Computational & Multiscale Mechanics of Materials

Non-local damage mean-field-homogenization
Stochastic multi-scale methods

FE2 homogenization of cellular structures

DG-based fracture
Nonlocal Gurson to crack transition

July 2020 - CM3 research projects
Direct links

• Data-driven approaches
  – Recurrent Neural Network-accelerated multi-scale simulations in elasto-plasticity
  – Bayesian identification of stochastic MFH model parameters

• Complex constitutive models for failure prediction under complex loading states
  – Shear and necking coalescence model for porous materials
  – Damage-enhanced viscoelastic-viscoplastic finite strain model for crosslinked resin

• Homogenization & Multi-Scale methods
  – Mean-Field-Homogenization for Elasto-Visco-Plastic Composites
  – Micro-structural simulation of fiber-reinforced highly crosslinked epoxy
  – Non-Local Damage Mean-Field-Homogenization
  – Stochastic Homogenization of Composite Materials
  – Stochastic 3-Scale Models for Polycrystalline Materials
  – Computational Homogenization For Cellular Materials
  – Boundary conditions and tangent operator in multi-physics FE
  – Stochastic Multi-Scale Model to Predict MEMS Stiction
  – Multi-Scale Modeling of Nano-Crystal Grain Boundary Sliding

• Fracture Mechanics
  – DG-Based Multi-Scale Fracture, DG-Based Dynamic Fracture
  – DG-Based Damage elastic damage to crack transition
  – Non-local Gurson damage model to crack transition
  – Stochastic Multi-Scale Fracture of Polycrystalline Films

• Smart Composite Materials – Shape Memory Effects
Recurrent Neural Network-accelerated multi-scale simulations in elasto-plasticity

MOAMMM project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 862015 for the project Multi-scale Optimisation for Additive Manufacturing of fatigue resistant shock-absorbing MetaMaterials (MOAMMM) of the H2020-EU.1.2.1. - FET Open Programme

July 2020 - CM3 research projects
Recurrence Neural Network-accelerated multi-scale simulations

- Introduction to non-linear multi-scale simulations
  - FE multi-scale simulations
    - Problems to be solved at two scales
    - Requires Newton-Raphson iterations at both scales
  - Use of surrogate models
    - Train a meso-scale surrogate model (off-line)
      - Requires extensive data
      - Obtained from RVE simulations
    - Use the trained surrogate model during analyses (on-line)
      - Surrogate acts as a homogenised constitutive law
      - Expected speed-up of several orders
Recurrent Neural Network-accelerated multi-scale simulations

• Definition of the surrogate model: Artificial Neural Network

  – Artificial neuron
    • Non-linear function on \( n_0 \) inputs \( u_k \)
    • Requires evaluation of weights \( w_k \)
    • Requires definition of activation function \( f \)

  – Feed-Forward Neuron Network
    • Simplest architecture
    • Layers of neurons
      – Input layer
      – \( N - 1 \) hidden layers
      – Output layers
    • Mapping \( \mathbb{R}^{n_0} \to \mathbb{R}^n: v = g(u) \)
Recurrent Neural Network-accelerated multi-scale simulations

- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for
- Recurrent neural network
  - Allows a history dependent relation
    - Input $u_t$
    - Output $v_t = g(u_t, h_{t-1})$
    - Internal variable $h_t = g(u_t, h_{t-1})$
  - Weights matrices $U, W, V$
    - Trained using sequences
      - Inputs $u_{t-n}^{(p)}, \ldots, u_t^{(p)}$
      - Output $v_{t-n}^{(p)}, \ldots, v_t^{(p)}$
Recurrent Neural Network-accelerated multi-scale simulations

- Recurrent neural network design
  - 1 Gated Recurrent Unit (GRU)
    - Rest gate: select past information to be forgotten
    - Update gate: select past information to be passed along
  - 2 feed-forward NNWs
    - NNW₁ to treat inputs $u_t$
    - NNW₀ to produce outputs $v_t$
  - Details
    - $u_t$: homogenised GL strain $E_M$ (symmetric)
    - $v_t$: homogenised 2nd PK stress $S_M$ (symmetric)
    - 100 hidden variables $h_t$
    - NNW₁ one hidden layer of 60 neurons
    - NNW₀ two hidden layers of 100 neurons
- Data generation
  - Elasto-plastic composite RVE
  - Training stage
    - Should cover full range of possible loading histories
    - Use random walking strategy (thousands)
    - Completes with random cyclic loading (tens)
    - Bounded by a sphere of 10% deformation
Recurrent Neural Network-accelerated multi-scale simulations

- Testing process (new data)
  - On random walk
Recurrent Neural Network-accelerated multi-scale simulations

- Testing process (new data)
  - On cyclic loading

![Image of 3D model and stress-strain curves](image)

**Graphs:**
- **FE vs. RNN**
  - $S_{MXY}$ vs. $E_{MXX}$
  - $S_{MXX}$ vs. $E_{MXX}$
  - $S_{MYY}$ vs. $E_{MXX}$

July 2020 - CM3 research projects
Recurrent Neural Network-accelerated multi-scale simulations

- Multiscale simulation
  - Elasto-plastic composite RVE
  - Comparison FE$^2$ vs. RNN-surrogate
  - Training data
    - Bounded at 10% deformation

<table>
<thead>
<tr>
<th></th>
<th>Off-line</th>
<th>FE$^2$</th>
<th>FE-RNN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data generation</td>
<td>-</td>
<td>-</td>
<td>9000 x 2 h-cpu</td>
</tr>
<tr>
<td>Training</td>
<td>-</td>
<td>-</td>
<td>3 day-cpu</td>
</tr>
<tr>
<td>Simulation</td>
<td>18000 h-cpu</td>
<td>0.5 h-cpu</td>
<td></td>
</tr>
</tbody>
</table>

![Diagram of multiscale simulation with abbreviations and data points A, B, C.](image)

July 2020 - CM3 research projects
Recurrent Neural Network-accelerated multi-scale simulations

- Multiscale simulation
  - Stress-strain distribution at point A
  - Strain within the 10% training range
Recurrent Neural Network-accelerated multi-scale simulations

- Multiscale simulation
  - Stress-strain distribution at point B
  - Strain just at 10% training range
Recurrent Neural Network-accelerated multi-scale simulations

- Multiscale simulation
  - Stress-strain distribution at point C
  - Strain out of 10% training range

[Graph showing reaction force vs. displacement with points A, B, and C labeled, and FE² and FE-RNN curves]

[Heatmaps showing strain distribution with labels EMYY and σMYY]
Recurrent Neural Network-accelerated multi-scale simulations

- MOAMMM FET-OPEN project (https://www.moammm.eu/)
  - ULiège, UCL (Belgium)
  - IMDEA Materials (Spain)
  - JKU (Austria)
  - cirp GmbH (Germany)

- Publications (doi)
  - 10.1016/j.cma.2020.113234
  - Data: 10.5281/zenodo.3902663
Mean-Field-Homogenization for Elasto-Visco-Plastic Composites

SIMUCOMP The research has been funded by the Walloon Region under the agreement no 1017232 (CT-EUC 2010-10-12) in the context of the ERA-NET+, Matera+ framework. The authors gratefully acknowledge the financial support from F.R.S-F.N.R.S. under the project number PDR T.1015.14 STOMMMAC The research has been funded by the Walloon Region under the agreement no 1410246-STOMMMAC (CT-INT 2013-03-28) in the context of M-ERA.NET Joint Call 2014.

July 2020 - CM3 research projects
Mean-Field-Homogenization for elasto-visco-plastic composites

- Multi-scale modeling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)

- Length-scales separation
  
  \[ L_{\text{macro}} \gg L_{\text{VE}} \gg L_{\text{micro}} \]

  For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

  To be statistically representative: Size of the meso-scale volume element larger than the characteristic length of the micro-structure
Mean-Field-Homogenization for elasto-visco-plastic composites

- Incremental-secant mean-field-homogenization
  - Linear Comparison Composite material
    - Defined from unloaded Composite material
  - Solve iteratively the system
    \[
    \begin{align*}
    \Delta \bar{\varepsilon}^r &= v_0 \Delta \varepsilon_0^r + v_1 \Delta \varepsilon_1^r \\
    \Delta \varepsilon_1^r &= \Delta \varepsilon_1 + \Delta \varepsilon_1^{\text{unload}} \\
    \Delta \varepsilon_0^r &= \Delta \varepsilon_0 + \Delta \varepsilon_0^{\text{unload}} \\
    \Delta \varepsilon_1^r &= B^\varepsilon (I, \bar{C}^{\text{Sr}}_0, \bar{C}^{\text{Sr}}_1) : \Delta \varepsilon_0^r
    \end{align*}
    \]
  - With the stress tensors
    \[
    \begin{align*}
    \bar{\sigma} &= v_0 \sigma_0 + v_1 \sigma_1 \\
    \sigma_1 &= \sigma_1^{\text{res}} + \bar{C}^{\text{Sr}}_1 : \Delta \varepsilon_1^r \\
    \sigma_0 &= \sigma_0^{\text{res}} + \bar{C}^{\text{Sr}}_0 : \Delta \varepsilon_0^r
    \end{align*}
    \]
  - For soft matrix response
    - Remove residual stress in matrix
      \[
      \Delta \varepsilon_1^r = B^\varepsilon (I, \bar{C}^{\text{Sr}}_0, \bar{C}^{\text{Sr}}_1) : \Delta \varepsilon_0^r
      \]
    - Or use second moment estimates
      \[
      \sigma_0 = \bar{C}^{\text{Sr}}_0 : \Delta \varepsilon_0^r
      \]

For elasto-plasticity: \( f(\sigma^{\text{eq}}, p) = 0 \)
&
For elasto-visco-plasticity: \( \Delta p = g_v(\sigma^{\text{eq}}, p) \Delta t \)
Mean-Field-Homogenization for elasto-visco-plastic composites

- Incremental-secant mean-field-homogenization
  - Stress tensor (2 forms)
    \[
    \sigma_{I/0} = \sigma^{\text{res}}_{I/0} + \bar{C}^{\text{Sr}}_{I/0} \cdot \Delta \varepsilon^r_{I/0}
    \]
    \[
    \sigma_{I/0} = \bar{C}^{S0}_{I/0} \cdot \Delta \varepsilon^r_{I/0}
    \]
  - Radial return direction toward residual stress
    - First order approximation in the strain increment (and not in the total strain)
    - Exact for the zero-incremental-secant method
  - The secant operators are naturally isotropic

\[
\begin{align*}
\bar{C}^{\text{Sr}} &= 3\kappa^{\text{el}} I^{\text{vol}} + 2 \left( \mu^{\text{el}} - 3 \frac{\mu^{\text{el}}^2 \Delta p}{(\sigma_{n+1} - \sigma^{\text{res}}_n)^{\text{eq}}} \right) I^{\text{vol}} \\
\bar{C}^{S0} &= 3\kappa^{\text{el}} I^{\text{vol}} + 2 \left( \mu^{\text{el}} - 3 \frac{\mu^{\text{el}}^2 \Delta p}{\sigma^{\text{eq}}_{n+1}} \right) I^{\text{vol}} 
\end{align*}
\]
Mean-Field-Homogenization for elasto-visco-plastic composites

- Incremental-secant mean-field-homogenization
  - Second-statistical moment estimation of the von Mises stress
    - First statistical moment (mean value) not fully representative
      \[ \bar{\sigma}_{I/0}^{\text{eq}} = \frac{3}{2} \bar{\sigma}_{I/0}^{\text{dev}} : \bar{\sigma}_{I/0}^{\text{dev}} \]
    - Use second statistical moment estimations to define the yield surface
      \[ \hat{\sigma}_{I/0}^{\text{eq}} = \sqrt{\frac{3}{2} I^{\text{dev}} : (\sigma_{I/0} \otimes \sigma_{I/0})} \geq \bar{\sigma}_{I/0}^{\text{eq}} \]

\[ f(\bar{\sigma}_{n}^{\text{eq}}, p_{n}) \]

\[ \Delta p = g_{v}(\bar{\sigma}_{n}^{\text{eq}}, p)\Delta t \]
Mean-Field-Homogenization for elasto-visco-plastic composites

- Non-proportional loading
  - Spherical inclusions
    - 17% volume fraction
    - Elastic
  - Elastic-perfectly-plastic matrix

\[ \varepsilon_{13} = \varepsilon_{23} \]
\[ \varepsilon_{33} = 2\varepsilon_{11} = 2\varepsilon_{22} \]
Mean-Field-Homogenization for elasto-visco-plastic composites

• Elasto-visco-plasticity
  – Elasto-visco-plastic short fibres
    • Spherical
    • 30 % volume fraction
  – Elasto-visco-plastic matrix

\[
\sigma_{11} \text{[MPa]} \quad \varepsilon_{11} \quad \dot{\varepsilon} = 10^{-3} \text{[1/s]}
\]

\[
\sigma_{\text{eq}} \text{[MPa]} \quad \varepsilon_{11} \quad \dot{\varepsilon} = 10^{-6} \text{[1/s]}
\]
• Extension to finite deformations
  – Formulate everything in terms of elastic left Cauchy-Green tensor
Mean-Field-Homogenization for elasto-visco-plastic composites

- Extension to finite deformations
  - Porous material: homogenized response
Mean-Field-Homogenization for elasto-visco-plastic composites

- Extension to finite deformations
  - Porous material: micro-structure evolution
Mean-Field-Homogenization for elasto-visco-plastic composites

- **SIMUCOMP ERA-NET project (incremental secant MFH)**
  - e-Xstream, CENAERO, ULiège (Belgium)
  - IMDEA Materials (Spain)
  - CRP Henri-Tudor (Luxemburg)

- **PDR T.1015.14 project (MFH with second-order moments)**
  - ULiège, UCL (Belgium)

- **STOMMMAC M.ERA-NET project (MFH for elasto-visco-plastic composites)**
  - e-Xstream, ULiège (Belgium)
  - BATZ (Spain)
  - JKU, AC (Austria)
  - U Luxembourg (Luxemburg)

- **Publications (doi)**
  - [10.1016/j.mechmat.2017.08.006](https://doi.org/10.1016/j.mechmat.2017.08.006)
  - [10.1080/14786435.2015.1087653](https://doi.org/10.1080/14786435.2015.1087653)
  - [10.1016/j.ijplas.2013.06.006](https://doi.org/10.1016/j.ijplas.2013.06.006)
Micro-structural characterization and simulation of fiber-reinforced highly crosslinked epoxy

