Homogenization, probabilistic realization, and macroscopic analysis of quasi-brittle materials

Reza Abedi
Mechanical, Aerospace & Biomedical Engineering
University of Tennessee Space Institute (UTSI) / Knoxville (UTK)

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- Motivation
Why spatial inhomogeneity is needed in (quasi-brittle) fracture?

- Cracks nucleate from weak points of the material, e.g. voids, microcracks, (grain boundaries), etc. ⇒
  - Deterministic models predict fracture at all points under uniform stress!

Realistic Expectations:

Homogeneous fracture properties ⇒
Everywhere fail at the same time!!

- While homogenized properties are typically suitable for elastic response, they are not appropriate for modeling fracture where from initial defects microcracks are nucleated, resulting in high stress concentration points and stress shielded regions even if the domain is under uniform stress field. This issue is even more important for quasi-brittle materials due to the lack of significant energy dissipative mechanisms in the bulk (e.g. plasticity).
Why randomness is important in (quasi-brittle) fracture?

Scatter in fracture patterns:
Same loading / geometry ⇒ Different fracture patterns (due to random distribution of defects)

Al-Ostaz 1997: Epoxy sheets with holes

Size effect:
as specimen size increases
1. Mean strength decreases
2. Scatter in fracture strength increases.

J Kozicki and J Tejchman (2007) (concrete fracture)

Almost no variability in elastic response

High variability in
• Ultimate strength
• Fracture toughness

Area under the curve

Quasi-brittle fracture of cellular ceramic (Genet 2014)
- RVEs and RVEs
- Homogenization
- Karhunen-Loeve Method
- Macroscopic fracture analysis
Representative Volume Elements (RVEs) versus Statistical Volume Elements (SVEs)

- RVEs are good for many elastic regime problems.
- For fracture modeling (particularly quasi-brittle material):
  - Need to preserve spatial inhomogeneity.
  - Randomness (sample to sample variations).

Ostoja-Starzewski 1998

SVE sizes: Material property is probabilistic.

RVE limit: \( l \) is very large.

SVEs appropriate for fracture modeling (still reduce problem size by homogenization).
1. By using SVEs material inhomogeneities & sample to sample variations (randomness) are preserved.
2. Still no need to resolve all microscale details!
3. A very efficient and accurate model for fracture modeling
Point-wise Statistics: Probability Density Function (PDF), \( P(\bar{s}) \)

- SVE1x1
- SVE2x2
- SVE4x4
- SVE8x8
- SVE16x16
Point-wise Statistics:
Observed size-effect

\[
\mu_{\bar{s}} - \sigma_{\bar{s}}
\]

\[
\mu_{\bar{s}} + \sigma_{\bar{s}}
\]
Computational moving window method:
A novel and simple way to characterize random media

SVE analysis on randomly generated domains and at different locations fully characterizes random material:
1. PDF of all points are obtained.
2. Covariance function is also obtained:

\[ \text{Cov}(a(x^1, x^2)) = \mathbb{E}[(a(x^1) - \mathbb{E}[a(x^1)])(a(x^2) - \mathbb{E}[a(x^2)])] \]

Experimental measurements
Moving window \(\Rightarrow\) auto- and cross-correlation functions

KL Random Field Fracture Strength $\bar{s}(x)$
Sample stochastic fracture results

Realizations for fracture strength based on

SVE1x1  SVE2x2  SVE8x8  Uniform fracture strength

Window sizes uses for statistical volume elements

Fracture patterns under uniform load in horizontal direction

Very unrealistic fracture pattern with uniform fracture strength model
Computational Domain & Loading Conditions

\[ \sigma = ct \]

\[ \Omega \]

\[ l \]

\[ \sigma = ct \]

\[ W \]

\( \sigma \): spatially uniform tensile stress

- Increase linearly with time
- Assumption breaks with onset of fracture

\( c \): load dependent constant
Effect of fracture strength randomness: e.g., SVE1x1

KL random fracture strength $\tilde{s}(x)$
Effect of fracture strength randomness: e.g., SVE1x1

KL random fracture strength $\bar{s}(x)$
Random $\bar{s}(x)$ vs. Homogeneous $\bar{s}(x) = c.t.e.$

Homogeneous $\bar{s}$

Random $\bar{s}$, SVE1x1 sampling
Effect of error tolerance: Space front

Coarse resolution, $\text{tol} = 10^{-8}$

Moderate resolution, $\text{tol} = 10^{-9}$

Fine resolution, $\text{tol} = 10^{-10}$
Effect of error tolerance: Energy analysis

