Gradient-Extended Damage Modeling Of Heterogeneous Microstructures Using The Fast Fourier Transforms Method

1. Introduction
2. Material Model Formulation
3. Damage Models
4. Coupling Scheme
5. Numerical Examples
6. Summary

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1. Introduction

The Object

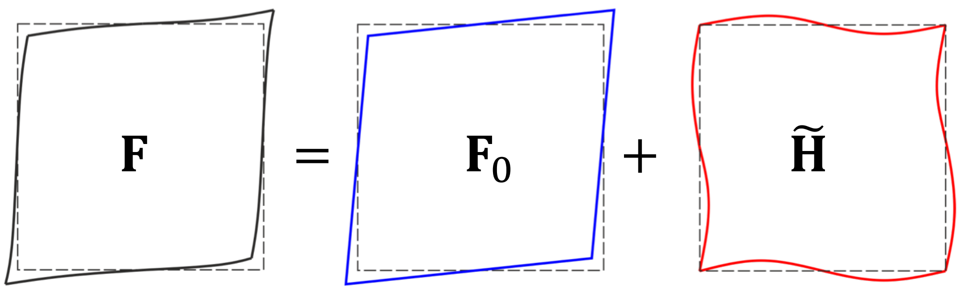
- Predict the homogenized mechanical response of a composite by means of the Fast Fourier Transform (FFT)

The Scope

- Isothermal quasi-static process (Helmholtz free energy)
- Large deformation model (Neo-Hookean)
- Matrix material shows isotropic elastic-damage behavior
- Fibers are isotropic elastic

2. Material Model Formulation

2.1 Boundary value problem



Deformation gradient decomposed into its average and fluctuation field

Periodic boundary conditions

- $\boldsymbol{u}$ periodic
- $\boldsymbol{t}$ anti-periodic

Field equations

- $\mathrm{Div}(\mathbf{P}(\boldsymbol{X})) = \mathbf{0}$ $\quad \boldsymbol{X}$ in Ω
- $\mathbf{F}(\boldsymbol{X}) = \mathbf{F}_0 + \widetilde{\mathbf{H}}(\boldsymbol{X})$ $\quad \boldsymbol{X}$ in Ω
- $\widetilde{\mathbf{H}}(\boldsymbol{X}) = \dfrac{\partial \widetilde{\boldsymbol{u}}}{\partial \boldsymbol{X}}$ $\quad \boldsymbol{X}$ in Ω

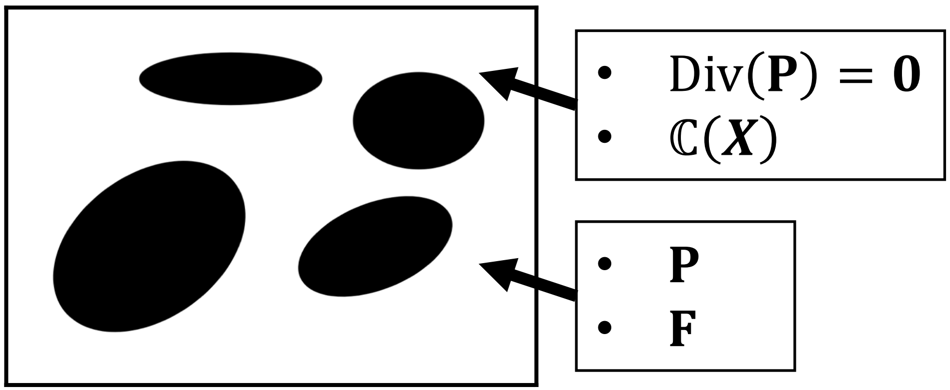
Average of deformation gradient

- $\mathbf{F}_0 = \dfrac{1}{\Omega} \int_{\Omega} \mathbf{F}(\boldsymbol{X})\, dV$ $\quad \boldsymbol{X}$ in Ω
- $\dfrac{1}{\Omega} \int_{\Omega} \widetilde{\mathbf{H}}(\boldsymbol{X})\, dV = \mathbf{0}$ $\quad \boldsymbol{X}$ in Ω

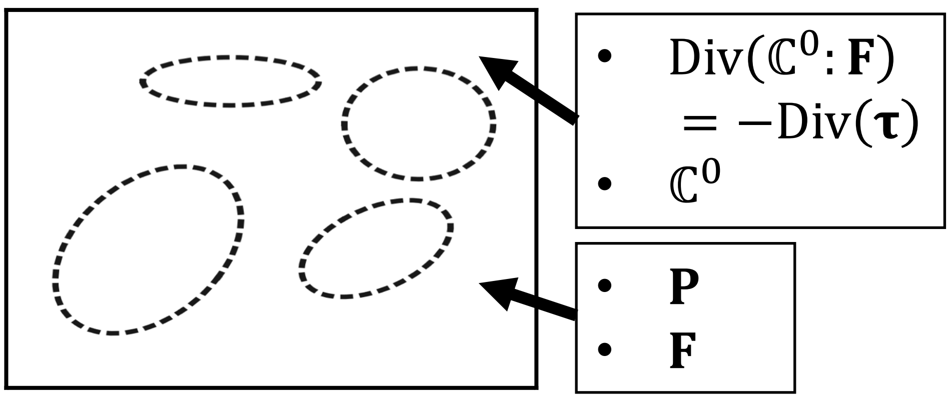
(P. Eisenlohr et al., 2013)

2. Material Model Formulation

2.2 Homogenization technique



Heterogeneous problem



Homogeneous problem

Heterogeneous problem

- $\mathbf{P}\big(\mathbb{C}(\boldsymbol{X}), \mathbf{F}(\boldsymbol{X})\big) = \mathbf{FS}(\boldsymbol{X})$ $\quad$ $\boldsymbol{X}$ in Ω
- $\mathrm{Div}(\mathbf{P}) = \mathbf{0}$ $\quad$ $\boldsymbol{X}$ in Ω

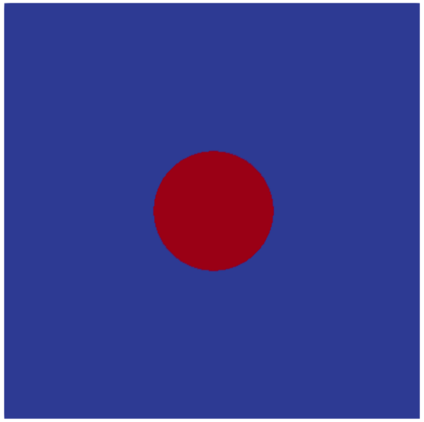
Homogeneous problem

- $\mathbf{P} = \mathbb{C}^0 : \mathbf{F} + \boldsymbol{\tau}(\boldsymbol{X})$ $\quad$ $\boldsymbol{X}$ in Ω
- $\boldsymbol{\tau} = \mathbb{C}^0 : \mathbf{F} - \mathbf{P}$ $\quad$ $\boldsymbol{X}$ in Ω
- $\mathrm{Div}(\mathbb{C}^0 : \mathbf{F}) = -\mathrm{Div}(\boldsymbol{\tau})$ $\quad$ $\boldsymbol{X}$ in Ω

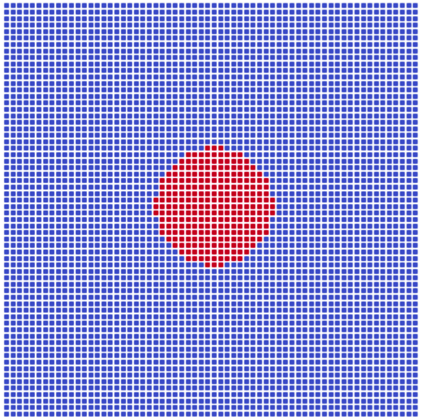
(P. Eisenlohr et al., 2013)

2. Material Model Formulation

2.3 Lippmann-Schwinger equation & spectral solution scheme



Original RVE



Discretized RVE (64×64)

Lippmann-Schwinger equation

- $\widetilde{\mathbf{H}} = -(\boldsymbol{\Gamma}^0 * \boldsymbol{\tau})(\boldsymbol{X})$ $\quad$ $\boldsymbol{X}$ in Ω
- $\mathbf{F} = \mathbf{F}_0 - (\boldsymbol{\Gamma}^0 * \boldsymbol{\tau})$ $\quad$ $\boldsymbol{X}$ in Ω

Spectral solution technique

- $\hat{\mathbf{F}}(\boldsymbol{\xi}) = -(\hat{\boldsymbol{\Gamma}}^0 : \hat{\boldsymbol{\tau}})(\boldsymbol{\xi})$ $\quad$ $\forall \boldsymbol{\xi} \neq \mathbf{0}$
- $\hat{\mathbf{F}}(\boldsymbol{\xi}) = \mathbf{F}_0$ $\quad$ $\forall \boldsymbol{\xi} = \mathbf{0}$
- $\mathbf{F}(\boldsymbol{X}) = \mathrm{FFT}^{-1}(\hat{\mathbf{F}}(\boldsymbol{\xi}))$

(P. Eisenlohr et al., 2013)

2. Material Model Formulation

2.4 Fixed-point scheme for inelastic materials

Initialization

- $\mathbf{F}^0(\boldsymbol{x}) = \mathbf{F}_0 \quad \forall \boldsymbol{x} \in \Omega$
- Calculate $\mathbf{P}^0(\mathbf{F}(\boldsymbol{x}))$ using a constitutive law $\quad \forall \boldsymbol{x} \in \Omega$

Iterate i+1

- (a) Calculate $\boldsymbol{\tau}^i(\boldsymbol{x}) = \mathbf{P}^i(\boldsymbol{x}) - \mathbb{C}^0(\boldsymbol{x}) : \mathbf{F}(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega$
- (b) $\hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) = \mathrm{FFT}\left(\boldsymbol{\tau}^i(\boldsymbol{x})\right) \quad \forall \boldsymbol{x} \in \Omega$
- (c) $\hat{\mathbf{F}}^{i+1}(\boldsymbol{\xi}) = -\hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}^i(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \neq \mathbf{0}, \quad \hat{\mathbf{F}}^{i+1}(\mathbf{0}) = \mathbf{F}_0$
- (d) $\mathbf{F}^{i+1} = \mathrm{FFT}^{-1}(\hat{\mathbf{F}}^{i+1}) \quad \forall \boldsymbol{x} \in \Omega$
- (e) Calculate $\mathbf{P}^{i+1}$ and inelastic state variables using material laws $\forall \boldsymbol{x} \in \Omega$
- (f) Check the convergence criterion: $error = \dfrac{\sum_{\Omega} ||\mathbf{F}^{i+1} - \mathbf{F}^i||}{N_x N_y N_z ||\mathbf{F}_0||}$
  - **If** $(error < tolerance)$ **return**
  - **Else** go to step (a)