The authors gratefully acknowledge the financial support from F.R.S.-F.N.R.S. under the project number PDR T.1015.14
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Resin behavior (experiments UCL)
  - Viscoelasto-Viscoplasticity
  - Saturated softening
  - Asymmetry tension-compression
  - Pressure-dependent yield

- To used in micro-structural analysis
  - Behavior in composite is different
  - Introduce a length-scale effect

\[ \frac{\sigma_{eq}}{\sigma_c} = \begin{cases} 
1 & (\text{Drucker-Prager}) \\
2 & (\text{Paraboloid}) \\
3.5 & \\
5 & 
\end{cases} \]

- Exp. Lesser 1997
- Exp. Hinde 2005
- Exp. Sauer 1977

July 2020 - CM3 research projects
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Material changes represented via internal variables
  - Constitutive law $P(F; Z(t'))$
    - Internal variables $Z(t')$
  - Multi-damage strategy
    $P = (1 - D_s)(1 - D_f)\hat{P}$

- Resin model implementation:
  - Requires non-local form [Bažant 1988]
    - Introduction of characteristic length $l_c$
    - Weighted average: $\tilde{Z}(x) = \int_{V_c} W(y; x, l_c) Z(y)dy$
  - Implicit form [Peerlings et al. 1998]
    - New degrees of freedom: $\tilde{Z}$
    - New Helmholtz-type equations: $\tilde{Z} - l_c^2 \Delta \tilde{Z} = Z$
  - Damage evolution laws

\[
\begin{align*}
\ddot{D}_{s/f} &= D_{s/f} (D_{s/f}, F(t), \chi_{s/f}(t); Z(\tau), \tau \in [0, t]) \dot{\chi}_{s/f} \\
\chi_{s/f}(t) &= \max_\tau (\tilde{\gamma}_{s/f}(\tau)) \\
\tilde{\gamma}_{s/f} - l_{s/f}^2 \Delta \tilde{\gamma}_{s/f} &= \gamma_{s/f}
\end{align*}
\]
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Resin model: hyperelastic-based formulation
  - Multiplicative decomposition
    \[ F = F^{ve} \cdot F^{vp}, \quad C^{ve} = F^{veT} \cdot F^{ve}, \quad J^{ve} = \det(F^{ve}) \]
  - Undamaged stress tensor definition
    - Elastic potential \( \psi(C^{ve}) \)
    - Undamaged first Piola-Kirchhoff stress tensor
      \[ \hat{P} = 2F^{ve} \cdot \frac{\partial \psi(C^{ve})}{\partial C^{ve}} \cdot F^{vp^{-T}} \]
    - Undamaged Kirchhoff stress tensors
      - In current configuration
        \[ \hat{\mathbf{r}} = \hat{P} \cdot F^{T} = 2F^{ve} \cdot \frac{\partial \psi(C^{ve})}{\partial C^{ve}} \cdot F^{veT} \]
      - In co-rotational space
        \[ \hat{\tau} = C^{ve} \cdot F^{ve^{-1}} \cdot \hat{\mathbf{r}} \cdot F^{ve^{-T}} = 2C^{ve} \cdot \frac{\partial \psi(C^{ve})}{\partial C^{ve}} \]
  - Apparent stress tensor
    - Piola-Kirchhoff stress
      \[ P = (1 - D_s)(1 - D_f) \hat{P} \]
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- **Resin model: logarithmic visco-elasticity**
  
  - Elastic potentials $\psi_i$:
    \[
    \psi_i(C^{ve}) = \frac{K_i}{2} \ln^2(J^{ve}) + \frac{G_i}{4} (\ln(C^{ve}))^{\text{dev}} : (\ln(C^{ve}))^{\text{dev}}
    \]
  
  - Dissipative potentials $\Upsilon_i$:
    \[
    \Upsilon_i(C^{ve}, q_i) = -q_i : \ln(C^{ve}) + \left[ \frac{1}{18K_i} \text{tr}^2(q_i) + \frac{1}{4G_i} q_i^{\text{dev}} : q_i^{\text{dev}} \right]
    \]

  \[
  \begin{align*}
  q_i^{\text{dev}} &= \frac{2G_i}{g_i} (\ln(C^{ve}))^{\text{dev}} - \frac{1}{g_i} q_i^{\text{dev}} \\
  \text{tr} (q_i) &= \frac{3K_i}{k_i} \ln^2(J^{ve}) - \frac{1}{k_i} \text{tr} (q_i)
  \end{align*}
  \]

  - Total potential $\psi$:
    \[
    \psi(C^{ve}, q_i) = \psi_{\infty}(C^{ve}) + \sum_i [\psi_i(C^{ve}) + \Upsilon_i(C^{ve}, q_i)]
    \]

    \[
    \hat{P} = 2F^{ve} \cdot \frac{\partial \psi(C^{ve})}{\partial C^{ve}} \cdot F^{vp^{-T}}
    \]
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- **Resin model: visco-plasticity**
  - Stress, back-stress
    \[ \varphi = \hat{\tau} - \hat{b} \]
  - Perzina plastic flow rule
    \[ \mathbf{D}^{vp} = \mathbf{F}^{vp} \cdot \mathbf{F}^{vp} = \frac{1}{\eta} \langle \phi \rangle \frac{\partial P}{\partial \hat{\tau}} \]
  - Pressure dependent yield surface
    \[
    \left\{ \begin{array}{l}
    \phi = \left( \frac{\varphi^{eq}}{\sigma_c} \right)^\alpha - \frac{m^\alpha - 1 \text{tr} \varphi}{m + 1} \frac{\sigma_t}{\sigma_c} - \frac{m^\alpha + m}{m + 1} \leq 0 \\
    m = \frac{\sigma_t}{\sigma_c}
    \end{array} \right.
    \]
  - Non-associated flow potential
    \[ p = (\varphi^{eq})^2 + \beta \left( \frac{\text{tr} \varphi}{3} \right)^2 \]
  - Equivalent plastic strain rate:
    \[
    \dot{\varphi} = \frac{\sqrt{\mathbf{D}^{vp} : \mathbf{D}^{vp}}}{\sqrt{1 + 2\nu_p^2}}
    \]
    \[ \nu_p = \frac{9 - 2\beta}{18 + 2\beta} \]
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Resin model: saturated softening
  - Damage evolution
    \[
    \dot{D}_s = H_s (\chi_s - \chi_{s0}) \dot{\varepsilon}_s (D_{s\infty} - D_s) \dot{\varepsilon}_s \\
    \chi_s = \max(\chi_{s0}, \bar{\gamma}_s(\tau)) \\
    \bar{\gamma}_s = l_s^2 \Delta \bar{\gamma}_s = \gamma
    \]
  - Calibration
    • Several hardening/softening combinations
    • Requires composite material tests
      - Length scale effect
        \[l_s = 3 \mu m \left(1 - \frac{D_s}{D_{s\infty}}\right)\]
      - Non-local BC at fiber interface \(\left[\dot{\gamma}_s\right] = 0\)

Pure resin uniaxial tests

- Composites

Experiment
- \(D_{s\infty} = 0.2\)
- \(D_{s\infty} = 0.31\)
- \(D_{s\infty} = 0.51\)
- \(D_{s\infty} = 0.62\)
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Resin model: failure softening
  - Failure surface
    
    \[
    \phi_f = \gamma - a \exp\left(-b \frac{\text{tr}(\hat{\varepsilon})}{3\hat{\varepsilon}^eq}\right) - c
    \]
    
    \[
    \phi_f - r \leq 0; \dot{r} \geq 0; \text{and } \dot{r}(\phi_f - r) = 0
    \]
    
    \[
    \dot{\gamma}_f = \dot{r}
    \]
  - Damage evolution
    
    \[
    \dot{D}_f = H_f (\chi_f) \zeta_f (1 - D_f)^{-\zeta_d} \dot{\chi}_f
    \]
    
    \[
    \chi_f = \max_{\tau} \left(\tilde{\gamma}_f(\tau)\right)
    \]
    
    \[
    \tilde{\gamma}_f - l_f^2 \Delta \tilde{\gamma}_f = \nu_f
    \]
    
    \[
    l_f = 3 \mu m \quad \nabla_0 \tilde{\gamma}_f \cdot \mathbf{N} = 0
    \]
  - Affect ductility
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Resin model: failure softening (2)
  - Damage evolution
    \[ \dot{D}_f = H_f (\chi_f)^{\xi_f} (1 - D_f)^{-\xi_d} \dot{\chi}_f \]
    \[ \tilde{\gamma}_f - l_f^2 \Delta \tilde{\gamma}_f = \gamma_f \]
  - Calibration
    - Recover the epoxy \( G_c \)
    - From localization simulation
      \[ G_c A = \gamma^{\text{end}} - \gamma^{\text{loc}} \]

July 2020 - CM3 research projects
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- **Resin model: Validation**
  - Compression without barrelling effect
  - With barrelling effect
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Composite model: Extraction of $G_c$

\begin{align*}
D & \begin{bmatrix} 1 & 0.5 & 0 \end{bmatrix} \\
\sigma & \begin{bmatrix} 20 \mu \text{m} \times 20 \mu \text{m} \\ 20 \mu \text{m} \times 40 \mu \text{m} \\ 20 \mu \text{m} \times 60 \mu \text{m} \\ 20 \mu \text{m} \times 80 \mu \text{m} \end{bmatrix}
\end{align*}

$\gamma = \frac{Y}{V_0} \left[ \text{MJ} \cdot \text{mm}^{-2} \right]$

$G_c = \frac{1}{2} \left[ \text{J} \cdot \text{m}^{-2} \right]$

$\text{RVE length} [\mu \text{m}]$

July 2020 - CM3 research projects
Micro-structural simulation of fiber-reinforced highly crosslinked epoxy

- Composite model: Validation
  - Compression test

- PDR T.1015.14 project
  - ULiège, UCL (Belgium)

- Publications
  - 10.1016/j.ijsolstr.2016.06.008
  - 10.1016/j.mechmat.2019.02.017
Stochastic Homogenization of Composite Materials

STOMMMAC The research has been funded by the Walloon Region under the agreement no 1410246-STOMMMAC (CT-INT 2013-03-28) in the context of M-ERA.NET Joint Call 2014.
Stochastic Homogenization of Composite Materials

- **Multi-scale modeling**
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem
      (on a meso-scale Volume Element)

- For structures not several orders larger than the micro-structure size
  \[ L_{\text{macro}} \gg L_{\text{VE}} \gg L_{\text{micro}} \]

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

Meso-scale volume element no longer statistically representative:
- Stochastic Volume Elements

July 2020 - CM3 research projects
Stochastic Homogenization of Composite Materials

- Material uncertainties affect structural behaviors

![Graph showing probability distributions and stochastic homogenization process.](image-url)

- Probabilistic homogenization
- Composite stiffness
- Material properties distribution
- Loading
- Stochastic structural analysis

**July 2020 - CM3 research projects**
**Proposed methodology for material:**

- To develop a stochastic Mean Field Homogenization method able to predict the probabilistic distribution of material response at an intermediate scale from micro-structural constituents characterization.

![Diagram showing stochastic homogenization process](image)
• Micro-structure stochastic model
  – 2000x and 3000x SEM images
  – Fibers detection
Stochastic Homogenization of Composite Materials

- Micro-structure stochastic model
  - Histograms of random micro-structures’ descriptors
• Micro-structure stochastic model
  – Dependent variables generated using their empirical copula

```
SEM sample
```

```
Generated sample
```

```
Directly from copula generator
```

```
Statistic result from generated SVE
```

Stochastic Homogenization of Composite Materials

```
Δd
```

```
Δd
```

```
Δd
```

July 2020 - CM3 research projects
Stochastic Homogenization of Composite Materials

• Micro-structure stochastic model
  – Dependent variables generated using their empirical copula

  – Fiber additive process
    1) Define $N$ seeds with first and second neighbors distances
    2) Generate first neighbor with its own first and second neighbors distances
    3) Generate second neighbor with its own first and second neighbors distances
    4) Change seeds & then change central fiber of the seeds
Stochastic Homogenization of Composite Materials

• Micro-structure stochastic model
  – Arbitrary size
  – Arbitrary number
  – Possibility to generate non-homogenous distributions

![Generated Micro-structure and SEM image](image)

Fiber radius in μm

Probability

0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5
2.2 2.4 2.6 2.8 3.0 3.2 3.4 3.6

Generated Micro-structure
SEM image
Stochastic Homogenization of Composite Materials

- Stochastic homogenization of SVEs
  - Extraction of Stochastic Volume Elements
    1. 2 sizes considered: \( l_{SVE} = 10 \, \mu m \) & \( l_{SVE} = 25 \, \mu m \)
    2. Window technique to capture correlation
       \[
       R_{rs}(\tau) = \frac{\mathbb{E}[(r(x) - \mathbb{E}(r))(s(x + \tau) - \mathbb{E}(s))]}{\sqrt{\mathbb{E}[(r - \mathbb{E}(r))^2]} \sqrt{\mathbb{E}[(s - \mathbb{E}(s))^2]}}
       \]
  - For each SVE
    1. Extract apparent homogenized material tensor \( \mathbb{C}_M \)
       \[
       \begin{align*}
       \varepsilon_M &= \frac{1}{V(\omega)} \int_{\omega} \varepsilon_m d\omega \\
       \sigma_M &= \frac{1}{V(\omega)} \int_{\omega} \sigma_m d\omega \\
       \mathbb{C}_M &= \frac{\partial \sigma_M}{\partial \mathbf{u}_M} \otimes \nabla_M
       \end{align*}
       \]
    2. Consistent boundary conditions:
       - Periodic (PBC)
       - Minimum kinematics (SUBC)
       - Kinematic (KUBC)
Stochastic Homogenization of Composite Materials

- Stochastic homogenization of SVEs
  - Apparent properties

Increasing $l_{SVE}$

When $l_{SVE}$ increases
- Average values for different BCs get closer (to PBC one)
- Distributions narrow
- Distributions get closer to normal
Stochastic Homogenization of Composite Materials

