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Peridynamic modelling of periodic microstructured materials

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Abstract

With the enhancement in additive manufacturing technology, microstructured materials has attracted significant attention during the last few years. Although these materials can show homogenised properties at the macroscopic scale, their microstructural properties can be very influential on the overall material behaviour especially on the fracture strength of the material since defects such as microcracks and voids can exist. Analysing each and every detail of the microstructure can be computationally expensive. Therefore, homogenisation approaches are widely used especially for periodic microstructured materials including composites. However, some of the existing homogenisation approaches can have limitations if defects exist since displacements become discontinuous if cracks occur in the structure which requires extra attention. As an alternative approach, peridynamics can be utilised since peridynamic equations are based on integro-differential equations and do not contain any spatial derivatives. Hence, in this study peridynamic modelling of periodic microstructured will be presented and the capability of the approach will be demonstrated with several numerical examples with and without defects.

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1. Introduction

With the enhancement in additive manufacturing technology, microstructured materials has attracted significant attention during the last few years. Although these materials can show homogenised properties at the macroscopic scale, their microstructural properties can be very influential on the overall material behaviour especially on the fracture strength of the material since defects such as microcracks and voids can exist. Analysing each and every detail of the microstructure can be computationally expensive. Therefore, homogenisation approaches are widely used especially for periodic microstructured materials including composites. However, some of the existing homogenisation approaches can have limitations if defects exist since displacements become discontinuous if cracks occur in the structure which requires extra attention. As an alternative approach, peridynamics (Silling, 2000) can be utilised since peridynamic equations are based on integro-differential equations and do not contain any spatial derivatives. Peridynamic equations are always valid regardless of discontinuities. There has been a rapid progress on peridynamics during the recent years. Peridynamics was utilised for the analysis of composite materials (Oterkus et al., 2010a; Oterkus and Madenci, 2012a,b; Madenci and Oterkus, 2014), polycrystalline materials (De Meo et. al., 2016, 2017; Zhu et. al., 2016) and graphene (Liu et. al., 2018), impact analysis (Oterkus, et. al., 2012), fatigue analysis (Oterkus et al., 2010b), analysis of microcrack-macrocrack interactions (Vazic et. al., 2017; Basoglu, et. al., 2019), beam and plate analysis (Diyaroglu et. al., 2019; Vazic et. al., 2020; Yang et. al., 2019, 2020), topology optimisation of cracked structures (Kefal et. al., 2019), analysis of dynamic fracture (Imachi et. al., 2019, 2020), homogenisation (Madenci et. al., 2018; Buryachenko, 2020) and analysis of other physical fields (De Meo et. al, 2017; Diyaroglu et. al., 2017a,b; Oterkus et. al., 2014; Wang et. al., 2018). An extensive review of peridynamics research was provided by Javili et. al. (2019). In this study, peridynamic modelling of periodic microstructured will be presented and the capability of the approach will be demonstrated with several numerical examples with and without defects.

2. Peridynamics homogenization

2.1. Representative volume element formulation

If the microscopic detail of a heterogeneous material can be defined by a “Representative Volume Element” (RVE) for a statistic homogeneous medium, microscopic analysis might be performed to obtain a homogenized description for this material. At least two distinct scales coexist in the process of homogenization: the macroscopic scale $\langle x \rangle$ and microscopic scale $\epsilon \langle y \rangle$.

For illustrative purposes, we will consider only linear elastic deformation. The constitutive relations for the original heterogeneous material can be assumed as

$$
\sigma^{\epsilon} (y) = C(y) \cdot \epsilon^{\epsilon} (y) \\
\epsilon^{\epsilon} (y) = S(y) \cdot \sigma^{\epsilon} (y)
$$

where $\mathbf{C}$ and $\mathbf{S}$ are functions of location and called stiffness tensor and compliance tensor, respectively, which are the inverse of each other $\mathbf{C} = \mathbf{S}^{-1}$. $\sigma^{\epsilon}$ and $\epsilon^{\epsilon}$ are called microscopic stress field and microscopic strain field.