Master's thesis, April 12, 2018 | Jaeyong Jung |
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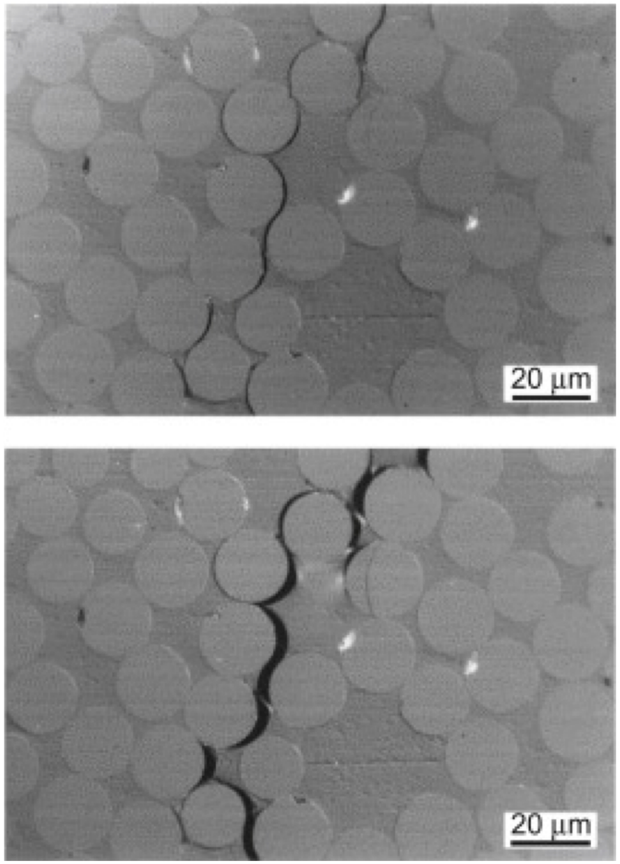
3. Damage Mechanics



Matrix and fiber–matrix interface cracking in composite materials, R. Talreja, 2016

Continuum damage models

- 2nd law of thermodynamics
- Damage loading criterion
- Scalar damage variables

Defect of local continuum damage models

- Ill-posedness in softening region (N. Triantafyllidis et al, 1986)

Nonlocal damage model

- Gradient-extended damage model (micromorphic approach)
- Micromorphic balance equation
- $D \approx \bar{D}$

(S. Forest, 2009)

3. Damage Mechanics

3.1 Local vs. nonlocal damage models

	Local damage	Nonlocal damage
Helmholtz free energy	$\Psi(\mathbf{C}, D, \xi_d) = f(D)\left[\frac{\mu}{2}\{\mathrm{tr}\mathbf{C} - 3 - \ln(\det\mathbf{C})\} + \frac{\Lambda}{4}\{\det\mathbf{C} - 1 - \ln(\det\mathbf{C})\}\right] + r\left\{\xi_d + \frac{\exp(-s\xi_d) - 1}{s}\right\}$	$\Psi(\mathbf{C}, D, \xi_d, \bar{D}, \nabla_0\bar{D}) = \Psi_{loc}(\mathbf{C}, D, \xi_d) + \frac{1}{2}H(D - \bar{D})^2 + \frac{1}{2}A\nabla_0\bar{D} \cdot \nabla_0\bar{D}$
Clausius-Duhem inequality	$-\dot{\Psi} + \mathbf{S}:\dot{\mathbf{E}} \geq 0$	$-\dot{\Psi} + \mathbf{S}:\dot{\mathbf{E}} + a_0\dot{\bar{D}} + \boldsymbol{b}_0 \cdot \nabla_0\dot{\bar{D}} \geq 0$
2nd Piola-Kirchhoff stress	$\mathbf{S} = 2\frac{\partial\Psi}{\partial\mathbf{C}} = f(D)\{\mu(\mathbf{I} - \mathbf{C}^{-1}) + \frac{\Lambda}{2}(\det\mathbf{C} - 1)\mathbf{C}^{-1}\}$	
Dissipation inequality	$Y\dot{D} - q_d\dot{\xi}_d \geq 0$	
Damage function	$f(D) = (1 - D)^2$	

3. Damage Mechanics

3.1 Local vs. nonlocal damage models

	Local damage	Nonlocal damage
Thermodynamic conjugate forces	$Y := -\frac{\partial \Psi}{\partial D} = -f'(D)\left[\frac{\mu}{2}\{\mathrm{tr}\mathbf{C} - 3 - \ln(\det\mathbf{C})\} + \frac{\Lambda}{4}\{\det\mathbf{C} - 1 - \ln(\det\mathbf{C})\}\right]$	$Y := -\frac{\partial \Psi}{\partial D} = Y_{loc} - H(D - \bar{D})$
	$q_d := \frac{\partial \Psi}{\partial \xi_d} = r\{1 - \exp(-s\xi_d)\}$	
Damage loading criterion	$\phi_d = Y - (Y_0 + q_d) \leq 0$	
Evolution equations	$\dot{D} = \dot{\lambda}\frac{\partial \phi_d}{\partial Y} = \dot{\lambda}, \quad \dot{\xi}_d = -\dot{\lambda}\frac{\partial \phi_d}{\partial \xi_d} = \dot{\lambda}$	
KKT conditions	$\dot{\lambda} \geq 0, \quad \phi_d \leq 0, \quad \dot{\lambda}\phi_d = 0$	
Micromorphic balance equation	-	$\bar{D} - \alpha\nabla_0^2\bar{D} = D, \quad \alpha = \frac{A}{H}$

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4. Coupling Scheme

4.1 Algorithm for the nonlocal damage model

FFT-based scheme
for
$\mathbf{F}^{i+1}$

Use $\mathbf{F}^{i+1}$ to calculate ($\bar{D}$ & D)

$\phi_d = 0$ &
$\bar{D} - \alpha \nabla_0^2 \bar{D} = D$
for
$(\bar{D}^{i+1}, D^{i+1})$

How to calculate ($\bar{D}$ & D) satisfying both?

Coupling scheme is required

Coupling Schemes (Simultaneous Scheme)

4.2 Simultaneous scheme for the nonlocal damage model

Residuals at each grid point (material point)

- $r_1(D, \overline{D}) = \overline{D} - \alpha\nabla^2\overline{D} - D = 0$ ($\nabla^2\overline{D}$ is expanded using finite-difference schemes)
- $r_2(D, \xi_d, \overline{D}) = \phi = Y(D, \xi_d, \overline{D}) - \left(Y_0 + q_d(\xi_d)\right) = 0$

Increments of state variables

- $\overline{D}^{n+1} = \overline{D}^n + \Delta\overline{D} = \overline{D}^n + \Delta\overline{D}$
- $D^{n+1} = D^n + \Delta D = D^n + \Delta\lambda$
- $\xi_d^{n+1} = \xi_d^n + \Delta\xi_d = \xi_d^n + \Delta\lambda$

Vectors of residuals and increments

- $\boldsymbol{r} = \begin{pmatrix} r_{1,(0,0,0)} \\ \vdots \\ r_{1,(N_x-1,N_y-1,N_z-1)} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ r_{2,(0,0,0)} \\ \vdots \\ r_{2,(N_x-1,N_y-1,N_z-1)} \end{pmatrix} \in \mathbb{R}^{2(N_xN_yN_z)}, \boldsymbol{x} = \begin{pmatrix} \Delta\overline{D}_{(0,0,0)} \\ \vdots \\ \Delta\overline{D}_{(N_x-1,N_y-1,N_z-1)} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \Delta\lambda_{(0,0,0)} \\ \vdots \\ \Delta\lambda_{(N_x-1,N_y-1,N_z-1)} \end{pmatrix} \in \mathbb{R}^{2(N_xN_yN_z)}$

Coupling Schemes (Simultaneous Scheme)

4.2 Simultaneous scheme for the nonlocal damage model

Application of the Newton-Raphson method

- $\boldsymbol{x}_0 = \boldsymbol{0}$
- $\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \Delta\boldsymbol{x}_i$
- $\boldsymbol{r}_{i+1} = \boldsymbol{r}_i + \left.\left(\frac{dr}{dx}\right)\right|_i \Delta\boldsymbol{x}_i = \boldsymbol{0}$
- $\Delta\boldsymbol{x}_i = -\left.\begin{pmatrix} \frac{\partial \boldsymbol{r}_1}{\partial \Delta\overline{\boldsymbol{D}}} & \frac{\partial \boldsymbol{r}_1}{\partial \Delta\boldsymbol{\lambda}} \\ \frac{\partial \boldsymbol{r}_2}{\partial \Delta\overline{\boldsymbol{D}}} & \frac{\partial \boldsymbol{r}_2}{\partial \Delta\boldsymbol{\lambda}} \end{pmatrix}^{-1}\right|_i \left.\begin{pmatrix} \boldsymbol{r}_1 \\ \boldsymbol{r}_2 \end{pmatrix}\right|_i$
- Submatrices $\in \mathbb{R}^{(N_x N_y N_z)\times(N_x N_y N_z)}$

Submatrix	Definition
$\frac{\partial \boldsymbol{r}_1}{\partial \Delta\overline{\boldsymbol{D}}}$	Approximation of $(\boldsymbol{I} - \alpha\nabla^2)$ using finite-difference schemes
$\frac{\partial \boldsymbol{r}_1}{\partial \Delta\boldsymbol{\lambda}}$	$\mathrm{diag}(-1)$
$\frac{\partial \boldsymbol{r}_2}{\partial \Delta\overline{\boldsymbol{D}}}$	$\mathrm{diag}(H)$
$\frac{\partial \boldsymbol{r}_2}{\partial \Delta\boldsymbol{\lambda}}$	$\mathrm{diag}(\frac{\partial \phi}{\partial \Delta\lambda})$

Methods to speed up computation

- Express $\frac{\partial \boldsymbol{r}_1}{\partial \Delta\overline{\boldsymbol{D}}}$ in sparse matrix form (CSR)
- Schur complement method
- Conjugate gradient method (SPD matrix)