- **Stochastic homogenization of SVEs**
  - Correlation study

![Cross-correlation plots for $l_{SVE} = 10 \mu m$ and $l_{SVE} = 25 \mu m$](image)

**Increasing $l_{SVE}$**

1. Auto/cross correlation vanishes at $\tau = l_{SVE}$
2. When $l_{SVE}$ increases, distributions get closer to normal

(1)+(2) Apparent properties are independent random variables

However the distribution depend on

- $l_{SVE}$
- The boundary conditions
Stochastic Homogenization of Composite Materials

- **Mean-Field-homogenization (MFH)**
  - Linear composites
    \[
    \begin{align*}
    \sigma_M &= \bar{\sigma} = v_0 \sigma_0 + v_1 \sigma_I \\
    \epsilon_M &= \bar{\epsilon} = v_0 \epsilon_0 + v_1 \epsilon_I \\
    \epsilon_I &= B^\epsilon(I, C_0, C_I, v_I) : \epsilon_0
    \end{align*}
    \]
    
    \[\hat{C}_M = \hat{C}_M(I, C_0, C_I, v_I)\]
    Defined as random variables

- **Consider an equivalent system**
  - For each SVE realization \(i\):
    \(C_M\) and \(v_I\) known
  - Anisotropy from \(C^i_M\)
    \(\theta\) is evaluated
  - Fiber behavior uniform
    \(\hat{C}_I\) for one SVE
  - Remaining optimization problem:
    \[
    \min_{\frac{a}{b}, \hat{E}_0, \hat{v}_0} \| C_M - \hat{C}_M \left( \frac{a}{b}, \hat{E}_0, \hat{v}_0 ; v_I, \theta, \hat{C}_I \right) \|
    \]
• Inverse stochastic identification
  - Comparison of homogenized properties from SVE realizations and stochastic MFH

\[ \mathbb{C}_M \approx \hat{\mathbb{C}}_M(\hat{I}, \hat{\mathbb{C}}_0, \hat{\mathbb{C}}_I, v_I, \theta) \]
Stochastic Homogenization of Composite Materials

- Incremental-secant Mean-Field-homogenization
  - Virtual elastic unloading from previous state
    - Composite material unloaded to reach the stress-free state
    - Residual stress in components
  - Define Linear Comparison Composite
    - From unloaded state
      \[
      \Delta \varepsilon_{I/0}^r = \Delta \varepsilon_{I/0}^u + \Delta \varepsilon_{I/0}^{unload}
      \]
    - Incremental-secant loading
      \[
      \begin{align*}
      \sigma_M &= \bar{\sigma} = v_0 \sigma_0 + v_1 \sigma_I \\
      \Delta \varepsilon_M^r &= \Delta \varepsilon = v_0 \Delta \varepsilon_0^r + v_1 \Delta \varepsilon_I^r \\
      \Delta \varepsilon_I^r &= \mathcal{B}^\varepsilon(I, C_0^S, C_I^S): \Delta \varepsilon_0^r
      \end{align*}
      \]
    - Incremental secant operator
      \[
      \Delta \sigma_M = C_M^S(I, C_0^S, C_I^S, v_1): \Delta \varepsilon_M^r
      \]
- Non-linear inverse identification
  - First step from elastic response
    \[ \mathbb{C}^{el}_M \approx \mathbb{C}^{el}_M(\mathbb{I}, \mathbb{C}^{el}_0, \mathbb{C}^{el}_I, \nu_I, \theta) \]
  - Second step from the LCC
    - New optimization problem
      \[ \Delta \sigma_M \approx \mathbb{C}^{S}_M(\mathbb{I}, \mathbb{C}^{S}_0, \mathbb{C}^{S}_I, \nu_I, \theta): \Delta \varepsilon_M^r \]
    - Extract the equivalent hardening \( \mathbb{R}(\hat{\rho}_0) \) from the incremental secant tensor
      \[ \mathbb{C}_0^{S} \approx \mathbb{C}_0^{S}(\mathbb{R}(\hat{\rho}_0); \hat{\mathbb{C}}_0^{el}) \]
Non-linear inverse identification
  - Comparison SVE vs. MFH

\[ C_{\text{M}} \simeq \hat{C}_{\text{M}}(\hat{I}, \hat{C}_{0}^{\text{el}}, \hat{C}_{I}^{\text{el}}, v_{I}, \theta) \]

\[ C_{0}^{S} \simeq \hat{C}_{0}^{S}(\hat{R}(\hat{\rho}^{0}); \hat{C}_{0}^{\text{el}}) \]
Damage-enhanced Mean-Field-homogenization

- Virtual elastic unloading from previous state
  - Composite material unloaded to reach the stress-free state
  - Residual stress in components

- Define Linear Comparison Composite
  - From elastic state
    \[ \Delta \varepsilon^r_{I/0} = \Delta \varepsilon_{I/0} + \Delta \varepsilon^\text{unload}_{I/0} \]
  - Incremental-secant loading
    \[ \sigma_M = \bar{\sigma} = v_0 \sigma_0 + v_1 \sigma_I \]
    \[ \Delta \varepsilon^r_M = \bar{\Delta \varepsilon} = v_0 \Delta \varepsilon^r_0 + v_1 \Delta \varepsilon^r_I \]
    \[ \Delta \varepsilon^r_I = B^e (I, (1 - D_0)C^S_0, C^S_I) : \Delta \varepsilon^r_0 \]
  - Incremental secant operator
    \[ \Delta \sigma_M = C^S_M (I, (1 - D_0)C^S_0, C^S_I, v_1) : \Delta \varepsilon^r_M \]
Stochastic Homogenization of Composite Materials

- Damage-enhanced inverse identification
  - Comparison SVE vs. MFH

\[
(1 - D_0)C_0 \approx (1 - \hat{D}_0(\hat{p}_0)) \hat{C}_0^S(R(\hat{p}_0); \hat{C}_0^{el})
\]
Stochastic Homogenization of Composite Materials

- Generation of random field
  - Comparison inverse identification vs. diffusion map –based generator

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson ratio</td>
<td>(\nu_1)</td>
<td>-</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>(E_0)</td>
<td>3000, 4000 (MPa)</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>(\nu_0)</td>
<td>0.25, 0.30 (-)</td>
</tr>
<tr>
<td>Yield stress</td>
<td>(\bar{\sigma}_{Y0})</td>
<td>10, 20, 30 (MPa)</td>
</tr>
<tr>
<td>Ratio of Young's moduli</td>
<td>(\bar{k}<em>{10}/\bar{k}</em>{10}^D)</td>
<td>-</td>
</tr>
<tr>
<td>Ratio of Young's moduli</td>
<td>(\bar{k}<em>{20}/\bar{k}</em>{20}^D)</td>
<td>-</td>
</tr>
<tr>
<td>Ratio of moments</td>
<td>(\bar{m}_0/\bar{m}_0^D)</td>
<td>-</td>
</tr>
<tr>
<td>Orientation angle</td>
<td>(\bar{\theta})</td>
<td>0, 0.5, 0.75</td>
</tr>
</tbody>
</table>

**Legend:**
- \(\times\) Inverse identification
- \(\Diamond\) Generated
Stochastic Homogenization of Composite Materials

- One single ply loading realization
  - Random field and finite elements discretizations
  - Non-uniform homogenized stress distributions
  - Creates damage localization

\[ \sigma_{M_{xx}} \text{ [Mpa]; } \varepsilon_{M_{xx}} = 2.6\% \]

\[ \hat{\sigma}_0 [-]; \varepsilon_{M_{xx}} = 2.6\% \]

\[ \hat{D}_0 [-]; \varepsilon_{M_{xx}} = 2.4\% \]

\[ \hat{D}_0 [-]; \varepsilon_{M_{xx}} = 2.6\% \]
Stochastic Homogenization of Composite Materials

- Ply loading realizations
  - Simple failure criterion at (homogenized stress) loss of ellipticity
  - Discrepancy in failure point
Stochastic Homogenization of Composite Materials

• **STOMM MAC M.ERA-NET project (MFH for elasto-visco-plastic composites)**
  – e-Xstream, ULiège (Belgium)
  – BATZ (Spain)
  – JKU, AC (Austria)
  – U Luxembourg (Luxemburg)

• **Publications (doi)**
  – [10.1016/j.compstruct.2018.01.051](https://doi.org/10.1016/j.compstruct.2018.01.051)
  – [10.1002/nme.5903](https://doi.org/10.1002/nme.5903)
Bayesian identification of stochastic Mean-Field Homogenization model parameters

STOMMAMAC The research has been funded by the Walloon Region under the agreement no 1410246-STOMMAMAC (CT-INT 2013-03-28) in the context of M-ERA.NET Joint Call 2014.
Bayesian identification of stochastic MFH model parameters

- Multi-scale modeling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem
      (on a meso-scale Volume Element)

Identification: Requires identification of micro-scale geometrical and material model parameters
Bayesian identification of stochastic MFH model parameters

- Proposed methodology
  - To develop a stochastic Mean Field Homogenization method whose missing micro-constituents properties are inferred from coupons tests

Micro-structure partly characterized

Multiscale model

Inference of missing microconstituents properties

Macro scale response UQ

Stochastic multiscale model
Bayesian identification of stochastic MFH model parameters

- Fibre distribution effect
  - 2-step homogenization

- For uniaxial tests along direction $\theta$: $\sigma_M = \sigma_M(I(\psi(p)), C_0, C_I ; \theta, \varepsilon_M)$
Bayesian identification of stochastic MFH model parameters

- Fibre distribution effect
  - Skin-core effect

- For uniaxial tests along direction $\theta$: $\sigma_M = \sigma_M \left( I(\psi(p)), c_0, c_1 ; \theta, \varepsilon_M \right)$

Pseudo grains $(k)$ of layer $(l)$

$\pi_p^{(l)}(p^{(k)})$

2-step

$\mathcal{C}_M^{(l)} \left( c_0, c_1, \nu_0^{(l)}, \pi_p^{(l)} \right)$

Voigt

$\mathcal{B}^\varepsilon = I$

$\mathcal{C}_M \left( c_0, c_1 ; l = 0..N \right)$
Bayesian identification of stochastic MFH model parameters

- Experimental characterization
  Fiber orientation and aspect ratio (JKU)
  Composite material response (BATZ)
Bayesian identification of stochastic MFH model parameters

- Assume a distribution of the matrix Young’s modulus
  - Beta distribution \( E_0 \sim \beta_{\alpha,\beta,a,b} \) with \( \beta_{\alpha,\beta,a,b}(y) = \frac{(y-a)^{\alpha-1}(y-b)^{\beta-1}}{(b-a)^{\alpha+\beta+1}B(\alpha,\beta)} \)
  - Matrix Young’s modulus corresponding to experimental measurements
    - \( E_{0c}^{(n)} \) with \( n = 1..n_{\text{total}} \), for all directions and positions
  - Bayes’ theorem
    \[
    \pi_{\text{post}}(\alpha, \beta, a, b | \hat{E}_{0c}) \propto \pi(\hat{E}_{0c} | \alpha, \beta, a, b) \pi_{\text{prior}}(\alpha) \pi_{\text{prior}}(\beta) \pi_{\text{prior}}(a) \pi_{\text{prior}}(b)
    \]
    - Priors: \( \pi_{\text{prior}}(x) = \Gamma_{\alpha,\beta,a,c} \) with \( \Gamma_{\alpha,\beta,a,c}(y) = \frac{(y-a)^{\alpha-1}e^{-\beta(y-a/c)}}{c^\alpha \Gamma(\alpha)} \)
    - Likelihood: \( \pi(\hat{E}_{0c} | \alpha, \beta, a, b) = \prod_{n=1}^{n_{\text{total}}} \beta_{\alpha,\beta,a,b}(E_{0c}^{(n)}) \)
    - Posterior:
      \[
      \pi_{\text{post}}(\alpha, \beta, a, b | \hat{E}_{0c}) \propto \prod_{n=1}^{n_{\text{total}}} \beta_{\alpha,\beta,a,c}(E_{0c}^{(n)}) \pi_{\text{prior}}(\alpha) \pi_{\text{prior}}(\beta) \pi_{\text{prior}}(a) \pi_{\text{prior}}(b)
      \]
Bayesian identification of stochastic MFH model parameters

• Assume a distribution of the matrix Young’s modulus
  
  \[ \pi_{\text{post}}(\alpha, \beta, a, b|\hat{E}_{0c}) \propto \prod_{n=1}^{n_{\text{total}}} \beta_{\alpha,\beta,a,c} \left(E_{0c}^{(n)}\right) \pi_{\text{prior}}(\alpha)\pi_{\text{prior}}(\beta)\pi_{\text{prior}}(a)\pi_{\text{prior}}(b) \]

• \( i = 1..n_{\text{pos}} \), with \( n_{\text{pos}} \) the number of positions tested (5, positions #1-#5)
Bayesian identification of stochastic MFH model parameters

- Validation
  - Evaluate stochastic response at Position 6
    - Perform stochastic homogenization from
      \[ \pi_{\text{post}}(\alpha, \beta, a, b | \bar{E}_{0c}) \]
    - From sampling of \([\alpha, \beta, a, b]\), evaluate
      \[ E_0 \sim \beta_{\alpha, \beta, a, b} \]
    - From sampling of \([E_0]\), evaluate composite response
      \[ E_{\text{MFH}} = E_{\text{MFH}}(I(p), a_r), E_0, \varnothing I, \theta) \]
  - Compare with experimental measurements \(E_{c}^{(6,j)}\)
Bayesian identification of stochastic MFH model parameters

- Extension to non-linear behavior
  - More parameters to infer
    - Matrix Young’s modulus $E_0$
    - Matrix yield stress $\sigma_{Y_0}$
    - Matrix hardening law
      \[ R(p_0) = h p_0^{m_1} (1 - \exp(-m_2 p_0)) \]
    - Effective aspect ratio $a_r$
  - 2-Step MFH model requires many iterations
    - Incremental secant approach
      \[
      \begin{align*}
      \sigma_M &= \bar{\sigma} = v_0 \sigma_0 + v_1 \sigma_I \\
      \Delta \epsilon_M &= \bar{\Delta \epsilon} = v_0 \Delta \epsilon_0^r + v_1 \Delta \epsilon_I^r \\
      \Delta \epsilon_I^r &= \mathbb{B}^\epsilon (I, C_0^S, C_I^S); \Delta \epsilon_0^r
      \end{align*}
      \]
      Too expensive for BI
  - Definition of parameters
Bayesian identification of stochastic MFH model parameters