Larger crack length
Lower average damage
But the same maximum stress & energy

Different tolerances -> same macroscopic energy response!
Automated homogenization-based fracture analysis (collaborative with OSU)
Three stages of two-scale model analysis:

1. Realistic image-based virtual microstructure reconstruction
2. Automated mesh generation using CISAMR.
   Evaluating homogenized elastic/fracture properties $C, \bar{s}_n(\theta), \bar{s}_l(\theta)$
3. Microscopic analysis
4. Formulation & calibration of macroscopic interfacial damage model
5. Mesh adaptive aSDG method for macroscopic fracture analysis
Stage 1: Automated microstructure construction and FEM analysis of SVEs (OSU)

- Microstructure reconstruction

Advanced statistical meshing geometry, and optimization algorithms are used to create (real or statistically consistent) high quality FEM meshes from material microstructure.

FEM mesh around inclusions
Stage 1: Automated microstructure construction and FEM analysis of SVEs (OSU)

- SVE analysis

SVEs are homogenized by using different forms of BCs
PDFs of elastic and fracture properties based on SVE size
Angle-dependency of properties

Fracture strength is angle-dependent (depending on the angle of loading), example below shows angular distribution of fracture strength for 4 different SVE sizes.
Size Effect:

Mean value and variations of homogenized properties change based on the size of SVE:

Bulk modulus

Normal strength
Stage 2:
Macroscopic fields for material properties

- Macroscopic field for fracture strength based on homogenization of SVEs
- Statistically consistent fields can also be constructed using known methods such as Karhunen-Loeve method.
Stage 3: Macroscopic fracture analysis

- Dynamic tensile loading
- Response very different from that of a homogeneous medium

Spall simulation can similarly be done
Stage 3: Macroscopic fracture analysis

Fragmentation due to high-rate thermal loading of the ceramic

(a) $\varepsilon_T = -1.0625 \times 10^{-4}$  
(b) $\varepsilon_T = -1.1562 \times 10^{-4}$  
(c) $\varepsilon_T = -1.2188 \times 10^{-4}$

(d) $\varepsilon_T = -1.3125 \times 10^{-4}$  
(e) $\varepsilon_T = -1.4062 \times 10^{-4}$  
(f) $\varepsilon_T = -1.4375 \times 10^{-4}$
- Rock Fracture:
  - Effect of randomness
Hydraulic Fracturing in Rock: Hydraulic Loading Rates

- Rate at which hydraulic loading is applied affects:
  - Perforation activation
  - Degree of crack penetration into rock
Comparison of deterministic and random fracture models

Not much difference at low loading rates:

Deterministic model

Weibull model

Loading rate: $t_r = 1 \text{ s}$
Comparison of deterministic and random fracture models

As loading rate increases deterministic model tends to generate more microcracks.

Deterministic model

Weibull model

Loading rate: $t_r = 100$ ms
Comparison of deterministic and random fracture models

And the fracture pattern from the two models deviates even further at higher loadings:

Loading rate: $t_r = 10 \text{ ms}$
Comparison of details of fracture patterns between the two models

Uniform strength causes very close microcracking as all points experience high stresses.

Nonuniform strength

More realistic response
Comparison of deterministic and random fracture models

Until deterministic model predicts very nonphysical fracture patterns!

Reason: Having weaker points where cracks can nucleate:
1) Releases stress in the neighborhood regions, preventing further crack nucleation.
2) Creates stress concentration ahead of the moving cracks.

Loading rate: \( t_r = 100 \ \mu s \)
Rate effect:

Increases loading rate:
1. Increases maximum stress
2. Increase or keep almost constant displacement jump at full damage
3. Increase or keep almost constant time at full damage
Rate effect:

Fracture energy increases as loading rate increase.

$k$: model parameter

$\log(\hat{\phi}/\phi_s)$ vs $\log(r^s)$
Effective stress

$D_{\text{static}} = f(\sigma_R^{\text{eff}}) =$ Damage that would happen under quasistatic loading.