If we assume the microstructure of a composite is periodic, the micromechanical analysis can be performed within a unit cell (UC). Any individual UC can be effectively approximated as a material point in the macroscopic analysis. Homogenization replaces the original heterogeneous material with a fictitious homogeneous medium which has the constitutive relations of

$$
\bar{\sigma}(x) = C^\ast (x) \cdot \bar{\epsilon} (x) \\
\bar{\epsilon} (x) = S^\ast (x) \cdot \bar{\sigma} (x)
$$

where $C^\ast$ and $S^\ast$ are the effective stiffness tensor and effective compliance tensor, respectively.
in which \( C^* \) and \( S^* \) are called effective stiffness tensor (or effective material property matrix) and effective compliance tensor, which satisfy the relations of \( C^* = S^{-1} \cdot \bar{\sigma} \) and \( \bar{\varepsilon} \) are called macroscopic stress and strain, respectively, which are constant values within a cell’s domain \( \varepsilon \).

It is assumed that the macroscopic displacement field \( \bar{u} \) can be expressed in terms of the microscopic displacement field \( u^\varepsilon \) as

\[
\bar{u}(x) = \frac{1}{V} \int u^\varepsilon(y; x) dV
\]

(3)

where \( V \) represents the volume of the UC, and microscopic displacement field \( u^\varepsilon \) can be expressed in terms of volume averaged displacement field and displacement fluctuation function \( \bar{u}^\varepsilon \) as

\[
u^\varepsilon(y; x) = \bar{u}(x) + \bar{\varepsilon}(x) \cdot x + \bar{u}^\varepsilon(y)
\]

(4)

in which \( \bar{\varepsilon}(x) \) is the average strain vector defined as

\[
\bar{\varepsilon}(x) = \frac{\partial \bar{u}(x)}{\partial x}
\]

(5)

In the absence of body force, the following equilibrium condition needs to be satisfied

\[
\sigma_{i,j} = 0
\]

(6)

which can also be rewritten as

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} + \frac{\partial \sigma_{yx}}{\partial y} = 0
\]

(7a)

\[
\frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + \frac{\partial \sigma_{yx}}{\partial x} = 0
\]

(7b)

\[
\frac{\partial \sigma_{zz}}{\partial z} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial x} = 0
\]

(7c)

where \( x, y \) and \( z \) are subject to microscopic scale parameter \( \varepsilon \). Then, according to average stress theorem, the volume average of the stress field inside the body is equal to the constant stress tensor \( \bar{\sigma}_{ij} \) along the border which can be expressed as

\[
\frac{1}{V} \int \sigma^\varepsilon dV = \bar{\sigma}
\]

(8)

Unlike finite element RVE homogenization method, boundary conditions in peridynamics homogenization is enforced on a fictitious boundary area with certain layers of nodes. Periodic boundary condition (PBC) in homogenization consists of two parts, namely the traction periodicity and the displacement periodicity.
\[
\begin{align*}
\mathbf{t}_i^* - \mathbf{t}_i &= 0 \\
\mathbf{u}_i^* &= \mathbf{u}_i^* + \mathbf{e}_0 \left( \mathbf{x}_i^* - \mathbf{x}_i \right)
\end{align*}
\]  
(9a)

(9b)

in which \( \mathbf{t} \) is the traction, \( \mathbf{u} \), is the displacement. Superscript represents the corresponding surface pairs.

Nodes from the fictitious area are child of their corresponding parent nodes from the real material domain. The displacement field of the child node is solely depending on the displacement of its parent node. Other peridynamics information such as node health for defects caused by bond breaking is also transferred from parent nodes to their corresponding child nodes.

From Eq. (4) and periodic boundary condition stated in Eq. (9), the microscopic strain field \( \mathbf{e}^\varepsilon \) can be obtained as

\[
\mathbf{e}^\varepsilon(y) = \mathbf{E}(x) + \mathbf{e}^\varepsilon(y)
\]  
(10)

If we substitute the microscopic strain given in Eq. (10) and constitutive relations given in Eq. (1) into Eq. (6), the displacement-based formulation for RVE homogenization analysis can be obtained as

\[
\mathbf{A}_0 \left[ \mathbf{C}(x)(\mathbf{E}(x) + \mathbf{e}^\varepsilon(y)) \right] = 0
\]  
(11)

in which \( \mathbf{A}_0 \) is the derivative operator:

\[
\mathbf{A}_0 = \begin{bmatrix}
\partial / \partial x & 0 & 0 & 0 \\
0 & \partial / \partial y & 0 & 0 \\
0 & 0 & \partial / \partial z & \partial / \partial y \\
0 & 0 & \partial / \partial z & \partial / \partial x \\
\end{bmatrix}
\]  
(12)

If we substitute Eq. (8) into the constitutive relations given in Eq. (2), effective material property tensor can be obtained as

\[
\mathbf{C}^* = \frac{1}{V} \int \mathbf{e}^\varepsilon dV
\]  
(13)