- Speed up the evaluation of the likelihood
  - Likelihood
    - \( \pi(\hat{\sigma}_M(t)|[\varepsilon_M(t' \leq t), \vartheta]) \)
  - With \( \vartheta = [E_0, \sigma_Y, h, m_1, m_2, a_r] \)
  - 2-Step MFH model
    - \( \sigma_{MFH}(t) \)
    - \( = \sigma_{MFH}(I(\psi(p), a_r), E_0) \)
  - Too expensive for BI
  - Use of a surrogate
    - \( \sigma_{NNW}(t) = \sigma_{NNW}(\varepsilon_M(t), \vartheta, \mathbb{C}_I ; \theta) \)
    - Constructed using artificial Neural Network
    - Trained fusing the 2-Step MFH model
      - \( \sigma_{MFH}(t) \)
      - \( = \sigma_{MFH}(I(\psi(p), a_r), E_0) \)
      - \(, \mathbb{C}_I, \varepsilon_M(t') \)
Bayesian identification of stochastic MFH model parameters

• Assume a noise in the measurements & use surrogate model
  – Measurements at strain $i$ in direction $\theta_j$:
    $$
    \Sigma_{c}^{(i,j,k)} = \sigma_{\text{NNW}}^{(i,j)} \left( \mathbf{e}_{M}^{(i,j)}, \mathbf{\theta}, C_{I} ; \theta_j \right) + \text{noise}^{(i,j)}
    $$
  
  $$
  \begin{align*}
  \pi \left( \Sigma_{c}^{(i,j,k)} \mid \left[ \mathbf{e}_{M}^{(i,j)}, \mathbf{\theta} \right] \right) &= \pi_{\text{noise}} \left( \Sigma_{c}^{(i,j,k)} - \sigma_{\text{NNW}}^{(i,j)} \left( \mathbf{e}_{M}^{(i,j)}, \mathbf{\theta}, C_{I} ; \theta_j \right) \right) \\
  j &= 1..n_{\text{dir}} \text{, with} \\
  n_{\text{dir}} \text{ the number of directions } \theta_j \text{ tested} \\
  i &= 1..n_{\epsilon}^{(j)} \text{, with} \\
  n_{\epsilon} \text{ the number of stress-strain points} \\
  k &= 1..n_{\text{test}}^{(i,j)} \text{, with} \\
  n_{\text{test}}^{(i,j)} \text{ the number of samples tested at point } i \text{ along direction } \theta_j
  
  \end{align*}
  $$

  \begin{align*}
  \pi_{\text{noise}}^{(i,j)} (y) &= \frac{1}{\sqrt{2\pi} \sigma_{\Sigma_{c}}^{(i,j)}} \exp \left( -\frac{y^2}{2\sigma_{\Sigma_{c}}^{(i,j)^2}} \right) \\
  \text{Bayes’ theory:} \\
  \pi_{\text{post}} (\mathbf{\theta} \mid \hat{\mathbf{e}}_{M}, \hat{\Sigma}_{c}) &\propto \pi_{\text{prior}} (\mathbf{\theta}) \prod_{j=1}^{n_{\text{dir}}} \prod_{i=1}^{n_{\epsilon}^{(j)}} \prod_{k=1}^{n_{\text{test}}^{(i,j)}} \pi_{\text{noise}}^{(i,j)} \left( \Sigma_{c}^{(i,j,k)} - \sigma_{\text{NNW}}^{(i,j)} \left( \mathbf{e}_{M}^{(i,j)}, \mathbf{\theta}, C_{I} ; \theta_j \right) \right)
  \end{align*}

July 2020 - CM3 research projects
Bayesian identification of stochastic MFH model parameters

- Results

\[
\pi_{\text{post}}(\theta | \hat{\epsilon}_M, \hat{\Sigma}_c) \propto \pi_{\text{prior}}(\theta) \prod_{j=1}^{n_{\text{dir}}} \prod_{i=1}^{n_{\epsilon}^{(j)}} \prod_{k=1}^{n_{\text{test}}^{(i,j)}} \pi_{\text{noise}} \left( \Sigma_c^{(i,j,k)} - \sigma_{\text{NNW}}^{(i,j)} (\epsilon_M^{(i,j)}, \theta, \mathcal{C}_I ; \theta_j) \right)
\]
Bayesian identification of stochastic MFH model parameters

- Verification

\[
\pi_{\text{post}}(\theta | \hat{\epsilon}_M, \hat{\Sigma}_c) \propto \pi_{\text{prior}}(\theta) \prod_{j=1}^{n_{\text{dir}}} \prod_{i=1}^{n_{\epsilon}^{(j)}} \prod_{k=1}^{n_{\text{test}}^{(i,j)}} \pi_{\text{noise}}^{(i,j)} \left( \Sigma_{c}^{(i,j,k)} - \sigma_{\text{NNW}}^{(i,j)}(\epsilon_{M}^{(i,j)}, \theta, C_{I} ; \theta_{j}) \right)
\]
Bayesian identification of stochastic MFH model parameters

- **STOMMMAC M.ERA-NET project (MFH for elasto-visco-plastic composites)**
  - e-Xstream, ULiège (Belgium)
  - BATZ (Spain)
  - JKU, AC (Austria)
  - U Luxembourg (Luxemburg)

- **Publications (doi)**
  - [10.1016/j.compstruct.2019.03.066](https://doi.org/10.1016/j.compstruct.2019.03.066)
Non-Local Damage Mean-Field-Homogenization

SIMUCOMP The research has been funded by the Walloon Region under the agreement no 1017232 (CT-EUC 2010-10-12) in the context of the ERA-NET +, Matera + framework.
Non-Local Damage Mean-Field-Homogenization

- **Multi-scale modeling**
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)

- **Length-scales separation**

\[ L_{\text{macro}} \gg L_{\text{VE}} \gg L_{\text{micro}} \]

**For accuracy:** Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

**To be statistically representative:** Size of the meso-scale volume element larger than the characteristic length of the microstructure
Non-Local Damage Mean-Field-Homogenization

- **Materials with strain softening**
  - Incremental forms
    - Strain increments in the same direction
      \[ \Delta \varepsilon_I = B \varepsilon \left( I, C_{0}^{alg}, C_{I}^{alg} \right) : \Delta \varepsilon_0 \]
  - Because of the damaging process, the fiber phase is elastically unloaded during matrix softening

- **Solution: new incremental-secant method**
  - We need to define the LCC from another stress state
• Based on the incremental-secant approach
  – Perform a virtual elastic unloading from previous solution
    • Composite material unloaded to reach the stress-free state
    • Residual stress in components
  – Apply MFH from unloaded state
    • New strain increments (>0)
      \[ \Delta \varepsilon_{I/0}^r = \Delta \varepsilon_{I/0} + \Delta \varepsilon_{I/0}^{unload} \]
    • Use of secant operators
      \[ \Delta \varepsilon_{I}^r = B^\varepsilon (I, (1 - D) \tilde{C}_{0}^{Sr}, \tilde{C}_{I}^{S0}) : \Delta \varepsilon_{0}^r \]
    • Possibility of unloading
      \[ \begin{cases} 
        \Delta \varepsilon_{I}^r > 0 \\
        \Delta \varepsilon_{I} < 0 
      \end{cases} \]
Non-Local Damage Mean-Field-Homogenization

- New results for damage
  - Fictitious composite
    - 50%-UD fibres
  - Elasto-plastic matrix with damage
Non-Local Damage Mean-Field-Homogenization

- **Material models**
  - Elasto-plastic material
    - Stress tensor \( \sigma = C^{el} : (\varepsilon - \varepsilon^{pl}) \)
    - Yield surface \( f(\sigma, p) = \sigma^{eq} - \sigma^Y - R(p) \leq 0 \)
    - Plastic flow \( \Delta \varepsilon^{pl} = \Delta p N \quad \& \quad N = \frac{\partial f}{\partial \sigma} \)
  - Local damage model
    - Apparent-effective stress tensors \( \sigma = (1 - D)\hat{\sigma} \)
    - Plastic flow in the effective stress space
    - Damage evolution \( \Delta D = F_D (\varepsilon, \Delta p) \)
  - Non-Local damage model \([\text{Peerlings et al.}, 1996]\)
    - Damage evolution \( \Delta D = F_D (\varepsilon, \Delta \hat{p}) \)
    - Anisotropic governing equation \( \hat{p} - \nabla \cdot (c_g \cdot \nabla \hat{p}) = p \)
Non-Local Damage Mean-Field-Homogenization

- **Laminate studies**
  - Bulk material law
    - Non-local damage-enhanced MFH
    - Intra-laminar failure
    - Account for anisotropy
  - Interface
    - DG/Cohesive zone model
    - Inter-laminar failure

\[ \begin{align*}
\Delta t & \quad \Delta n \\
\Gamma_{Li} & \quad \Gamma_{Li+1} \\
\Omega_i & \quad \Omega_{i+1} \\
\end{align*} \]
Non-Local Damage Mean-Field-Homogenization

- $[45^\circ_4 / -45^\circ_4]_S$- open hole laminate (epoxy- with 60% UD CF)

Intra-laminar failure along fiber directions

Inter-laminar failure matches experimental results
Non-Local Damage Mean-Field-Homogenization

- $[90^\circ / 45^\circ / -45^\circ / 90^\circ / 0^\circ]_S$- open hole laminate
  - Intra-laminar failure along fiber directions (experiments: IMDEA Materials)
Non-Local Damage Mean-Field-Homogenization

- \([90^\circ / 45^\circ / -45^\circ / 90^\circ / 0^\circ]_s\) - open hole laminate
  - Inter-laminar failure compared to experimental results (experiments: IMDEA Materials)
Non-Local Damage Mean-Field-Homogenization

• SIMUCOMP ERA-NET project
  – e-Xstream, CENAERO, ULiège (Belgium)
  – IMDEA Materials (Spain)
  – CRP Henri-Tudor (Luxemburg)

• Publications (doi)
  – 10.1016/j.compstruct.2015.02.070
  – 10.1016/j.ijsolstr.2013.07.022
  – 10.1016/j.ijplas.2013.06.006
  – 10.1007/978-1-4614-4553-1_13
Boundary conditions and tangent operator in multi-physics computational homogenization

ARC 09/14-02 BRIDGING - From imaging to geometrical modelling of complex micro structured materials: Bridging computational engineering and material science
The authors gratefully acknowledge the financial support from F.R.S-F.N.R.S. under the project number PDR T.1015.14

July 2020 - CM3 research projects
Boundary conditions and tangent operator in FE$^2$

- **Multi-scale modeling**
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)

- **Length-scales separation**

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

To be statistically representative: Size of the meso-scale volume element larger than the characteristic length of the microstructure
Boundary conditions and tangent operator in FE²

- Generalized multi-physics representation
  - Strong form \( \mathcal{P} \cdot \nabla_0 = 0 \)
  - Fully-coupled constitutive law \( \mathcal{P} = \mathcal{P}(\mathcal{X}^c, \mathcal{F}; \mathcal{Z}) \)
    - \( \mathcal{F} \): generalized deformation gradient, \( \mathcal{X}^c \): fields appearing in the constitutive relations
    - \( \mathcal{Z} \): internal variables
  - Tangent operators \( \mathcal{L} = \frac{\partial \mathcal{P}}{\partial \mathcal{F}} \) & \( \mathcal{J} = \frac{\partial \mathcal{P}}{\partial \mathcal{X}^c} \) but also \( \mathcal{Y}_F = \frac{\partial \mathcal{Z}}{\partial \mathcal{F}} \) & \( \mathcal{Y}_{\mathcal{X}^c} = \frac{\partial \mathcal{Z}}{\partial \mathcal{X}^c} \)

- Two-scale procedure
  - Macro-scale
    - \( \mathcal{P}_M, \frac{\partial \mathcal{P}_M}{\partial \mathcal{F}_M}, \frac{\partial \mathcal{P}_M}{\partial \mathcal{X}_M^c}, \frac{\partial \mathcal{Z}_M}{\partial \mathcal{F}_M}, \frac{\partial \mathcal{Z}_M}{\partial \mathcal{X}_M^c} \)
  - Microscopic
    - \( \mathcal{P}_m, \mathcal{X}_m^c \)
    - \( \mathcal{P}_m \cdot \nabla_0 = 0 \)
    - \( \mathcal{P}_m(\mathcal{X}_m^c, \mathcal{F}_m; \mathcal{Z}_m) \)
  - Generalized Hill-Mandel condition

July 2020 - CM3 research projects
Boundary conditions and tangent operator in FE²

- **Generalized microscopic boundary conditions**
  - Arbitrary field $k$ kinematics: \( X_m^k = X_M^k + F_M^k \cdot X_m + W_m^k \)
  - Constrained field $k$ equivalence: \( \int_{\omega_0} C_m^k X_m^c^k \, d\omega = \int_{\omega_0} C_m^k d\omega X_M^c^k \)
  - E.g. periodic boundary conditions

Define an interpolant map
\[ S^i = \sum \mathbb{N}_k^i (X_m) a_k^i \]
Substitute fluctuation fields
\[ W_m^k (X_m^+) = S^i (X_m^-) = W_m^k (X_m^-) \]
Boundary conditions and tangent operator in $\text{FE}^2$