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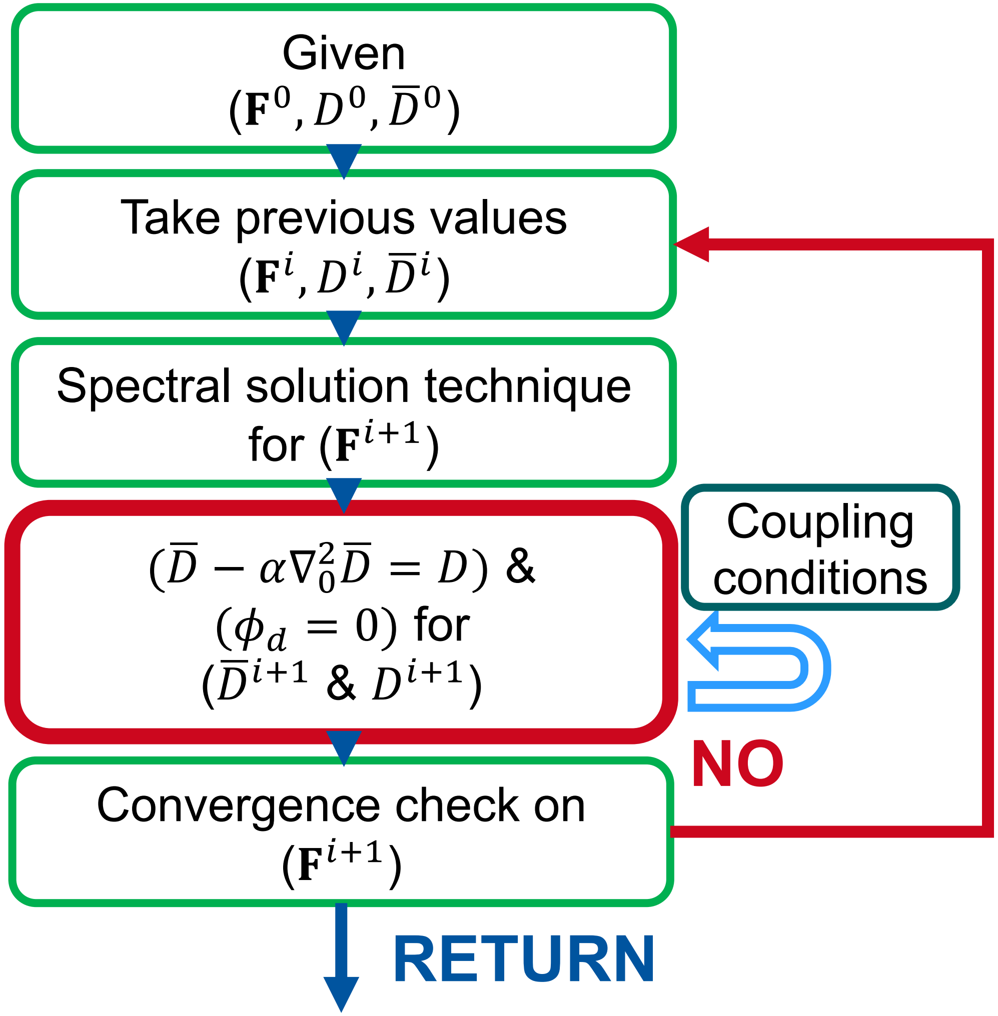
4. Coupling Scheme

4.2 Simultaneous scheme for the nonlocal damage model



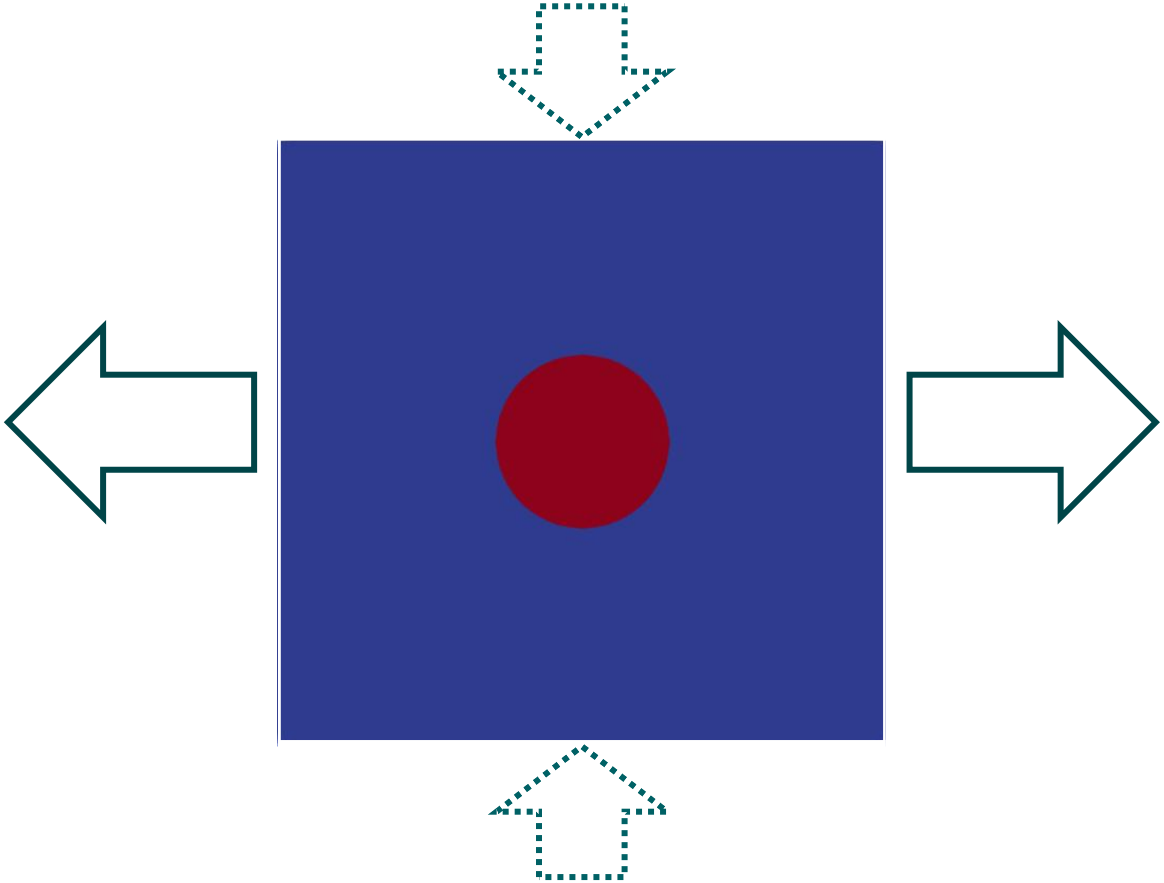
Simultaneous scheme

- Solve multiple equations simultaneously
  - $\overline{D} - \alpha \nabla_0^2 \overline{D} = D$
  - $\phi_d = 0$ (damage loading)
- Newton-Raphson method is applied to both equations

Coupling conditions

- $\left|\overline{D}(\boldsymbol{X}) - \alpha \nabla_0^2 \overline{D}(\boldsymbol{X}) - D(\boldsymbol{X})\right| < tolerance$
- $\phi_d \leq tolerance$

5.1 Single fiber, uniaxial stretch



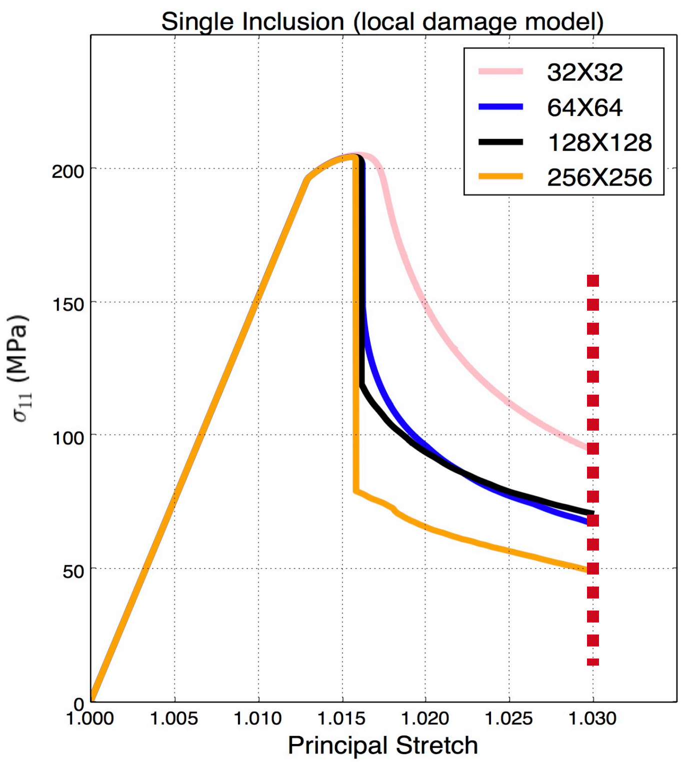
$$\mathbf{F}_0 = \begin{pmatrix} l_i & 0 & 0 \\ 0 & 1/l_i & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$l_i \in [1, 1.3]$$

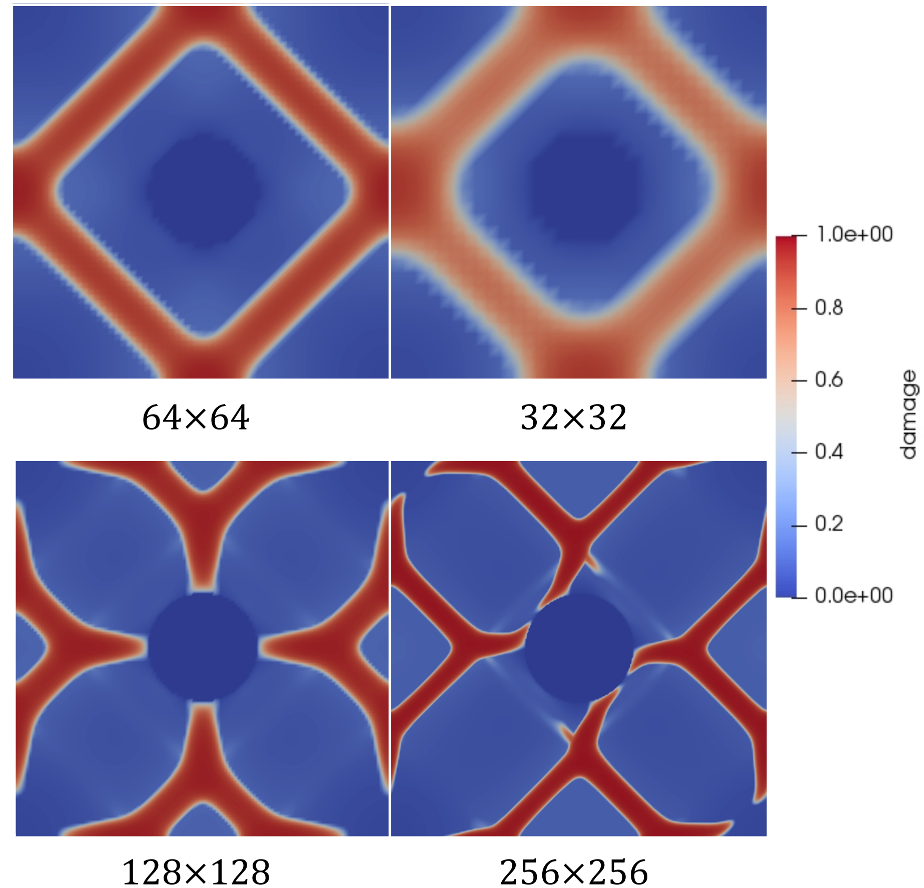
Symbols	Value	Unit
Λ	5000	MPa
μ	7500	MPa
Y_0	5	MPa
r	50	MPa
s	0.5	-
H	10^4	MPa
α	2.5×10^{-8}	MPa mm^2