- $\tilde{\sigma}_B$: Bonded mode Riemann traction that drives damage evolution.

\[
\tilde{\sigma}_B = \frac{w^i Z^i - w^i Z^i}{Z^i + Z^i} = \frac{s^i Z^i - s^i Z^i}{Z^i + Z^i} + \frac{Z^i Z^i}{Z^i + Z^i} [v_i]
\]

Failure criteria:
In Mohr-Coulomb representation:

Two different effective stress models are used
Contact/damage examples

Color: \( \log(\text{strain energy}) \);
Height: \( \text{velocity} \)

Mode I: cyclic loading

cyclic loading for a stiff circular inclusion with an initial defect
Refracturing example

Beginning of unloading

Cracks start to close $\Rightarrow$ high frequency wave scattering

Cracks gradually close during the ambient pressure phases
Refracturing example

Cracks reopen from the source of fluid pressure in the second phase of loading

Time $t = 8.6$ ms

Time $t = 9.2$ ms

Time $t = 9.5$ ms

movie
Refracturing example:
Lower loading rate
Refracturing example: Lower loading rate

The medium is anisotropic with explicit representation of microcracks. At lower loading rate only two cracks are activated.
Compressive mode fracture: Explosive loading

(a) Time $t = 15 \, \mu$s  (b) Time $t = 20 \, \mu$s  (c) Time $t = 25 \, \mu$s

(d) Time $t = 30 \, \mu$s  (e) Time $t = 37.5 \, \mu$s  (f) Time $t = 57.5 \, \mu$s

Rapid unloading
Compressive mode fracture: Uniaxial compressive loading

Comparison of slip lines:

\[ A_0 = 1 \]

\[ A_0 = 0.1 \]

\[ A_0 = 0.01 \]

\[ A_0 = 0.001 \]

For the \( l^2 \) model:
- Fewer cracks experience slip.
- Less coherent slip lines.

For the MC model:
- \( A_0 \) increases:
  - Fewer cracks experience slip.
  - Less coherent slip lines.
- Rock Fracture:
  - Modeling anisotropy (Implicit)
Animation of crack propagation:
Example from dynamic hydraulic fracturing

YouTube link
Dynamic hydraulic fracturing / angular bias

Explosive
Duration: 10-100 Microseconds

Propellant
Duration: 1-10 Milliseconds

Hydraulic
Duration: 1000 Seconds
Implicit modeling of anisotropy
- Rock Fracture:
  - Modeling anisotropy (Explicit)
Explicit modeling of anisotropy

(a) $\theta_0 = 10^\circ$.
(b) $\theta_0 = 20^\circ$.
(c) $\theta_0 = 30^\circ$.
(d) $\theta_0 = 40^\circ$.
(e) $\theta_0 = 60^\circ$.
(f) $\theta_0 = 90^\circ$. 
- Rock Fracture:
  - Homogenizing anisotropic rock
Averaging scheme for angle-dependent crack strength

Circular SVEs
Isotropic rock
Examples of microcrack distribution in rock

Rock with angular bias in microcrack orientation
Anisotropic rock
- Rock Fracture:
  - Macroscopic fracture of homogenized anisotropic rock
Macroscopic fracture response: Hydrostatic tensile stress

Isotropic

Anisotropic, -20 degrees bedding planes
Ongoing works:
Elasticity & fracture random fields

Statistical analysis of multiple related random fields

Realization of multiple random fields

Macroscopic fracture analysis

Arash Noshadravan (Texas A&M)

Soheil Soghrati (OSU) & UT

*Macroscopic fracture analysis (inhomogeneous / anisotropic – elasticity & strength)*
Ongoing works:
Bulk vs. interfacial damage models

Interfacial vs. bulk damage models

Homogeneous

Interfacial

Bulk

Homogeneous

Inhomogeneous

Bulk
Bias in homogenized values based on SVE geometry: shear strength, Square

Small SVE: $\delta = 3.125$
- High strength
- Low strength

Large SVE: $\delta = 12.5$

Square SVEs: shear strength
Bias in homogenized values based on SVE geometry: normal strength, Voronoi

Small SVE: \( \delta = 3.125 \)

Large SVE: \( \delta = 12.5 \)

Isotropic!

Voronoi SVEs: normal strength
Conclusions

1. Material randomness modeled with two different approaches:
   a) Weibull model for fracture strength.
   b) Statistical Volume Elements (SVEs): In this approach homogenized material properties maintain material inhomogeneity and sample-to-sample variations.

2. Stages for SVE-based homogenizations:
   a) Microstructure realized and homogenized by finite element method.
   b) Statistics of homogenized properties is derived (PDF, correlation function).
   c) Random fields consistent with these fields are constructed.
   d) Macroscopic fracture simulations were performed by the aSDG method.

3. Incorporating inhomogeneity in material properties is very important particularly for problems with no macroscopic stress concentration points (e.g. fragmentation problems).

4. In many materials such as rock, modeling anisotropy is as important as modeling inhomogeneity.