- **Microscale BVP**
  - Weak formulation
    \[
    \begin{aligned}
    \mathbf{P}_m \cdot \nabla \omega_0 &= 0 \quad \text{with} \quad \mathbf{P}_m (\mathbf{X}_m^C, \mathbf{F}_m; \mathbf{Z}_m) \\
    \mathbf{X}_m^k &= \mathbf{X}_M^k + \mathbf{F}_M^k \cdot \mathbf{X}_m + \mathbf{W}_m^k \\
    \int_{\omega_0} C_m^k \mathbf{X}_m^C^k \, d\omega &= \int_{\omega_0} C_m^k d\omega \mathbf{X}_M^C^k
    \end{aligned}
    \]
  - Weak finite element constrained form ($\omega_0 = \mathbf{U}_e \omega^e$)
    \[
    \begin{aligned}
    \mathbf{f}_m (\mathbf{U}_m) - \mathbf{C}^T \mathbf{\lambda} &= 0 \\
    \mathbf{C} \mathbf{U}_m - \mathbf{S} \left [ \begin{array}{c} \mathbf{F}_M \\ \mathbf{X}_M^C \end{array} \right ] &= 0
    \end{aligned}
    \]
  - System linearization
    \[
    \begin{aligned}
    \mathbf{Q}^T \frac{\partial \mathbf{f}_m}{\partial \mathbf{U}_m} \mathbf{Q} \delta \mathbf{U}_m + \mathbf{r} - \mathbf{Q}^T \frac{\partial \mathbf{f}_m}{\partial \mathbf{U}_m} \mathbf{C}^T (\mathbf{C}^T)^{-1} \left ( \mathbf{r}_c - \mathbf{S} \left [ \begin{array}{c} \delta \mathbf{F}_M \\ \delta \mathbf{X}_M^C \end{array} \right ] \right ) &= 0 \\
    \mathbf{C} \delta \mathbf{U}_m + \mathbf{r}_c - \mathbf{S} \left [ \begin{array}{c} \delta \mathbf{F}_M \\ \delta \mathbf{X}_M^C \end{array} \right ] &= 0 \quad \& \quad \mathbf{Q} = \mathbf{I} - \mathbf{C}^T (\mathbf{C}^T)^{-1} \mathbf{C}
    \end{aligned}
    \]
Boundary conditions and tangent operator in FE²

- **Multi-scale resolution**
  - System linearization
    \[
    \begin{align*}
    & Q^T \frac{\partial f_m}{\partial \mathbf{u}_m} Q \delta \mathbf{u}_m + \mathbf{r} - Q^T \frac{\partial f_m}{\partial \mathbf{u}_m} C^T (CC^T)^{-1} \left( \mathbf{r}_c - S \left[ \frac{\delta F_M}{\delta \chi^C_M} \right] \right) = 0 \\
    & C \delta \mathbf{u}_m + \mathbf{r}_c - S \left[ \frac{\delta F_M}{\delta \chi^C_M} \right] = 0 \quad \& \quad Q = I - C^T (CC^T)^{-1} C
    \end{align*}
    \]
  - FEM resolution: \( \delta F_M = \delta \chi^C_M = 0 \)
    \[
    \delta \mathbf{u}_m = -\tilde{K}^{-1} \left( \mathbf{r} + \left( C^T - Q^T \frac{\partial f_m}{\partial \mathbf{u}_m} C^T (CC^T)^{-1} \right) \mathbf{r}_c \right)
    \]
  - Constraints effect: \( \mathbf{r} = \mathbf{r}_c = 0 \)
    \[
    \frac{\partial \mathbf{u}_m}{\partial [F_M \chi^C_M]^T} = \tilde{K}^{-1} \left( C^T - Q^T \frac{\partial f_m}{\partial \mathbf{u}_m} C^T (CC^T)^{-1} \right) S
    \]
  - Macro-scale operators at low cost
    \[
    \begin{bmatrix}
    \frac{\partial P_M}{\partial F_M} & \frac{\partial P_M}{\partial \chi^C_M} \\
    \frac{\partial P_M}{\partial Z_M} & \frac{\partial P_M}{\partial \chi^C_M}
    \end{bmatrix} = \left( \bigwedge_{\omega^e} \frac{1}{V(\omega)} \right) \int_{\omega^e_t} \frac{\partial P_m}{\partial F_m} B^e \frac{\partial P_m}{\partial \chi^C_m} N^e \left( \frac{\partial P_m}{\partial Z_m} B^e \frac{\partial P_m}{\partial \chi^C_m} N^e \right) d\omega \begin{bmatrix}
    \frac{\partial \mathbf{u}_m}{\partial [F_M \chi^C_M]^T}
    \end{bmatrix}
    \]
    Only one matrix to factorize
    \[
    \tilde{K} = C^T C + Q^T \frac{\partial f_m}{\partial \mathbf{u}_m} Q
    \]
Boundary conditions and tangent operator in FE²

- Thermo-elasto-plasticity

\[ \begin{align*}
\mathbf{P}_M &= \frac{1}{V(\omega_0)} \int_{\omega_0} \mathbf{P}_m \, d\omega \\
\mathbf{q}_M &= \frac{1}{V(\omega_0)} \int_{\omega_0} \mathbf{q}_m \, d\omega \\
\rho_M C_{vM} &= \frac{1}{V(\omega_0)} \int \rho_m C_{vm} \, d\omega \\
\mathbf{D}_M &= \frac{1}{V(\omega_0)} \int \mathbf{D}_m \, d\omega
\end{align*} \]

\[ \begin{align*}
\frac{\partial \mathbf{P}_M}{\partial \mathbf{F}_M}, & \frac{\partial \mathbf{P}_M}{\partial \mathbf{q}_M}, \frac{\partial \mathbf{P}_M}{\partial \mathbf{D}_M} \\
\frac{\partial \mathbf{q}_M}{\partial \mathbf{F}_M}, & \frac{\partial \mathbf{q}_M}{\partial \mathbf{q}_M}, \frac{\partial \mathbf{q}_M}{\partial \mathbf{D}_M} \\
\frac{\partial \mathbf{D}_M}{\partial \mathbf{F}_M}, & \frac{\partial \mathbf{D}_M}{\partial \mathbf{q}_M}, \frac{\partial \mathbf{D}_M}{\partial \mathbf{D}_M}
\end{align*} \]

\[ \begin{align*}
\mathbf{P}_M \cdot \mathbf{V}_0 &= 0 \\
\rho_M C_{vM} \dot{\mathbf{\varphi}}_M - \mathbf{D}_M + \mathbf{q}_M \cdot \mathbf{V}_0 &= 0
\end{align*} \]
Boundary conditions and tangent operator in FE²

- Thermo-elasto-plasticity

  Thermal-softening hardening
  \[ \tau = (\sigma_0 + H_p)(1 - \omega_T(T - T_0)) \]
Boundary conditions and tangent operator in FE$^2$

- **BRIDGING ARC project (Periodic boundary conditions)**
  - ULiège, Applied Sciences (A&M, EEI, ICD)
  - ULiège, Sciences (CERM)

- **PDR T.1015.14 project (MFH with second-order moments)**
  - ULiège, UCL (Belgium)

- **Publications**
  - [10.1007/s00466-016-1358-z](https://doi.org/10.1007/s00466-016-1358-z)
  - [10.1016/j.commatsci.2011.10.017](https://doi.org/10.1016/j.commatsci.2011.10.017)
Computational & Multiscale Mechanics of Materials

Computational Homogenization For Cellular Materials

ARC 09/14-02 BRIDGING - From imaging to geometrical modelling of complex micro structured materials: Bridging computational engineering and material science

July 2020 - CM3 research projects
Computational Homogenization For Cellular Materials

- Multi-scale modeling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)

- What if homogenized properties loose ellipticity?
  - Buckling of honeycomb structures
Computational Homogenization For Cellular Materials

- **DG-based second-order FE^2**
  - **Macro-scale**
    - High-order Strain-Gradient formulation
    - C^1 weakly enforced by DG
    - Partitioned mesh (∥∥)

  - **Transition**
    - Gauss points on different processors
    - Each Gauss point is associated to one mesh and one solver

  - **Micro-scale**
    - Usual 3D finite elements
    - High-order periodic boundary conditions
      - Non-conforming mesh
      - Use of interpolant functions

\[ \frac{\partial P_M}{\partial F_M} \]
\[ \frac{\partial Q_M}{\partial \nabla F_M} \]
\[ \frac{\partial P_M}{\partial \nabla F_M} \]
\[ \frac{\partial Q_M}{\partial F_M} \]

LIÈGE université
Computational Homogenization For Cellular Materials

- **Instabilities**
  - Micro-scale: buckling
  - Macro-scale: localization bands
  - Captured owing to
    - Second-order homogenization
    - Ad-hoc periodic boundary conditions
    - Path following method
Computational Homogenization For Cellular Materials

• Open-hole plate

• BRIDGING ARC project
  – ULiège, Applied Sciences (A&M, EEI, ICD)
  – ULiège, Sciences (CERM)

• Publications
  – 10.1016/j.mechmat.2015.07.004
  – 10.1016/j.ijsolstr.2014.02.029
  – 10.1016/j.cma.2013.03.024
Stochastic 3-Scale Models for Polycrystalline Materials

3SMVIB: The research has been funded by the Walloon Region under the agreement no 1117477 (CT-INT 2011-11-14) in the context of the ERA-NET MNT framework.
Stochastic 3-Scale Models

- Multi-scale modeling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem
      (on a meso-scale Volume Element)

- For structures not several orders larger than the micro-structure size
  \[ L_{\text{macro}} \gg L_{\text{VE}} \sim L_{\text{micro}} \]

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

Meso-scale volume element no longer statistically representative:
  - Stochastic Volume Elements
Stochastic 3-Scale Models

- Key idea

<table>
<thead>
<tr>
<th>Micro-scale</th>
<th>Meso-scale</th>
<th>Macro-scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>➢ Samples of stochastic volume elements</td>
<td>➢ Intermediate scale</td>
<td>➢ Uncertainty quantification of the macro-scale quantity</td>
</tr>
<tr>
<td>➢ Random microstructure</td>
<td>➢ The distribution of the material property $\mathbb{P}(C)$ is defined</td>
<td>➢ Quantity of interest distribution $\mathbb{P}(Q)$</td>
</tr>
</tbody>
</table>

- Stochastic Homogenization

- Mean value of material property

- Variance of material property

- SFEM

- Probability density

- Quantity of interest
Stochastic 3-Scale Models

- Material structure: grain orientation distribution
  - Grain orientation by XRD (X-ray Diffraction) measurements on 2 µm-thick poly-silicon films

<table>
<thead>
<tr>
<th>Deposition temperature [°C]</th>
<th>580</th>
<th>610</th>
<th>630</th>
<th>650</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;111&gt; [%]</td>
<td>12.57</td>
<td>19.96</td>
<td>12.88</td>
<td>11.72</td>
</tr>
<tr>
<td>&lt;220&gt; [%]</td>
<td>7.19</td>
<td>13.67</td>
<td>7.96</td>
<td>7.59</td>
</tr>
<tr>
<td>&lt;311&gt; [%]</td>
<td>42.83</td>
<td>28.83</td>
<td>39.08</td>
<td>38.47</td>
</tr>
<tr>
<td>&lt;400&gt; [%]</td>
<td>4.28</td>
<td>5.54</td>
<td>3.13</td>
<td>3.93</td>
</tr>
<tr>
<td>&lt;331&gt; [%]</td>
<td>17.97</td>
<td>18.14</td>
<td>21.32</td>
<td>20.45</td>
</tr>
<tr>
<td>&lt;422&gt; [%]</td>
<td>15.15</td>
<td>13.86</td>
<td>15.63</td>
<td>17.84</td>
</tr>
</tbody>
</table>

XRD images provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

July 2020 - CM3 research projects
Stochastic 3-Scale Models

- Application to polycrystalline materials: The micro-scale to meso-scale transition
  - Stochastic homogenization
    \[ \sigma_{m_i} = \mathbf{C}_i : \mathbf{e}_{m_i}, \forall i \]
    Stochastic Homogenization
    \[ \sigma_M = \mathbf{C}_M : \mathbf{e}_M \]
    Samples of the meso-scale homogenized elasticity tensors

- Homogenized Young’s modulus distribution

\[ \text{COV} = \frac{\sqrt{\text{Variance}}}{\text{mean}} \cdot 100\% \]
Stochastic 3-Scale Models

• Application to polycrystalline materials: The meso-scale spatial correlation
  
  – Use of the window technique

  \[
  R_{\mathcal{C}}^{(r,s)}(\tau) = \frac{\mathbb{E} \left[ \left( \mathbb{E}(\mathcal{C}(r)) - \mathbb{E}(\mathcal{C}(r)) \right) \left( \mathbb{E}(\mathcal{C}(s)) \mathbf{x} + \mathbf{\tau} - \mathbb{E}(\mathcal{C}(s)) \right) \right]}{\sqrt{\mathbb{E} \left[ \left( \mathbb{E}(\mathcal{C}(r)) - \mathbb{E}(\mathcal{C}(r)) \right)^2 \right] \mathbb{E} \left[ \left( \mathbb{E}(\mathcal{C}(s)) - \mathbb{E}(\mathcal{C}(s)) \right)^2 \right]}}
  \]

  – Definition of the correlation length

  \[
  L_{\mathcal{C}}^{(r,s)} = \frac{\int_{-\infty}^{\infty} R_{\mathcal{C}}^{(r,s)}(\tau) \, d\tau}{R_{\mathcal{C}}^{(r,s)}(0)}
  \]
Stochastic 3-Scale Models

- Application to polycrystalline materials: The meso-scale random field
  - Accounts for the meso-scale distribution & spatial correlation
  - Needs to be generated using a stochastic model

\( l_{SVE} = 0.1 \, \mu m \)

Random field with different SVEs sizes

\( l_{SVE} = 0.4 \, \mu m \)

- Stochastic model

\[ \mathbb{E}[E_x] \]
\[ \mathbb{E}[E_x] \pm \sigma_{E_x} \]
\[ \text{Samples of the random field} \]

\( \mu_{l_{SVE}} = 0 \)

\( \mu_{l_{SVE}} = 0.4 \)

Random field with different SVEs sizes
Stochastic 3-Scale Models

- Stochastic model of Gaussian meso-scale random fields
  - Define the homogenous zero-mean random field $\mathcal{A}'(x, \theta)$
    - Elasticity tensor $C_M(x, \theta)$ (matrix form $C_M$) is bounded
      $\varepsilon : (C_M - C_L) : \varepsilon > 0 \quad \forall \varepsilon$
    - Use a Cholesky decomposition
      
      $C_M(x, \theta) = C_L + (\bar{A} + \mathcal{A}'(x, \theta))^T (\bar{A} + \mathcal{A}'(x, \theta))$

  - Evaluate the covariance function
    
    $R^{(rs)}_{\mathcal{A}'}(\tau) = \sigma_{\mathcal{A}'(r)}\sigma_{\mathcal{A}'(s)}R^{(rs)}_{\mathcal{A}'}(\tau) = \mathbb{E} \left[ \left( \mathcal{A}'(r)(x) \right) \left( \mathcal{A}'(s)(x + \tau) \right) \right]$