5. Numerical Examples

5.1.1 Single, local, uniaxial



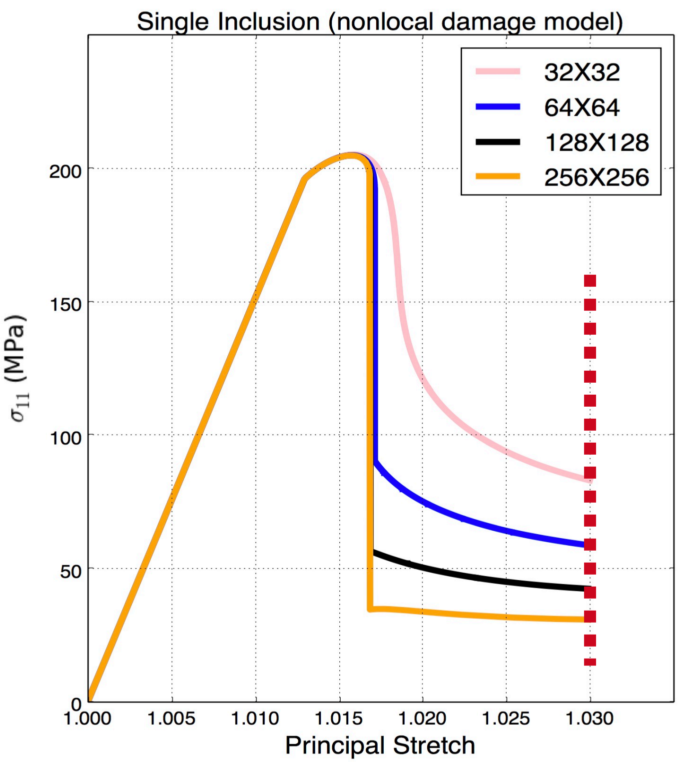
Stress-principal stretch curve of uniaxial-stretch simulation

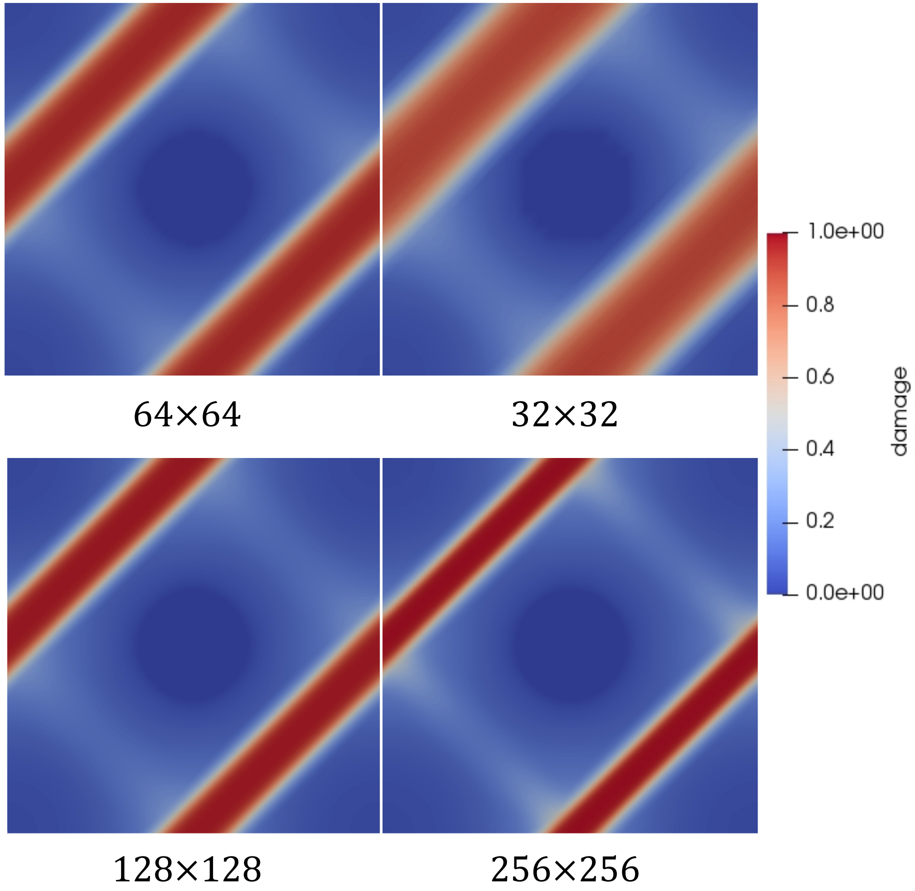


Fractured configurations at principal stretch 1.03

5. Numerical Examples

5.1.2 Single, nonlocal, uniaxial



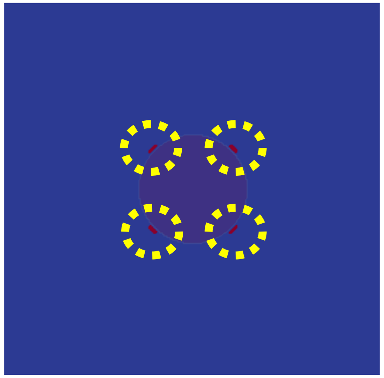


Stress-principal stretch curve of uniaxial-stretch simulation

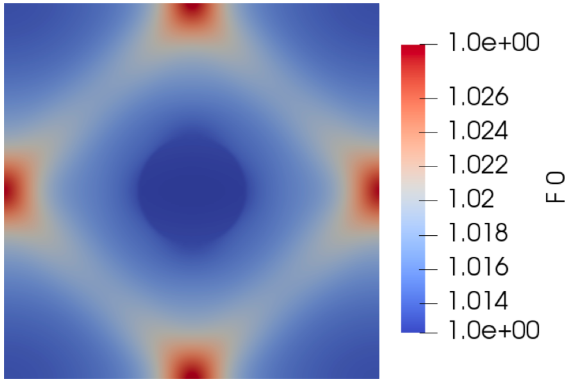
Fractured configurations at principal stretch 1.03

5. Numerical Examples

5.1.3 Investigations



Damage nucleation sites (256X256)



$\mathbf{F}_0$ just before crack propagation

Observations on the nucleation

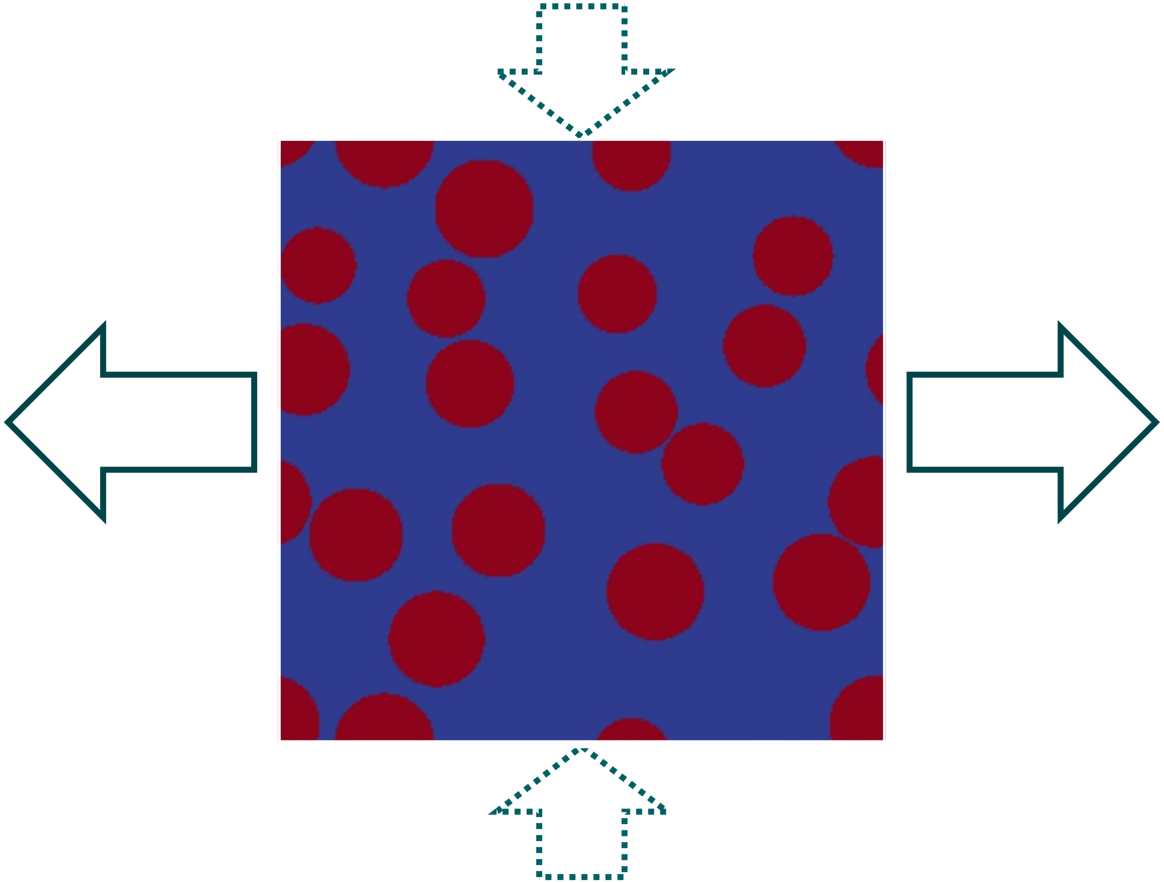
- The damage nucleation happens nearby the fiber
- However, $\mathrm{tr}(\mathbf{C})$ is the largest between fibers (large Y)
- Crack goes across mostly damaged regions

