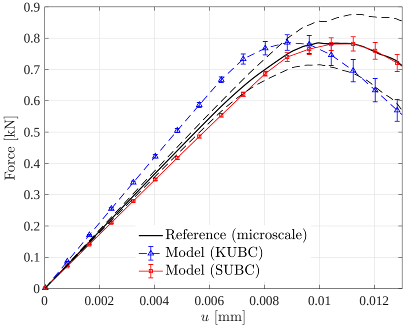

FIGURE 16 – Validation on the macroscopic response

Optimization problem

The toughness is identified by imposing a match in mean for the peak force

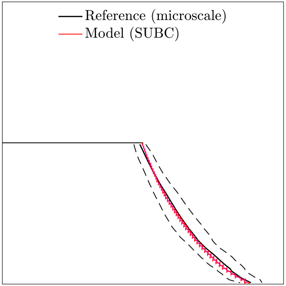

FIGURE 17 – Validation on the crack path (SUBC)

Note that

- similar results are obtained with microstructural and model-based samples
- the variability can be increased (no mesoscale standpoint)
- the correlation between the moduli has no effect

Outline

Conclusion

Mesoscopic perspective on crack propagation in heterogeneous materials :

- Phase-field approach to simulate crack propagation
- Construction and identification of a stochastic model
- Validation on crack path and macroscopic response

It was shown that :

- The framework performs well to predict the mean peak force
- The influence of the BC is significant
- In particular, SUBC provides a better approximation

Ongoing works are focused on

- extending the approach to more complex behaviors ;
- incorporating real experiments ; and
- approaching the whole calibration as an inverse problem

This work has benefited from a French Government grant managed by ANR within the frame of the national program Investments for the Future ANR-11-LABX-022-01

Thank you for the attention