  - Evaluate the spectral density matrix from periodized zero-padded matrix $\tilde{R}^p_{\mathcal{A}'}(\tau)$
    
    $S^{(rs)}_{\mathcal{A}'}[\omega^{(m)}] = \sum_n \tilde{R}^p_{\mathcal{A}'}[\tau^{(n)}] e^{-2\pi i \tau^{(n)} \cdot \omega^{(m)}} \quad \& \quad S_{\mathcal{A}'}[\omega^{(m)}] = H_{\mathcal{A}'}[\omega^{(m)}] H_{\mathcal{A}'}^*[\omega^{(m)}]$

  - Generate a Gaussian random field $\mathcal{A}'(x, \theta)$
    
    $\mathcal{A}'(r)(x, \theta) = \sqrt{2\Delta \omega} \Re \left( \sum_s \sum_m H^{(rs)}_{\mathcal{A}'}[\omega^{(m)}] \eta(s,m) e^{2\pi i (x \cdot \omega^{(m)} + \theta(s,m))} \right)$
Stochastic 3-Scale Models

- Stochastic model of non-Gaussian meso-scale random fields
  - Start from micro-sampling of the stochastic homogenization
    - The continuous form of the targeted PSD function
      \[
      S^{(rs)}_T(\omega) = \Delta \tau S^{(rs)}_V[\omega^{(m)}] = \Delta \tau \sum_n \tilde{R}^{(rs)}_{\mathcal{A}'(r)}[\tau^{(n)}] e^{-2\pi i \tau^{(n)} \cdot \omega^{(m)}}
      \]
    - The targeted marginal distribution density function \(F^{NG(r)}\) of the random variable \(\mathcal{A}'(r)\)
    - A marginal Gaussian distribution \(F^{G(r)}\) of zero-mean and targeted variance \(\sigma_{\mathcal{A}'(r)}\)
  - Iterate

```
Generate Gaussian random vector \(\mathcal{A}'^G(x)\) from \(S^{(rs)}(\omega)\)

Map \(\mathcal{A}'^G(x)\) to a non-Gaussian field:
\[
\mathcal{A}'^{NG(r)}(x) = F^{-1}_{NG(r)} \left( F^{G(r)} \left( \mathcal{A}'^G(r)(x) \right) \right)
\]

Evaluate the PSD \(S^{NG(rs)}(\omega)\) of \(\mathcal{V}^{NG}(x)\)
```

\[
S^{(rs)}(\omega) \leftarrow S^{(rs)}(\omega) \frac{S^{(rr)}_{T}(\omega)S^{(ss)}_{T}(\omega)}{S^{NG(rr)}(\omega)S^{NG(ss)}(\omega)}
\]

No

\[
S^{NG(rs)} \approx S^{T(rs)} ?
\]

July 2020 - CM3 research projects
Stochastic 3-Scale Models

- The meso-scale stochastic model
  - Application to film deposited at 610°C:
  - Comparison between micro-samples and generated fields

![Graph showing probability density](image1)

- Micro-Samples
- Generator

![3D graphs](image2)

- Normalized $\hat{R}_{A'}^{(1,1)}$
- $C_{M11} [\text{GPa}]$

July 2020 - CM3 research projects
Stochastic 3-Scale Models

- Application to polycrystalline materials: The meso-scale to macro-scale transition
  - Convergence in terms of $\alpha = \frac{l_c}{l_{\text{mesh}}}$, the correlation length and macro-mesh ratio
  - The results converge
    - With the mesh size for all the SVE sizes
    - Toward the direct Monte Carlo simulations results

\[
COV = \frac{\sqrt{\text{Variance}}}{\text{mean}} \cdot 100\%
\]

- $l_{\text{SVE}} = 0.1 \, \mu m$
- $l_{\text{SVE}} = 0.2 \, \mu m$
- $l_{\text{SVE}} = 0.4 \, \mu m$
- $l_{\text{SVE}} = 0.6 \, \mu m$
- Direct procedure

Coarse macro-scale mesh
Fine macro-scale mesh
Stochastic 3-Scale Models

• Application to polycrystalline materials: The meso-scale to macro-scale transition
  – Comparison with direct Monte Carlo simulations

Relative difference in the mean: 0.57 %

Relative difference in the mean: 0.44 %
Thermo-mechanical homogenization

- Down-scaling

\[
\varepsilon_M = \frac{1}{V(\omega)} \int_\omega \varepsilon_m d\omega
\]

\[
\nabla_M \vartheta_M = \frac{1}{V(\omega)} \int_\omega \nabla_m \vartheta_m d\omega
\]

\[
\vartheta_M = \frac{1}{V(\omega)} \int_\omega \frac{\rho_m C_{vm}}{\rho_M C_{VM}} \vartheta_m d\omega
\]

- Up-scaling

\[
\sigma_M = \frac{1}{V(\omega)} \int_\omega \sigma_m d\omega
\]

\[
q_M = \frac{1}{V(\omega)} \int_\omega q_m d\omega
\]

\[
\rho_M C_{VM} = \frac{1}{V(\omega)} \int \rho_m C_{vm} dV
\]

- Consistency Satisfied by periodic boundary conditions
Stochastic 3-Scale Models

• Quality factor
  – Micro-resonators
    • Temperature changes with compression/traction
    • Energy dissipation
  – Eigen values problem
    • Governing equations
    \[
    \begin{bmatrix}
    M & 0 \\
    0 & 0
    \end{bmatrix}
    \begin{bmatrix}
    \ddot{u} \\
    \ddot{\theta}
    \end{bmatrix}
    +
    \begin{bmatrix}
    0 & 0 \\
    D_{u\theta}(\theta) & D_{\theta\theta}
    \end{bmatrix}
    \begin{bmatrix}
    \dot{u} \\
    \dot{\theta}
    \end{bmatrix}
    +
    \begin{bmatrix}
    K_{uu}(\theta) & K_{u\theta}(\theta) \\
    K_{u\theta}(\theta) & K_{\theta\theta}(\theta)
    \end{bmatrix}
    \begin{bmatrix}
    u \\
    \theta
    \end{bmatrix}
    =
    \begin{bmatrix}
    F_u \\
    F_{\theta}
    \end{bmatrix}
    \]
    • Free vibrating problem
    \[
    \begin{bmatrix}
    u(t) \\
    \theta(t)
    \end{bmatrix}
    =
    \begin{bmatrix}
    u_0 \\
    \theta_0
    \end{bmatrix}
    e^{i\omega t}
    \]
    • Quality factor
    • From the dissipated energy per cycle
    \[
    Q^{-1} = \frac{2|\Im \omega |}{\sqrt{(\Im \omega)^2 + (\Re \omega)^2}}
    \]
Stochastic 3-Scale Models

- Application of the 3-Scale method to extract the quality factor distribution
  - 3D models readily available
  - The effect of the anchor can be studied

15 \times 3 \times 2 \mu m^3\text{-beam,}\quad \text{deposited at } 610\degree C

15 \times 3 \times 2 \mu m^3\text{-beam & anchor,}\quad \text{deposited at } 610\degree C
**Stochastic 3-Scale Models**

- **Surface topology: asperity distribution**
  - Upper surface topology by AFM (Atomic Force Microscope) measurements on 2 µm-thick poly-silicon films

<table>
<thead>
<tr>
<th>Deposition temperature [°C]</th>
<th>580</th>
<th>610</th>
<th>630</th>
<th>650</th>
</tr>
</thead>
<tbody>
<tr>
<td>Std deviation [nm]</td>
<td>35.6</td>
<td>60.3</td>
<td>90.7</td>
<td>88.3</td>
</tr>
</tbody>
</table>

AFM data provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

July 2020 - CM3 research projects
- Accounting for roughness
  - Second-order homogenization

\[
\tilde{n}_M = \mathbb{C}_M \cdot \varepsilon_M + \mathbb{C}_M^2 \cdot \kappa_M \\
\tilde{m}_M = \mathbb{C}_M^3 \cdot \varepsilon_M + \mathbb{C}_M^4 \cdot \kappa_M
\]

- Stochastic homogenization
  - Several SVE realizations
  - For each SVE $\omega_j = \bigcup_i \omega_i$
  - The density per unit area is now non-constant

Stochastic 3-Scale Models

\[
\begin{align*}
\omega & = \bigcup_i \omega_i \\
\mathbb{C}_M & = \mathbb{C}_M^1, \mathbb{C}_M^2, \mathbb{C}_M^3, \mathbb{C}_M^4 \quad \rightarrow \quad U_M^j \\
\bar{\rho}_M^j
\end{align*}
\]

Meso-scale BVP resolution
Computational homogenization

July 2020 - CM3 research projects
Stochastic 3-Scale Models

- Accounting for roughness
  - Cantilever of $8 \times 3 \times t \mu m^3$ deposited at 610 °C

Flat SVEs (no roughness) - F
Rough SVEs (Polysilicon film deposited at 610 °C) - R
Grain orientation following XRD measurements – $Si_{pref}$
Grain orientation uniformly distributed – $Si_{uni}$
Reference isotropic material – Iso

Roughness effect is the most important for $8 \times 3 \times 0.5 \mu m^3$ cantilevers
Roughness effect is of same importance as orientation for $8 \times 3 \times 2 \mu m^3$ cantilevers
Stochastic 3-Scale Models

• Application to robust design
  – Determination of probabilistic meso-scale properties
  – Propagate uncertainties to higher scale
  – Vibro-meter sensors:
    • Uncertainties in resonance frequency / Q factor

• 3SMVIB MNT.ERA-NET project
  – Open-Engineering, V2i, ULiège (Belgium)
  – Polit. Warszawska (Poland)
  – IMT, Univ. Cluj-Napoca (Romania)

• Publications (doi)
  – 10.1002/nme.5452
  – 10.1016/j.cma.2016.07.042
  – 10.1016/j.cma.2015.05.019
DG-Based (Multi-Scale) Fracture

The research has been funded by the Belgian National Fund for Education at the Research in Industry and Farming. SIMUCOMP The research has been funded by the Walloon Region under the agreement no 1017232 (CT-EUC 2010-10-12) in the context of the ERA-NET +, Matera + framework. The research has been funded by the Walloon Region under the agreement no. 7581-MRIPF in the context of the 16th MECATECH call.

July 2020 - CM3 research projects
**DG-Based Fracture**

- **Hybrid DG/cohesive law formulation**
  - Discontinuous Galerkin method
    - Finite-element discretization
    - Same **discontinuous** polynomial approximations for the
      - **Test** functions $\varphi_h$ and
      - **Trial** functions $\delta \varphi$
  - Can easily be combined with a cohesive law for fracture analyses
    - Interface elements already exist
    - Easy to shift from un-fractured to fractured states
    - Remains accurate before fracture onset (DG formulation)
    - Efficient // implementation
- **Publications (doi)**
  - [10.1016/j.cma.2010.08.014](http://dx.doi.org/10.1016/j.cma.2010.08.014)
• Multi-scale modeling
  – 2 problems are solved concurrently
    • The macro-scale problem
    • The meso-scale problem (on a meso-scale Volume Element)

• For meso-scale volume elements embedding crack propagation
  \[ L_{\text{macro}} \gg L_{\text{VE}} \Rightarrow L_{\text{micro}} \]

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

The crack induces a loss of statistical representativeness
  • Should recover consistency lost due to the discontinuity
Micro-Meso fracture model for intra-laminar failure
  - Epoxy-CF (60%), transverse loading
  - 3 stages captured

Elastic response

Damage due to debonding

Meso-crack

July 2020 - CM3 research projects
• Micro-Meso fracture model for intra-laminar failure (2)
  – Scale transition after softening onset
    • Should not depend on the RVE size
    • Extraction of the meso-scale TSL ($\bar{t}_M$ vs. $\Delta_M$) [Verhoosel et al., IJNME 2010]

• SIMUCOMP ERA-NET project
  – e-Xstream, CENAERO, ULiège (Belgium)
  – IMDEA Materials (Spain)
  – CRP Henri-Tudor (Luxemburg)

• Publication (doi)
  – 10.1016/j.engfracmech.2013.03.018
DG-Based Dynamic Fracture

- Fracture of thin structures

\[ N, M \]

\[ \Delta r, \Delta x \]

- FNRS-FRIA fellowship

- Publications (doi)
  - 10.1002/nme.4381
  - 10.1007/s10704-012-9748-5
  - 10.1016/j.cma.2011.07.008
  - 10.1002/nme.3008

Blast loaded cylinder

Detonated pipe

Fragmented disk

July 2020 - CM3 research projects
DG-Based elastic damage to crack transition

- Capture triaxiality effects: Cohesive Band Model (CBM)
  - Introduction of a uniform band of given thickness $h_b$ [Remmers et al. 2013]

- Methodology
  1. Bulk stress $\sigma$ using non-local damage law
  2. Compute a “band” deformation gradient
     \[ F_b = F + \frac{[u] \otimes N}{h_b} + \frac{1}{2} \nabla_T [u] \]
  3. Band stress $\sigma_b$ using the (local) damage law
  4. Recover traction forces $t([u], F) = \sigma_b \cdot n$

- The cohesive band thickness
  - Evaluated to ensure energy consistency
  - Same dissipated energy as with a damage model
DG-Based elastic damage to crack transition

- Slit plate

$$\begin{align*}
F_x &= k F_y \\
W
\end{align*}$$

Force evolution for $k = 0$

Dissipated energy for $k = 0$

- Non-Local + CBM
- Non-Local

July 2020 - CM3 research projects
DG-Based elastic damage to crack transition

• Slit plate
  – Triaxiality effect through ratio $k$

Force evolution for $k = -0.5$

Dissipated energy for $k = -0.5$

Force evolution for $k = 0.5$

Dissipated energy for $k = 0.5$

Non-Local only
Non-Local + CZM
Non-Local + CBM
DG-Based elastic damage to crack transition

- Comparison with phase field
  - Single edge notched specimen [Miehe et al. 2010]
  - Calibration of damage and CBM parameters with 1D case [Leclerc et al. 2018]
• Compact Tension Specimen:
  – Non-Local damage law combined to cohesive band model improves accuracy

• MRIPF MECATECH project
  – GDTech, UCL, FZ, MECAR, Capital People (Belgium)