Evaluation of the nonlocal model

- Reasonably predicts damage nucleation
- Consistent crack propagations
- Adhesive elements will make the crack more realistic (Nguyen et al., 2010)

5. Numerical Examples

5.2 Multiple fibers, uniaxial stretch



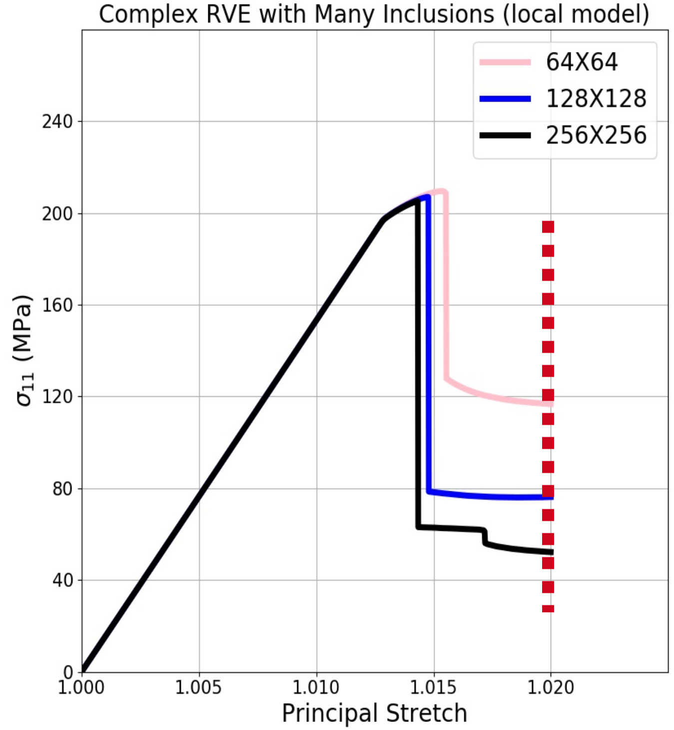
$$\mathbf{F}_0 = \begin{pmatrix} l_i & 0 & 0 \\ 0 & 1/l_i & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$l_i \in [1, 1.2]$$

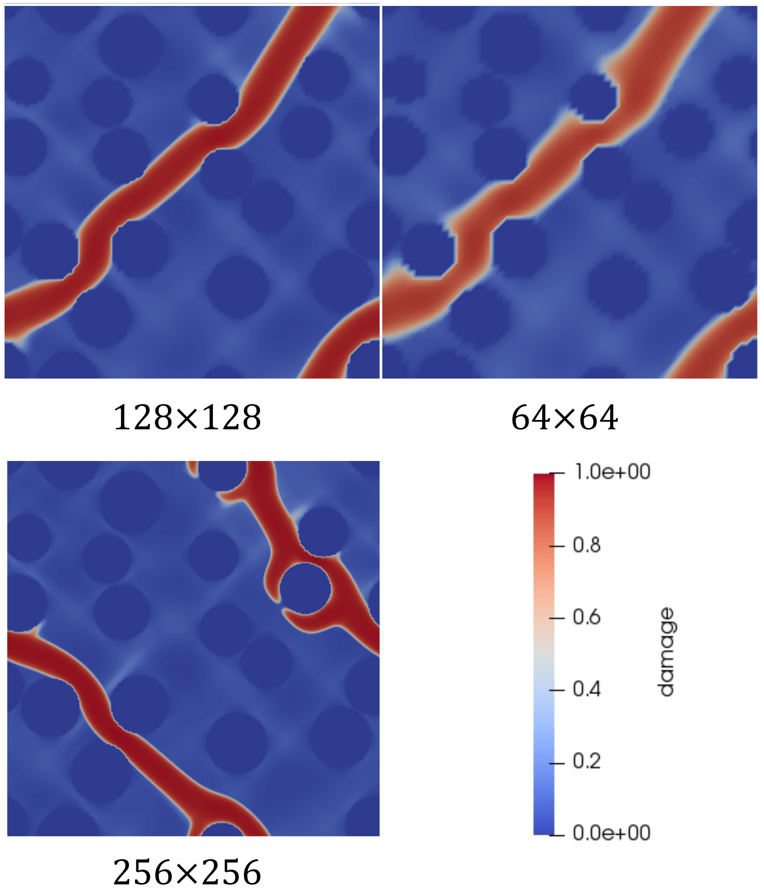
Symbols	Value	Unit
Λ	5000	MPa
μ	7500	MPa
Y_0	5	MPa
r	50	MPa
s	0.5	-
H	10^4	MPa
α	2.5×10^{-8}	MPa mm^2

5. Numerical Examples

5.2.1 Multiple, local, uniaxial



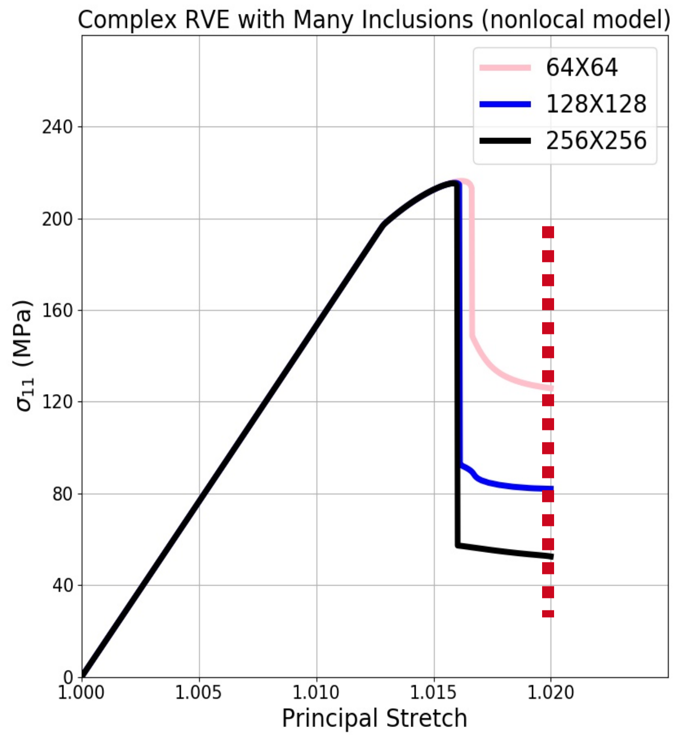
Stress-principal stretch curve of uniaxial-stretch simulation



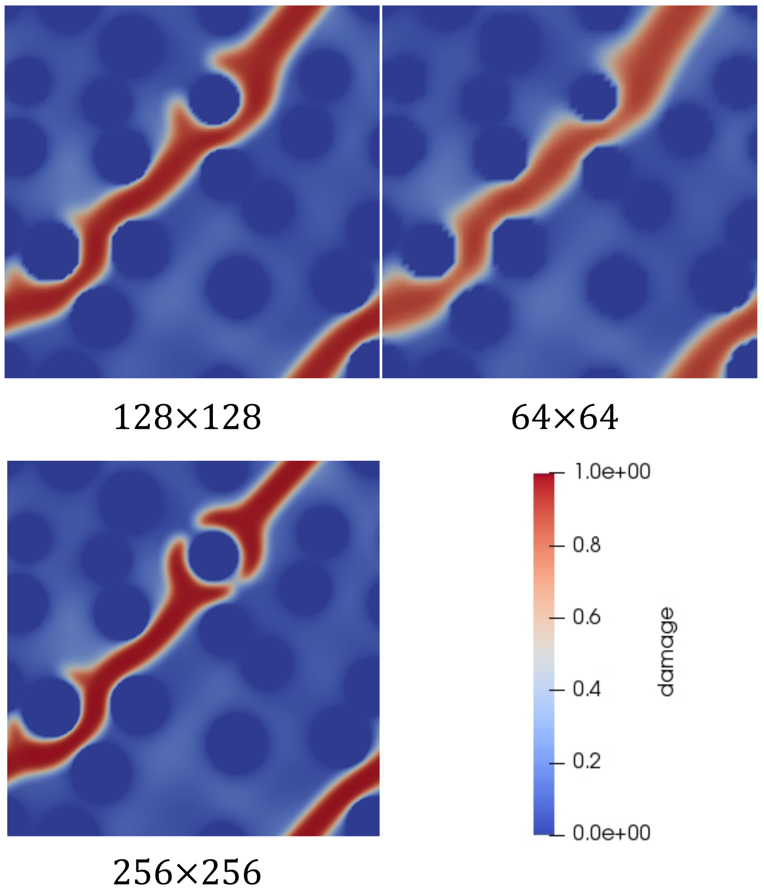
Fractured configurations at principal stretch 1.02

5. Numerical Examples

5.2.2 Multiple, nonlocal, uniaxial



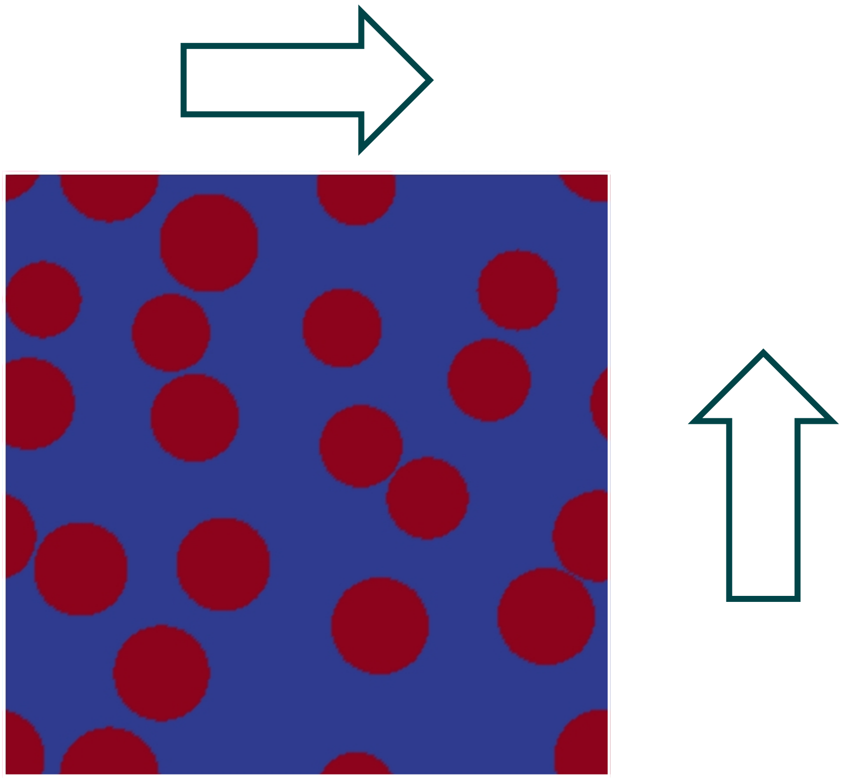
Stress-principal stretch curve of uniaxial-stretch simulation



Fractured configurations at principal stretch 1.02

5. Numerical Examples

5.3 Multiple inclusions, shear deformation



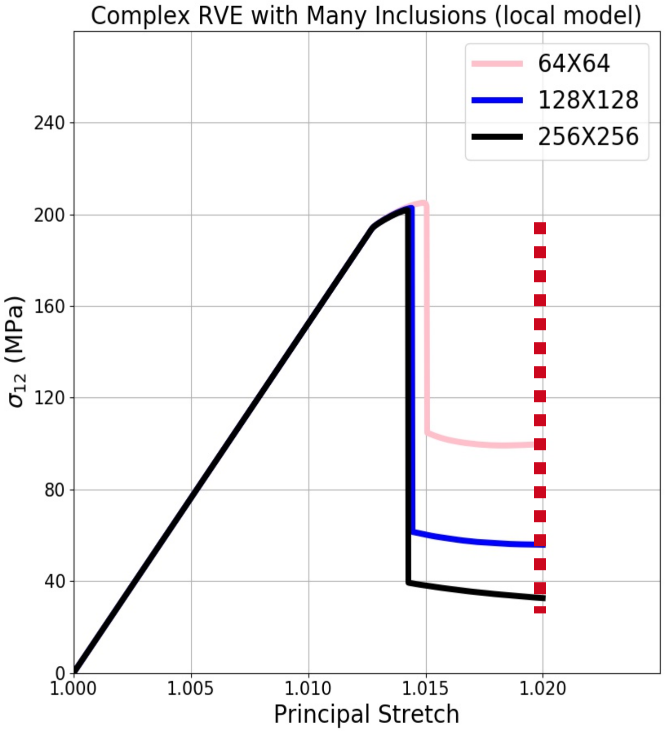
$$\mathbf{F}_0 = \begin{pmatrix} 1 & l_i & 0 \\ l_i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$l_i \in [1, l_f]$$

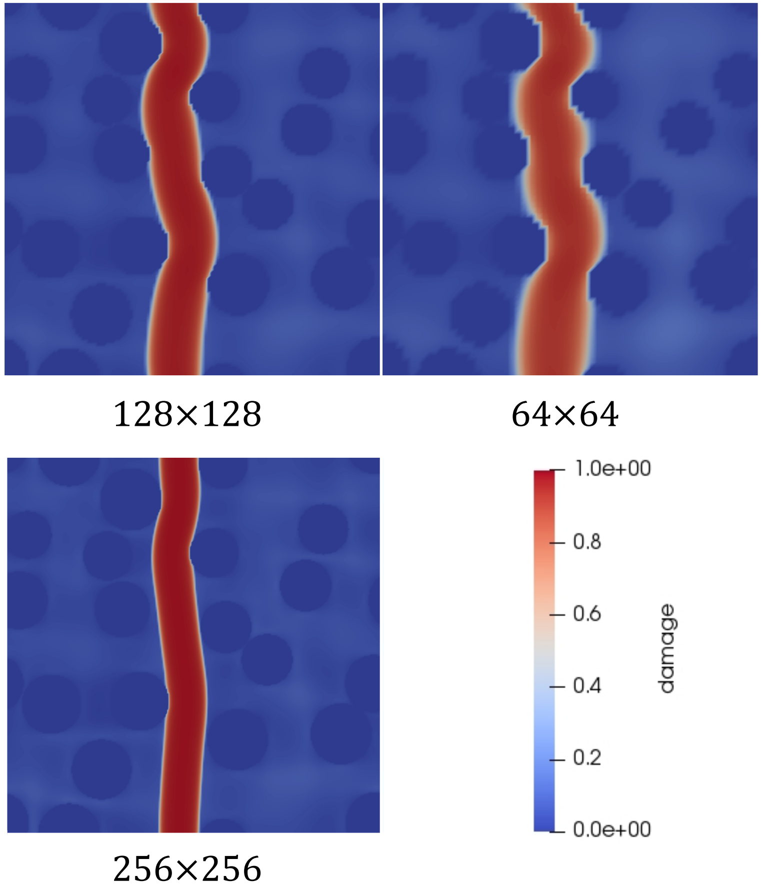
Symbols	Value	Unit
Λ	5000	MPa
μ	7500	MPa
Y_0	5	MPa
r	50	MPa
s	0.5	-
H	10^4	MPa
α	1.0×10^{-8}	MPa mm^2

5. Numerical Examples

5.3.1 Multiple, local, shear



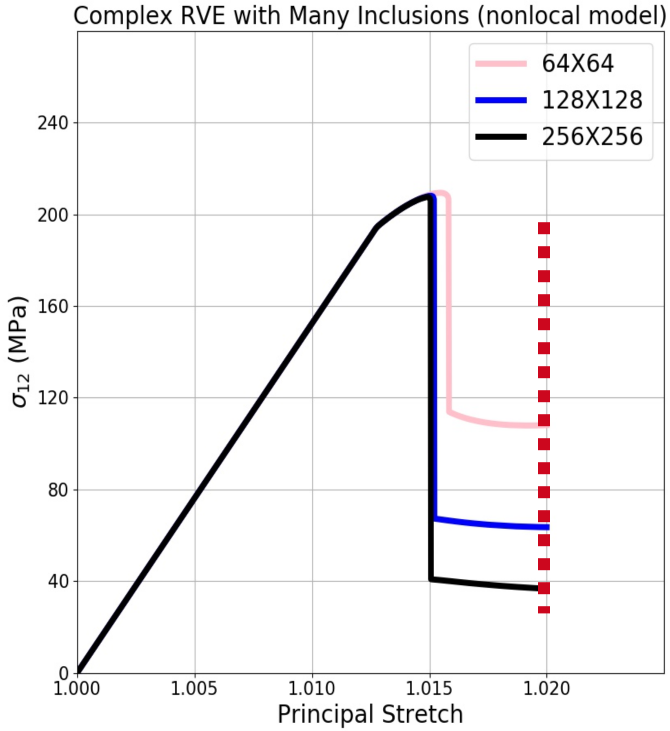
Stress-principal stretch curve of shear deformation simulation

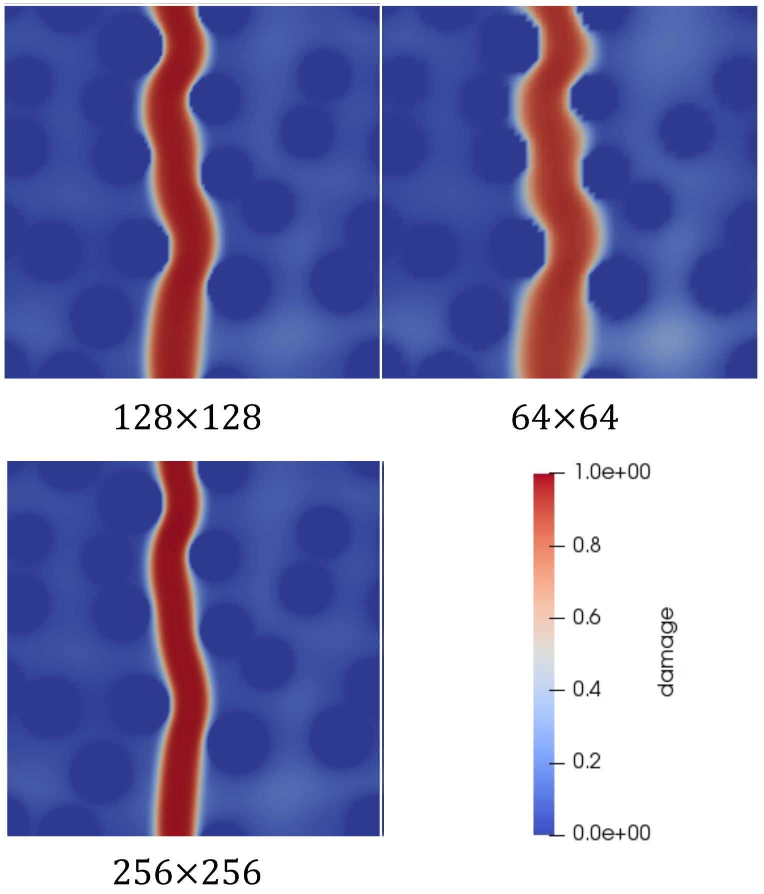


Fractured configurations at principal stretch 1.02

5. Numerical Examples

5.3.2 Multiple, nonlocal, shear





Stress-principal stretch curve of shear deformation simulation

Fractured configurations at principal stretch 1.02

6. Conclusions

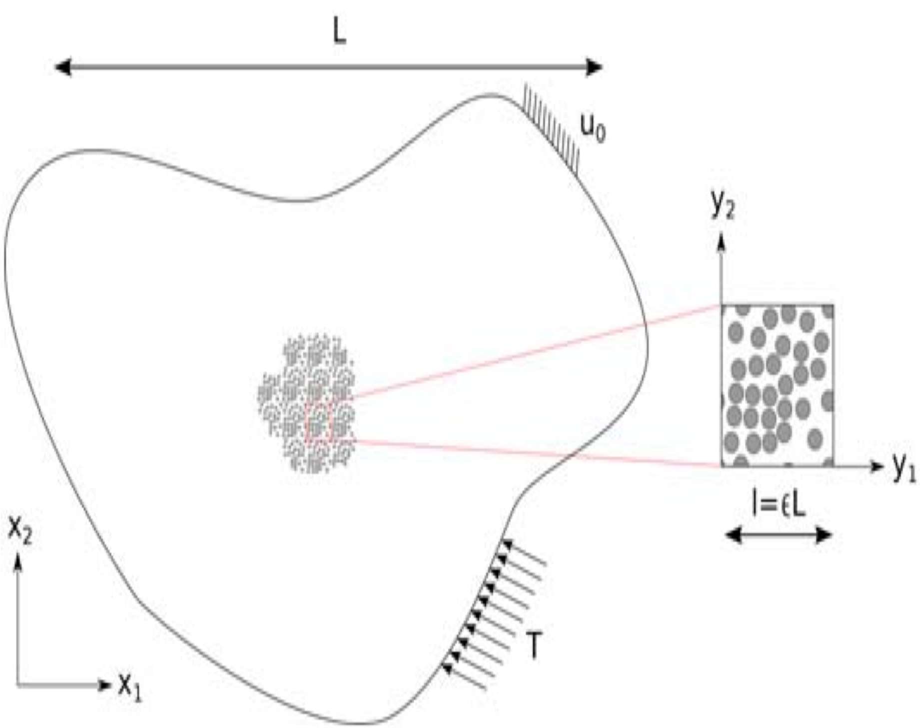
Summary

- Development of the numerical scheme for the prediction of elastic-damage behavior in composite materials
  - Nonlocal damage model shows more convincing results