• Publication (doi)
  – 10.1002/nme.5618
  – 10.1016/j.cma.2014.06.031
Shear and necking coalescence mechanisms for porous materials

The research has been funded by the Walloon Region under the agreement no. 1610154- EntroTough in the context of the 2016 WallInnov call
Shear and necking coalescence mechanisms for porous materials

- **Objective:**
  - To develop a non-local ductile failure model accounting for complex loading stress states

- **Porous plasticity**

![Diagram showing voids nucleation, growth, and coalescence](image)
Shear and necking coalescence mechanisms for porous materials

- Ductile failure: stress-state dependent fracture strain
  - Stress triaxiality dependent
    \[
    \eta = \frac{p'}{\sigma_{eq}} \in \left[ -\infty, \infty \right] \quad p = \frac{\text{tr} (\sigma)}{3} \quad \sigma_{eq} = \sqrt{\frac{3}{2} \text{dev}(\sigma) : \text{dev}(\sigma)}
    \]
  - Lode dependent
    \[
    \theta = \frac{1}{3} \arccos \left( \frac{27 J_3}{2 \sigma_{eq}^3} \right) \quad J_3 = \text{det}(\text{dev}(\sigma))
    \]

Fracture locus for 2024-T351 aluminum alloy

(Bai & Wierzbicki 2010)
Shear and necking coalescence mechanisms for porous materials

- Hyperelastic-based formulation
  - Multiplicative decomposition
    \[ F = F^e \cdot F^p, \quad C^e = F^{eT} \cdot F^e, \quad J^e = \det(F^e) \]
  - Stress tensor definition
    - Elastic potential \( \psi(C^e) \)
    - First Piola-Kirchhoff stress tensor
      \[ P = 2F^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \cdot F^{p-T} \]
    - Kirchhoff stress tensors
      - In current configuration
        \[ \kappa = P \cdot F^T = 2F^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \cdot F^{eT} \]
      - In co-rotational space
        \[ \tau = C^e \cdot F^{e-1} \cdot \kappa \cdot F^{-T} = 2C^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \]
  - Logarithmic deformation
    - Elastic potential \( \psi \):
      \[ \psi(C^e) = \frac{K}{2} \ln^2(\lambda^e) + \frac{G}{4} \left( \ln(C^e) \right)^{\text{dev}} \cdot \left( \ln(C^e) \right)^{\text{dev}} \]
    - Stress tensor in co-rotational space
      \[ \tau = \frac{K \ln(J^e)}{p} I + G \left( \ln(C^e) \right)^{\text{dev}} \]
Shear and necking coalescence mechanisms for porous materials

- Material changes represented via internal variables
  - Constitutive law $\sigma(\varepsilon; Z(t'))$
  - Internal variables $Z(t')$
    - Plastic flow normal to yield surface $\Phi$
      $$\mathbf{D}^p = \dot{\mathbf{F}}^p \mathbf{F}^{-1} = \dot{\mu} \frac{\partial \Phi}{\partial \sigma}$$
    - Matrix plastic strain rate $\dot{\varepsilon}_m = \frac{\sigma: \mathbf{D}^p}{(1 - f)\sigma_Y}$
    - Volumetric plastic deformation $\dot{\varepsilon}_v = \text{tr} (\mathbf{D}^p)$
    - Deviatoric plastic deformation $\dot{\varepsilon}_d = \sqrt{\frac{2}{3} \text{dev}(\mathbf{D}^p): \text{dev}(\mathbf{D}^p)}$
  - Voids characteristics $\mathbf{Y}$
    - Porosity: $f$
    - Void ligament ratio: $\chi$
    - Void aspect ratio: $W$
    - Void spacing ratio: $\lambda$
Shear and necking coalescence mechanisms for porous materials

- **Non-local formalism**
  - Local form
    - Mesh dependency
  - Requires non-local form [Bažant 1988]
    - Introduction of characteristic length $l_c$
    - Weighted average: $\tilde{Z}_k(x) = \int_{V_c} W(y; x, l_c) Z_k(y) dy$
  - Implicit form [Peerlings et al. 1998]
    - New degrees of freedom: $\tilde{Z}_k$
    - New Helmholtz-type equations: $\tilde{Z}_k - l_c^2 \Delta \tilde{Z}_k = Z_k$
  - Constitutive law $\sigma(\varepsilon, \tilde{Z}(t'); Z(t'))$

- **Non-local multi-mechanisms**

  \[
  \begin{align*}
  \dot{\varepsilon}_m &= \frac{\sigma : D^p}{(1 - f)\sigma_Y} \\
  \dot{\varepsilon}_v &= \text{tr} (D^p) \\
  \dot{\varepsilon}_d &= \sqrt{\frac{2}{3}} \text{dev}(D^p) : \text{dev}(D^p)
  \end{align*}
  \]
  \[
  \begin{align*}
  \dot{\varepsilon}_m - l_c^2 \Delta \varepsilon_m &= \varepsilon_m \\
  \dot{\varepsilon}_v - l_c^2 \Delta \varepsilon_v &= \varepsilon_v \\
  \dot{\varepsilon}_d - l_c^2 \Delta \varepsilon_d &= \varepsilon_d
  \end{align*}
  \]
Shear and necking coalescence mechanisms for porous materials

- Different yield surfaces: void growth
  - Classical GTN model
    - Non-local porosity evolution
      \[ \dot{f} = \dot{f}_{\text{gr}} + \dot{f}_{\text{nu}} + \dot{f}_{\text{sh}} \]
      \[ \dot{f}_{\text{gr}} = (1 - f) \dot{\varepsilon}_v \]
      \[ \dot{f}_{\text{nu}} = A_n (\dot{\varepsilon}_m) \dot{\varepsilon}_m \]
      \[ \dot{f}_{\text{sh}} = k_w \phi_n \left( \frac{p}{\sigma_{\text{eq}}} \right) \phi_\omega (\cos 3\theta) f \dot{\varepsilon}_d \]
    - Yield surface
      \[ \phi_G = \frac{\sigma_{\text{eq}}^2}{\sigma_Y^2} + 2q_1 f \cosh \left( \frac{q_2 p}{2\sigma_Y} \right) - 1 - q_3 f^2 \leq 0 \]
Shear and necking coalescence mechanisms for porous materials

- Different yield surfaces: coalescence
  - Coalescence by necking
    - Yield surface
      \[
      \phi_T = \frac{2}{3} \sigma_{eq} \cos \theta + |p| - C_T^f (\chi, W) \sigma_Y \leq 0
      \]
    - Limit load factor
      \[
      C_T^f (\chi, W) = (1 - \chi^2) \left[ h \left( \frac{1 - \chi}{W} \right)^2 + g \sqrt{\frac{1}{\chi}} \right]
      \]
  - Coalescence by shearing
    - Yield surface
      \[
      \phi_S = \sqrt{3} \tau - C_S^f (\chi) \sigma_Y = \sigma_{eq} \left( \frac{\sin \theta}{2} + \frac{\sqrt{3} \cos \theta}{2} \right) - C_S^f (\chi) \sigma_Y \leq 0
      \]
    - Limit load factor
      \[
      C_S^f (\chi) = \xi (1 - \chi^2)
      \]
Shear and necking coalescence mechanisms for porous materials

- Multi-surface model
  - Effective yield surface

\[ \phi_e = \left( (\phi_G + 1)^m + (\phi_T + 1)^m + (\phi_S + 1)^m \right)^{1/m} \]
Shear and necking coalescence mechanisms for porous materials

- Solution under proportional loadings
  - Constant
    - Stress triaxiality ($\frac{p}{\sigma_{eq}}$); and
    - Normalized Lode angle ($\bar{\theta} = 1 - \frac{6\theta}{\pi}$)
  - $\varepsilon_{dc}$ - ductility = plastic deformation at coalescence onset

\[
\bar{\theta} = 1 \\
\bar{\theta} = 0.5 \\
\bar{\theta} = 0.25 \\
\bar{\theta} = 0. \\
\bar{\theta} = -0.25 \\
\bar{\theta} = -0.5 \\
\bar{\theta} = -1
\]
Shear and necking coalescence mechanisms for porous materials

- Plane strain smooth specimen under tensile loading
  - Verification of the nonlocal model: mesh convergence

\[
L = 12.5 \text{ mm} \\
e_0 = 3 \text{ mm} \\
\xi = 1.015 (\varepsilon_{ds} = 0.95)
\]

Distribution of void ligament ratio \( \chi \)

Capture slant fracture
Shear and necking coalescence mechanisms for porous materials

- Plane strain smooth specimen under tensile loading
  - Effect of $\xi$

  \[
  L = 12.5 \text{ mm} \quad e_0 = 3 \text{ mm}
  \]

Distribution of void ligament ratio $\chi$

- $\varepsilon_{ds} = 0$
- $\varepsilon_{ds} = 0.4$
- $\varepsilon_{ds} = 0.95$
- $\varepsilon_{ds} = 1.25$
- $\varepsilon_{ds} = 1.5$
- No shear
Shear and necking coalescence mechanisms for porous materials

- Axisymmetric (notched) specimens under tensile loading
  - Different notch radii: \( R_0/R_n = 0, 0.2, 0.6, 1, 1.5 \)

- EntroTough WallInnov project: UCL, ULB (Belgium)
  - Publication (doi): 10.1016/j.jmps.2020.103891

\[
R_0 = 3 \text{ mm} \\
R_1 = 6 \text{ mm} \\
L = 25 \text{ mm} \\
\xi = 1.015 \ (\varepsilon_{ds} = 0.95)
\]
Shear and necking coalescence mechanisms for porous materials

- Grooved plate

- EntroTough WalInnov project
  - UCL, ULB (Belgium)

- Publication (doi)
  - 10.1016/j.jmps.2020.103891
Non-local Gurson damage model to crack transition

The research has been funded by the Walloon Region under the agreement no. 7581-MRIPF in the context of the 16th MECATECH call.
Non-local Gurson damage model to crack transition

**Objective:**
- To develop high fidelity numerical methods for ductile failure

**Numerical approach:**
- Combination of 2 complementary methods in a single finite element framework:
  - continuous (damage model)
  - + transition to
  - discontinuous (cohesive band model including triaxiality / strain rate effects)

![Diagram showing the process of crack initiation, propagation, and final failure with stages: Elastic regime, beginning of softening, localization, crack initiation and propagation, and final failure.](image)
Non-local Gurson damage model to crack transition

• Material changes represented via internal variables
  – Constitutive law \( \sigma(\varepsilon;Z(t')) \)
    • Internal variables \( Z(t') \)
  – Different models
    • Lemaitre-Chaboche (degraded properties)
    • Gurson model (yield surface in terms of porosity \( f \))

• Model implementation:
  – Local form
    • Mesh dependency
  – Requires non-local form [Bažant 1988]
    • Introduction of characteristic length \( l_c \)
    • Weighted average: \( \tilde{Z}(x) = \int_{V_c} W(y; x, l_c) Z(y)dy \)
  – Implicit form [Peerlings et al. 1998]
    • New degrees of freedom: \( \tilde{Z} \)
    • New Helmholtz-type equations: \( \tilde{Z} - l_c^2 \Delta \tilde{Z} = Z \)

The numerical results change without convergence

July 2020 - CM3 research projects
Non-local Gurson damage model to crack transition

- **Hyperelastic-based formulation**
  - Multiplicative decomposition
    \[ F = F^e \cdot F^p, \quad C^e = F^{eT} \cdot F^e, \quad J^e = \det(F^e) \]
  - Stress tensor definition
    - Elastic potential \( \psi(C^e) \)
    - First Piola-Kirchhoff stress tensor
      \[ P = 2F^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \cdot F^{p-T} \]
    - Kirchhoff stress tensors
      - In current configuration
        \[ \kappa = P \cdot F^T = 2F^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \cdot F^{eT} \]
      - In co-rotational space
        \[ \tau = C^e \cdot F^{e-1} \cdot \kappa \cdot F^{e-T} = 2C^e \cdot \frac{\partial \psi(C^e)}{\partial C^e} \]
- **Logarithmic deformation**
  - Elastic potential \( \psi \):
    \[ \psi(C^e) = \frac{K}{2} \ln^2(J^e) + \frac{G}{4} (\ln(C^e))^{\text{dev}} : (\ln(C^e))^{\text{dev}} \]
  - Stress tensor in co-rotational space
    \[ \tau = K \ln(J^e) I + G (\ln(C^e))^{\text{dev}} \]
Non-local Gurson damage model to crack transition

- Porous plasticity (or Gurson) approach
  - Competition between 2 plastic modes:

**Growth mode:**
Gurson model

\[
\phi_G = \frac{\tau_{eq}^2}{\tau_Y^2} + 2q_1 \bar{f} \cosh\left(\frac{q_2 p}{2\tau_Y}\right) - 1 - q_3 \bar{f}^2 \leq 0
\]

**Coalescence mode:**
Thomason model

\[
\phi_T = \frac{2}{3} \tau_{eq} + |p| - C_T^f (\chi) \tau_Y \leq 0
\]
Non-local Gurson damage model to crack transition

- Hybrid DG model: use of a Cohesive Band Model (CBM)
  - Principles
    - Substitute TSL of CZM by the behavior of a uniform band of thickness $h_b$ [Remmers et al. 2013]
  - Localization criterion
    - Thomason: $N \cdot \tau \cdot N - C^f_I \tau_y \geq 0$
  - Methodology [Leclerc et al. 2018]
    1. Compute a band strain tensor $F_b = F + \left[ u \right] \otimes N + \frac{1}{2} \nabla_T \left[ u \right]$
    2. Compute a band stress tensor $\sigma_b(F_b; Z(\tau))$ using the same CDM as bulk elements
    3. Recover a surface traction $t(\left[ u \right], F) = \sigma_b \cdot n$

- What is the effect of $h_b$ (band thickness)
  - Recover the fracture energy
Non-local Gurson damage model to crack transition

- Comparison with literature [Huespe2012, Besson2003]

Slanted plane strain specimen

Cup-cone in round bar

$\hat{p}$ $\begin{array}{c} 0 \\ 0.75 \\ > 1.5 \end{array}$
Non-local Gurson damage model to crack transition

• Grooved plate

![Image of grooved plate]

• MRIPF MECATECH project
  – GDTech, UCL, FZ, MECAR, Capital People (Belgium)