Suggestions for improvements

- More realistic simulations
  - Adhesive elements bonding matrix and fibers
  - Viscoplastic-damage models
  - Uncertainty quantification of the influence of microvoids (D. A. Vajari)
  - Data-driven modeling and parameter estimation using machine learning
- GPGPU acceleration for calculating FFT and inelasticities
- Phase-field damage modeling
  - Possible crack path doesn’t have to be known
- Numerical techniques for healing snap-back can be implemented
  - Artificial viscosity models
  - FEA with arc-length solver

Appendix
Multiscale Modeling



Homogenization of a microstructure. Source: CALTECH, found at http://www.pellegrino.caltech.edu/multiscale-homogenization-of-viscoelastic-unidirectional-composites/

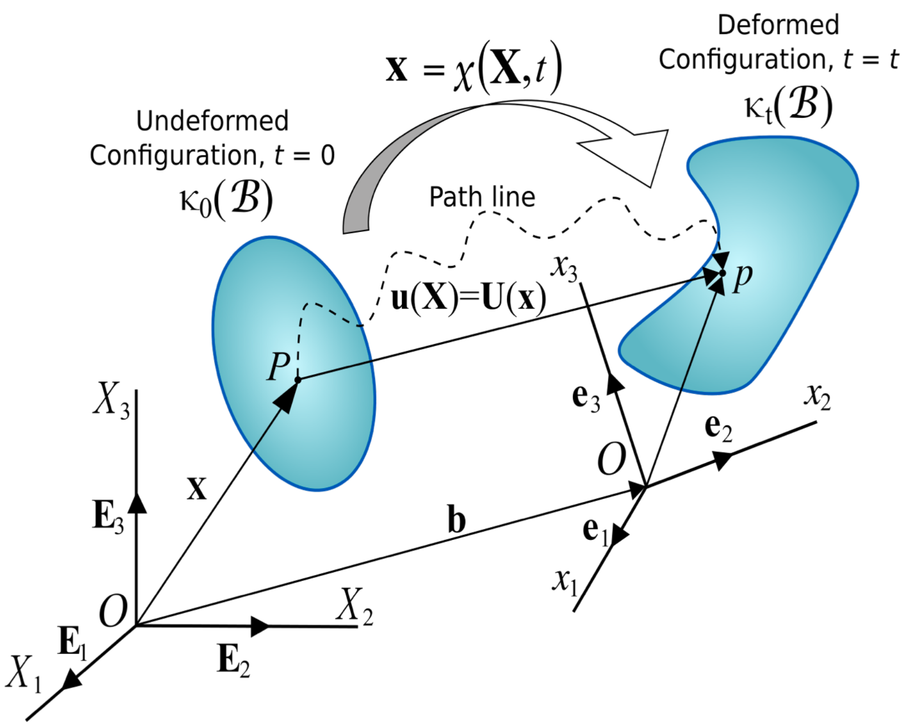
Separation of length scales

- $\epsilon = \frac{l}{L} \ll 1$
- Macroscopic material point = microstructure

Representative Volume Element (RVE)

- Microstructure exhibiting the same physical response
- Domain of simulations

Appendix
Large Deformation Kinematic



Displacement of a continuum body, from a reference configuration to the current configuration. *Source: Wikipedia, found at https://commons.wikimedia.org/wiki/File:Displacement_of_a_continuum.svg*

Deplacement vector

- $\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{X}$

Deformation and displacement gradient

- $\mathbf{F}(\boldsymbol{x}) = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \mathbf{H}(\boldsymbol{x}) + \mathbf{I}$
- $\mathbf{H}(\boldsymbol{x}) = \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{X}}$

Right Cauchy-Green deformation tensor

- $\mathbf{C}(\boldsymbol{x}) = \mathbf{F}^{\mathrm{T}}\mathbf{F}$

Green-Lagrange strain tensor

- $\mathbf{E}(\boldsymbol{x}) = \frac{1}{2}(\mathbf{F}^{\mathrm{T}}\mathbf{F} - \mathbf{I}) = \frac{1}{2}(\mathbf{C} - \mathbf{I})$

Appendix
FFT-Based Scheme (Lipp.-Sch. Equation in Fourier Space)

The Formulation of solution technique

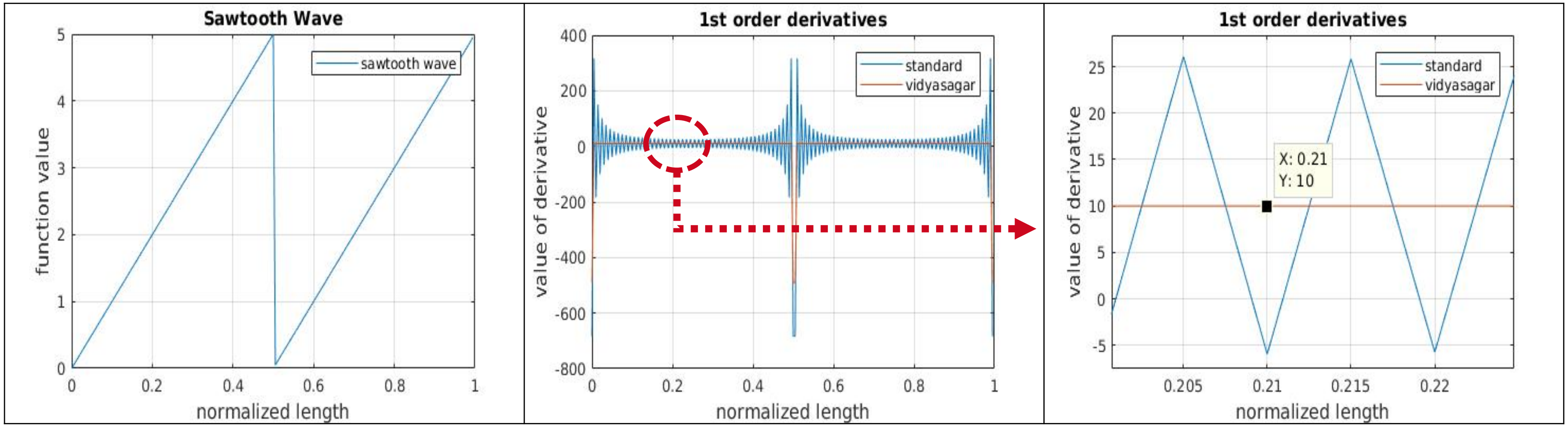
	Real space	Fourier space
Deformation gradient	$\mathbf{F}(\boldsymbol{x}) = \dfrac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}$	$\hat{F}_{mn}(\boldsymbol{\xi}) = \hat{\imath}\hat{u}_m(\boldsymbol{\xi})\xi_n$
First Piola-Kirchhoff stress	$\mathbf{P} = \mathbb{C}^0(\boldsymbol{x}) : \mathbf{F} + \boldsymbol{\tau}(\boldsymbol{x})$	$\hat{P}_{kl}(\boldsymbol{\xi}) = \mathbb{C}^0_{klmn}\hat{\mathrm{F}}_{mn} + \hat{\tau}_{kl}(\boldsymbol{\xi})$ $\Leftrightarrow \hat{\imath}\mathbb{C}^0_{klmn}\hat{u}_m(\boldsymbol{\xi})\xi_n + \hat{\tau}_{kl}(\boldsymbol{\xi})$
Divergence free condition	$\mathrm{Div}(\mathbf{P}) = \mathbf{0}$	$\hat{\imath}\hat{P}_{kl}\xi_l = 0$
Displacement	$\boldsymbol{u}(\boldsymbol{x})$	$\hat{u}_m(\boldsymbol{\xi}) = \hat{\imath}\hat{G}^0_{mk}\hat{\tau}_{kl}\xi_l$
Deformation gradient	$\mathbf{F} = \mathbf{F}_0 - (\boldsymbol{\Gamma}^0 * \boldsymbol{\tau})$	$\hat{F}_{kl} = -\hat{\Gamma}^0{}_{klmn}\hat{\tau}_{mn}$
Green's operator	$\boldsymbol{\Gamma}^0$	$\hat{\Gamma}^0{}_{kLmN}(\boldsymbol{\xi}) = \dfrac{\delta_{km}\xi_L\xi_N}{2\mu_0\lvert\boldsymbol{\xi}\rvert^2} - \dfrac{\Lambda_0\xi_k\xi_L\xi_m\xi_N}{2\mu_0(\Lambda_0 + 2\mu_0)\lvert\boldsymbol{\xi}\rvert^4}$
Acoustic tensor	$\mathbf{G}^0$	$\hat{G}^0(\boldsymbol{\xi}) = \dfrac{(\Lambda_0 + 2\mu_0)\lvert\boldsymbol{\xi}\rvert^2\mathbf{I} - \Lambda_0\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{2\mu_0(\Lambda_0 + 2\mu_0)\lvert\boldsymbol{\xi}\rvert^4}$

Appendix
FFT-Based Scheme (Defect of Spectral Differentiation)

Limitation of spectral differentiation
- Spectral differentiation is not accurate when derivatives are discontinuous

Remedy
- Approximate differential operators using finite-difference scheme, A. Vidyasagar
- Use $\boldsymbol{\xi}_{ijk} = [\xi_i, \xi_j, \xi_k] = [\frac{\sin(2\pi i/N_x)}{dx}, \frac{\sin(2\pi j/N_y)}{dy}, \frac{\sin(2\pi k/N_z)}{dz}]$

Example



Appendix
Coupling Schemes

Partitioned approaches

- Solve each numerical model individually in a sequence
  - Solve M.B.E. for $\overline{D}$
  - D.L.C. for D

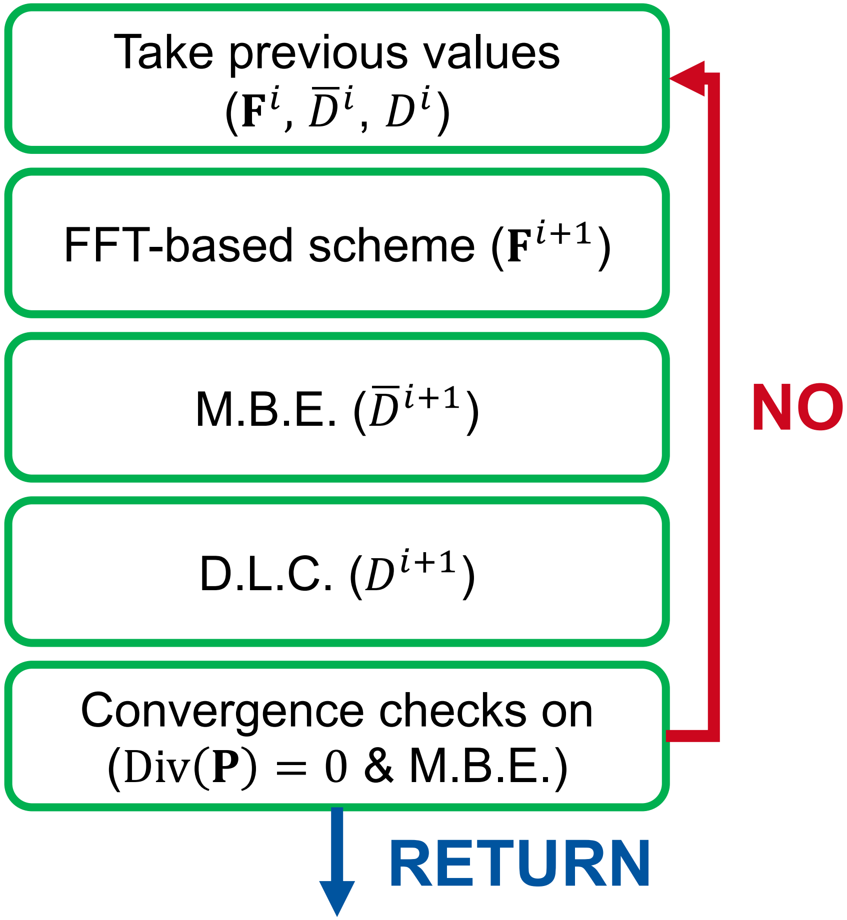
- Schemes
  - Staggered scheme
    - Coupling condition is not checked
  - Iteratively staggered scheme
    - Solution procedure continues until coupling condition is fulfilled
    - Coupling conditions
      - $\left|\overline{D}(\boldsymbol{X}) - \alpha\nabla_0^2\overline{D}(\boldsymbol{X}) - D(\boldsymbol{X})\right| < tolerance$
      - $\phi_d \leq tolerance$

Simultaneous scheme

- Solve every numerical model at the same time

Appendix
Coupling Schemes (Partitioned Approaches)

Staggered scheme



Solution techniques

- M.B.E. solved using spectral method
- D.L.C. solved using return-mapping algorithm

Spectral method

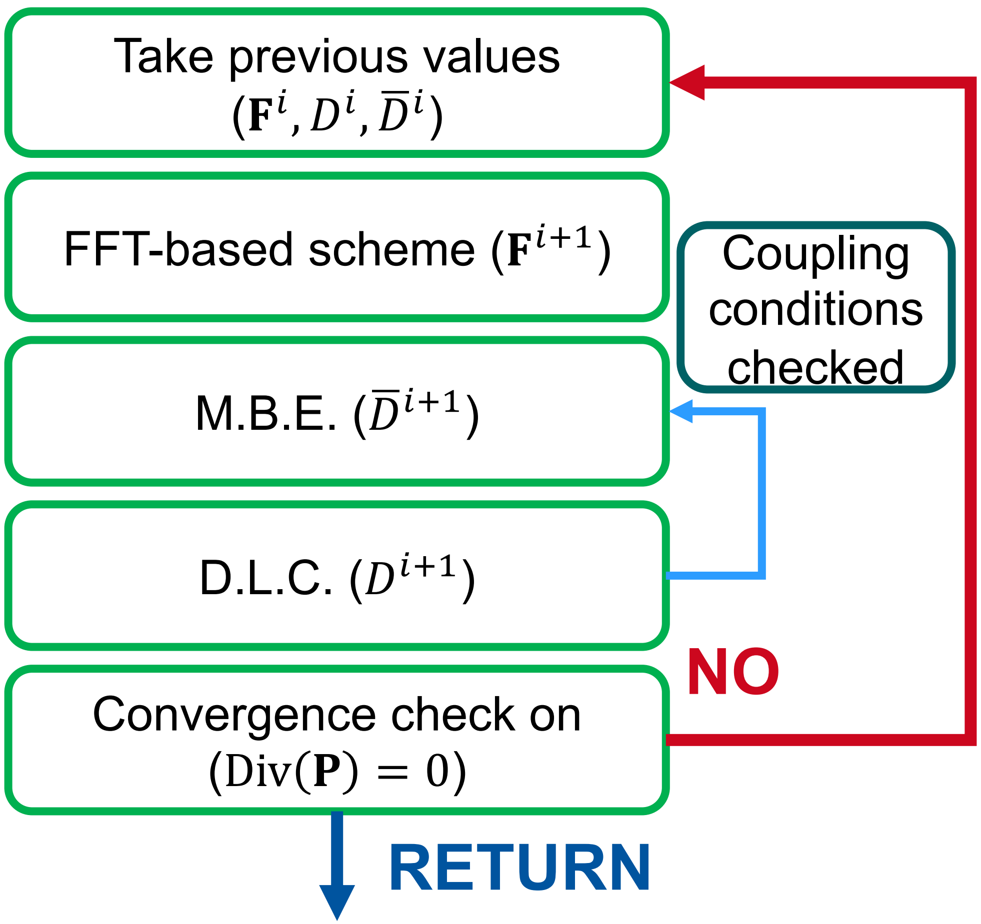
- $\nabla_0^2 \overline{D}(\boldsymbol{X}) = \widehat{\overline{D}}(\boldsymbol{X})|\xi|^2$
- $\widehat{\overline{D}} = \frac{\widehat{D}}{1+\alpha|\xi|^2}$

Possible instability

- Solving (M.B.E. & D.L.C) with $\mathbf{F}^{i+1}$ once is not enough to yield converged solution

Appendix
Coupling Schemes (Partitioned Approaches)

Iteratively staggered scheme



Iteration b.t.w. M.B.E. & D.L.C.

- For a given $\mathbf{F}^{i+1}$, keep iterating the staggered scheme until coupling conditions are fulfilled

Coupling conditions

- $\left|\overline{D}(\boldsymbol{X}) - \alpha \nabla_0^2 \overline{D}(\boldsymbol{X}) - D(\boldsymbol{X})\right| < tolerance$
- $\phi_d \leq tolerance$

Appendix
Coupling Schemes (Validations of Implementations)

Validation using a homogeneous problem

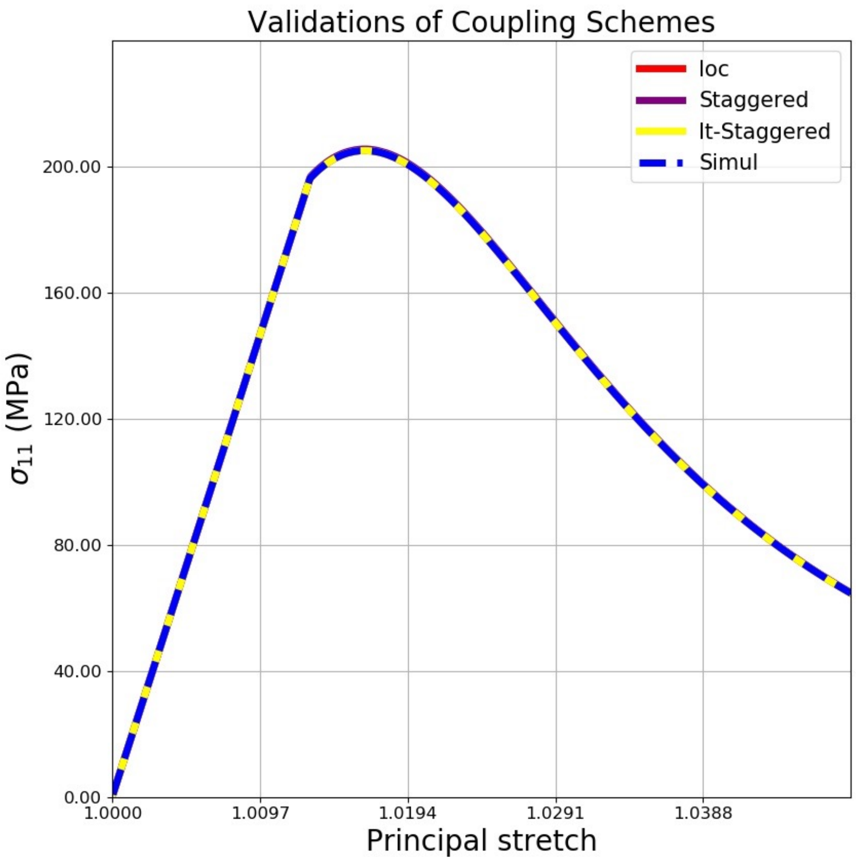
- Macroscopic deformation gradient at each loading step
  - $$\mathbf{F}_0 = \begin{pmatrix} l_i & 0 & 0 \\ 0 & 1/l_i & 0 \\ 0 & 0 & 1/l_i \end{pmatrix} \qquad l_i \in [1, l_f]$$
- Material parameters

Parameters	Symbol	Value	Unit
Lamé's first parameter	Λ	5000	MPa
Lamé's second parameter	μ	7500	MPa
Initial damage threshold	Y_0	5	MPa
Damage parameter	r	50	MPa
Exponential damage parameter	s	0.5	-
Penalty constant	H	10^4	MPa
Internal length scale	α	10^{-6}	MPa mm^2

Appendix
Coupling Schemes (Validations of Implementations)

Results

- Comparison between different implementations of nonlocal damage model



Appendix
Coupling Schemes (Validations of Implementations)

Runtime comparison