• Publication (doi)
  – 10.1002/nme.5618
  – 10.1016/j.ijplas.2019.11.010
Stochastic Multi-Scale Fracture of Polycrystalline Films

Robust design of MEMS: Financial support from F. R. S. - F. N. R. S. under the project number FRFC 2.4508.11

July 2020 - CM3 research projects
Stochastic Multi-Scale Fracture of Polycrystalline Films

- **Multi-scale modeling**
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem
      (on a meso-scale Volume Element)

- For meso-scale volume elements not several orders larger than the micro-structure size and embedding crack propagations

\[ L_{\text{macro}} \gg L_{\text{VE}} \approx ? L_{\text{micro}} \]

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

Meso-scale volume element no longer statistically representative:
- Stochastic Volume Elements
- Should recover consistency lost due to the discontinuity
Stochastic Multi-Scale Fracture of Polycrystalline Films

- Micro-scale model: Silicon crystal
  - Different fracture strengths and critical energy release rates
  - Define a “continuous” strength mapping
Stochastic Multi-Scale Fracture of Polycrystalline Films

- Micro-scale model: Polycrystalline films
  - Discontinuous Galerkin method
  - Extrinsic cohesive law
  - Intra/Inter granular fracture
  - Accounts for interface orientation

\[ \Delta (t) \]

\[ \tau_c [\text{GPa}] \]

\[ \theta \]

\[ \phi \]

\[ G_c \]

\[ \Delta_c \]

\[ \Delta \]
Stochastic Multi-Scale Fracture of Polycrystalline Films

- Stochastic micro-scale to meso-scale model
  - Several SVE realizations (random grain orientation)
  - Extraction of consistent meso-scale cohesive laws
    - $\bar{t}_M$ vs. $\Delta_M$
    - for each SVE sample
  - Resulting meso-scale cohesive law distribution

\[ \delta \bar{t}_M = \delta \sigma_M \cdot e_X \]
\[ \delta \Delta_M = \delta u^m - L_{\text{cell}} C_M^{-1} : e_X \otimes e_X \cdot \delta \bar{t}_M \]
Stochastic Multi-Scale Fracture of Polycrystalline Films

• **Macro-scale simulation**
  – Finite element model non-conforming to the grains
  – Use homogenized (random) meso-scale cohesive laws as input

• **Collaboration for experiments**
  – UcL (T. Pardoen, J.-P Raskin)

• **Publications**
  – [10.1007/s00466-014-1083-4](https://doi.org/10.1007/s00466-014-1083-4)
Smart Composite Materials

This project has been funded with support of the European Commission under the grant number 2012-2624/001-001-EM. This publication reflects the view only of the author, and the Commission cannot be held responsible for any use which may be made of the information contained therein.
Smart Composite Materials

- **Electro-thermo-mechanical coupling**
  - Finite field variation formulation
  - Strong coupling

\[
\begin{align*}
\frac{\partial N}{\partial \Omega} & = 0 \\
\frac{\partial D}{\partial \Omega} & = 0 \\
\mathbf{x} = \varphi(X) \\
\partial_D \Omega_0 & = \partial_D \Omega
\end{align*}
\]

**Conservation of electric charge**

\[
\begin{align*}
J_e \cdot \mathbf{V}_0 & = 0 \\
J_e & = J_e(F, \mathbf{V}_0, V, \mathbf{V}_0 \vartheta, \vartheta; Z)
\end{align*}
\]

**Conservation of energy**

\[
\begin{align*}
\rho C_v \dot{\vartheta} - D + J_y \cdot \mathbf{V}_0 & = 0 \\
J_y & = \mathbf{q} + \nabla J_e \\
\mathbf{q} & = \mathbf{q}(F, V, \mathbf{V}_0 \vartheta, \vartheta; Z)
\end{align*}
\]

**Conservation of momentum balance**

\[
\begin{align*}
\mathbf{P} \cdot \mathbf{V}_0 & = 0 \\
\mathbf{P} & = \mathbf{P}(F, \vartheta; Z) \\
D & = \beta \dot{p} + \vartheta \frac{\partial W^e}{\partial \vartheta}
\end{align*}
\]
Two-way electro-thermal coupling

- Seebeck coefficient $\alpha$
- Finite strain conductivities $\mathbf{K}(V, \vartheta) = \mathbf{F}^{-1} \cdot \mathbf{k}(V, \vartheta) \cdot \mathbf{F}^{-T} \mathbf{J}$ and $\mathbf{L}(V, \vartheta) = \mathbf{F}^{-1} \cdot \mathbf{l}(V, \vartheta) \cdot \mathbf{F}^{-T} \mathbf{J}$

\[
\begin{pmatrix}
\mathbf{J}_x \\
\mathbf{J}_y
\end{pmatrix} =
\begin{pmatrix}
\mathbf{L}(V, \vartheta) & \alpha \mathbf{L}(V, \vartheta) \\
\mathbf{V} \mathbf{L}(V, \vartheta) + \alpha \mathbf{T} \mathbf{L}(V, \vartheta) & \mathbf{K}(V, \vartheta) + \alpha \mathbf{V} \mathbf{L}(V, \vartheta) + \alpha^2 \mathbf{T} \mathbf{L}(V, \vartheta)
\end{pmatrix}
\begin{pmatrix}
-\nabla_0 V \\
-\nabla_0 \vartheta
\end{pmatrix}
\]

Non energetically conjugated

Change of variables

\[
\begin{align*}
 f_V &= -\frac{V}{\vartheta} \\
 f_\vartheta &= \frac{1}{\vartheta}
\end{align*}
\]

\[
\begin{pmatrix}
\mathbf{J}_x \\
\mathbf{J}_y
\end{pmatrix} =
\mathbf{Z}(\mathbf{F}, f_V, f_\vartheta)
\begin{pmatrix}
\nabla_0 f_V \\
\nabla_0 f_\vartheta
\end{pmatrix}
\]

- The coefficients matrix $\mathbf{Z}(\mathbf{F}, f_V, f_\vartheta)$ is symmetric and definite positive
Smart Composite Materials

- **Thermo-mechanical shape memory polymer**
  - Deformations above glass transition temperature $\vartheta_g$ (1)
  - Fixed once cooled down below $\vartheta_g$ (2 & 3)
  - Recovery once heated up (4)

- **Elasto-visco-plastic model constitutive behavior**
  - Different mechanisms ($\alpha$)
    - Multiplicative decomposition
      \[ F(\alpha) = F^e(\alpha)F^p(\alpha) \]
    - Free energy
      \[ \psi = \sum_\alpha \psi(\alpha) \left( C^e(\alpha), \vartheta \right) \]
    - Thermo-visco-plasticity
      \[ \tau(\alpha) = T \left( C^e(\alpha), F^p(\alpha), \dot{\vartheta}(\alpha), \vartheta, \xi(\alpha) \right) \]
  - Stress and dissipation
    \[ P = P(F, \vartheta; F^p(\alpha), p(\alpha), \xi(\alpha)) \]
    \[ D = \beta \dot{p}(\alpha) \tau(\alpha) \]

[V. Srivastav et. al, 2010]
Smart Composite Materials

- Elasto-visco-plastic behavior of thermo-mechanical shape memory polymer

Refs. by [V. Srivastav et. al, 2010]
• Recovery of a shape memory composite unit cell
  – Carbon Fiber reinforced SMP
  – Shape memory effect triggered by Joule effect
  – Test with compressive force recovery:
    • #1: Compression deformation obtained above $\vartheta_g$
    • #2: Fixation of the deformation above $\vartheta_g$
    • #3: Reheat above $\vartheta_g$ at constant deformation:
      recovery force, the cell wants to expend
    • #4: Release deformation/stress
      recovery force vanishes
Smart Composite Materials

- **Recovery of a shape memory composite unit cell**
  - Carbon Fiber reinforced SMP
  - Triggered by Joule effect

![Graph showing the relationship between various parameters such as voltage (U), stress (σ), temperature (θ), and strain (ε). The graph illustrates the recovery process of a shape memory composite unit cell.]
Smart Composite Materials

- **Discontinuous Galerkin implementation**
  - Finite-element discretization
  - Same *discontinuous* polynomial approximations for the
    - **Test** functions $\varphi_h$ and
    - **Trial** functions $\delta \varphi$
  - Extended to non-linear electro-thermo-mechanical coupling

- **Publication (doi)**
  - 10.1007/s11012-017-0743-9
  - 10.1016/j.jcp.2017.07.028
Multi-Scale Modeling of Nano-Crystal Grain Boundary Sliding
Multi-Scale Modeling of Nano-Crystal Grain Boundary Sliding

- 2-scale framework
  - Macro-scale: Finite Elements
  - Micro-scale: Quasi-Continuum

Grain-boundary sliding/opening characterization

Crystal plasticity characterization by nano-indentation
Multi-Scale Modeling of Nano-Crystal Grain Boundary Sliding

- **Grain size effect**
  - Competition between inter-intra granular

Grain size: 6.56 nm

Grain size: 3.28 nm

- **Effect of nano-voids in the grain boundaries**
  - Different deformation mechanism
  - Lower yield stress

- **Collaboration**
  - EC Nantes, Univ. of Vermont, Oxford

- **Publications**
  - [10.1016/j.commatsci.2014.03.070](https://doi.org/10.1016/j.commatsci.2014.03.070)
  - [10.1016/j.actamat.2013.10.056](https://doi.org/10.1016/j.actamat.2013.10.056)
  - [10.1016/j.jmps.2013.04.009](https://doi.org/10.1016/j.jmps.2013.04.009)
Stochastic Multi-Scale Model to Predict MEMS Stiction

3SMVIB: The research has been funded by the Walloon Region under the agreement no 1117477 (CT-INT 2011-11-14) in the context of the ERA-NET MNT framework. The research has been funded by the Belgian National Fund for Education at the Research in Industry and Farming.
Stochastic Multi-Scale Model to Predict MEMS Stiction

- **Stiction (adhesion of MEMS)**
  - Different physics at the different scales
  - Elastic or Elasto-plastic behaviors
  - Due to van der Waals (dry environment) and/or capillary (humid environment) forces

- **Requires surfaces topology knowledge (AFM measures)**
  - Subject to uncertainties
Stochastic Multi-Scale Model to Predict MEMS Stiction

- Deterministic multi-scale models for van der Waals forces
  - Extraction of meso-scale adhesive forces
  - Using statistical representations of the rough surface (average solution)
  - Account for induced elasto-plasticity (cyclic loading)

\[
F_n \quad 2a \quad z_0 \\
2c \\
\text{van der Waals/Hertz forces at the asperity level}
\]

MEMS stiction

\[
t \quad g \\
s \quad l \\
\text{AFM measurement}
\]

Loading cycle

\[
F_{n=1}/(N/\sigma_\gamma) \\
\text{Meso-scale adhesive forces in terms of loading cycle}
\]
Stochastic Multi-Scale Model to Predict MEMS Stiction

- New multi-scale models with capillary effect
  - Extraction of meso-scale adhesive-forces from a single surface measurement
  - Depends on the surface sample measurement location
  - Motivates the development of a stochastic multi-scale method

![AFM measurement](image)

![Capillary/Hertz forces model](image)

![Humidity 0.7](image)

Meso-scale adhesive forces in terms of surface sample
Stochastic Multi-Scale Model to Predict MEMS Stiction

• Stochastic multi-scale model: From the AFM to virtual surfaces

Enforce statistical moments with maximum entropy method

\[
m_i = \int_R z^i p_Z(z) \, dz
\]
\[
p_Z = \arg \max - \int_R p_Z(z) \ln(p_Z(z)) \, dz
\]

Evaluate PSD from covariance

\[
\tilde{R}(\tau) = \mathbb{E}[z(x), z(x + \tau)]
\]
\[
S_Z(\tau) = \int_{R^2} \exp(-i\zeta \cdot \tau) \tilde{R}_Z(\tau) \, d\zeta
\]

AFM measurement

Height Probability Density Function

Power spectrum density

Generated non-Gaussian surface samples
Stochastic Multi-Scale Model to Predict MEMS Stiction

- Stochastic multi-scale model: Evaluate meso-scale surface forces

Generated non-Gaussian surface samples

Computed meso-scale adhesive forces
**Stochastic Multi-Scale Model to Predict MEMS Stiction**

- **Stochastic multi-scale model:** Stochastic model of meso-scale adhesion forces

**Definition of parameter vector** $\nu$

$$\tilde{f}(\tilde{d}) = \Phi(\tilde{d}, \nu)$$

**Enforce physical constraints**

$$\nu^{(i)} \rightarrow q^{(i)}$$

**Principal component analysis from covariance matrix $[\tilde{R}_q]$ of vectors $q^{(i)}$**

$$\eta^T = (q - \bar{q})^T [A][\lambda]^{-1/2}$$

**Polynomial chaos expansion**

$$\eta^{PC} = \sum c_\alpha \Psi_\alpha(\xi)$$

**Computed meso-scale adhesive forces**

**Generated adhesive forces**

July 2020 - CM3 research projects
Stochastic Multi-Scale Model to Predict MEMS Stiction

- Stochastic multi-scale model: Stochastic MEMS stiction analyzes

Stochastic finite elements (random contact law variable)

Generated meso-scale adhesive forces

Stiction risk

[Exp data] [Xue et al. 2008]

Num results: mean

Num results: 95% range

Num results: 60% range

Non-Gaussian

Gaussian
Stochastic Multi-Scale Model to Predict MEMS Stiction

- Application to robust design
  - Determination of probabilistic meso-scale properties
  - Propagate uncertainties to higher scale
  - Vibro-meter sensors:
    - Uncertainties in stiction risk

- 3SMVIB MNT.ERA-NET project
  - Open-Engineering, V2i, ULiège (Belgium)
  - Polit. Warszawska (Poland)
  - IMT, Univ. Cluj-Napoca (Romania)

- FNRS-FRIA fellowship

- Publications (doi)
  - 10.1109/JMEMS.2018.2797133
  - 10.1016/j.triboint.2016.10.007
  - 10.1007/978-3-319-42228-2_1
  - 10.1016/j.cam.2015.02.022
  - 10.1016/j.triboint.2012.08.003
  - 10.1007/978-1-4614-4436-7_11
  - 10.1109/JMEMS.2011.2153823
  - 10.1063/1.3260248