2.2. Numerical implementation in ordinary state-based peridynamics

Effective material property tensor given in Eq. (13) can be evaluated numerically by considering the stress field fluctuation resulted from the following macroscopic strain boundary conditions \( \mathbf{e}_i (i = 1, \ldots, 6) \)

\[
\begin{align*}
\mathbf{e}_1^* &= [c_x, 0, 0, 0, 0, 0] \\
\mathbf{e}_2^* &= [0, c_x, 0, 0, 0, 0] \\
\mathbf{e}_3^* &= [0, 0, c_x, 0, 0, 0] \\
\mathbf{e}_4^* &= [0, 0, 0, c_x / 2, 0, 0] \\
\mathbf{e}_5^* &= [0, 0, 0, 0, c_x / 2] \\
\mathbf{e}_6^* &= [0, 0, 0, 0, 0, c_x / 2]
\end{align*}
\]  
(13a)

(13b)

(13c)

(13d)

(13e)

(13f)
in which $c_s$ is the scale factor and equal to a small number. Effective property matrix $C^*$ can then be assembled from

$$
\begin{pmatrix}
C_{1,i} \\
C_{2,i} \\
C_{3,i} \\
C_{4,i} \\
C_{5,i} \\
C_{6,i}
\end{pmatrix} = \begin{pmatrix}
\langle \sigma_{i}^{xx} \rangle \\
\langle \sigma_{i}^{xy} \rangle \\
\langle \sigma_{i}^{xz} \rangle \\
\langle \sigma_{i}^{yx} \rangle \\
\langle \sigma_{i}^{zx} \rangle \\
\langle \sigma_{i}^{yy} \rangle
\end{pmatrix} / c_s, \quad (i = 1, \ldots, 6)
$$

(14)

in which the angle brackets denote the volume average over cell domain.

3. Verification and numerical results

3.1. Verification of method

A single cell from a fiber-reinforced composite as shown in Fig. 1 is used for the evaluation of its effective material properties using the current method.

![Fig. 1. Example composite cell](image)

Material properties of the selected cell are given in Table 1.

<table>
<thead>
<tr>
<th>Material name</th>
<th>Elastic modulus $E$ (Pa)</th>
<th>Poisson’s Ratio $v$</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>$2 \times 10^9$</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>Fiber</td>
<td>$3 \times 10^9$</td>
<td>0.4</td>
<td>0.4</td>
</tr>
</tbody>
</table>

To achieve convergence for the homogenization solution, a 120 by 120 peridynamics mesh is used in this study. The effective stiffness tensor for the plane perpendicular to the fiber direction is then obtained as

$$
\begin{pmatrix}
2.6619369 \times 10^{8} & 8.9981233 \times 10^{7} & 9.5836894 \times 10^{7} \\
8.9981233 \times 10^{7} & 2.6619369 \times 10^{8} & 1.2902814 \times 10^{8} \\
9.5836894 \times 10^{7} & 1.2902814 \times 10^{8} & 8.7409126 \times 10^{7}
\end{pmatrix}
$$

(15)
in which \( s \) is the scale factor and equal to a small number. Effective property matrix \( \mathbf{C} \) can then be assembled from

\[
\begin{bmatrix}
2.6619369 \times 10^9 & 8.9981233 \times 10^8 & -9.5836894 \times 10^{-6} \\
8.9981233 \times 10^8 & 2.6619369 \times 10^9 & -1.2902814 \times 10^{-5} \\
-9.5836894 \times 10^{-6} & -1.2902814 \times 10^{-5} & 8.7409126 \times 10^8
\end{bmatrix} \text{ Pa}
\]

(15)

The effective material properties obtained from the current method is compared with the homogenization result of finite element analysis (FEA) based homogenization method given in Yu and Tang (2007) as shown in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>( E_2 ) (Pa)</th>
<th>( E_3 ) (Pa)</th>
<th>( G_{23} ) (Pa)</th>
<th>( v_{23} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peridynamic</td>
<td>2.3577740 \times 10^9</td>
<td>2.3577740 \times 10^9</td>
<td>8.7409126 \times 10^8</td>
<td>0.33802918</td>
</tr>
<tr>
<td>FEA(MSG)</td>
<td>2.3425347 \times 10^9</td>
<td>2.3425347 \times 10^9</td>
<td>8.7738943 \times 10^8</td>
<td>0.34529092</td>
</tr>
</tbody>
</table>

3.2. Composite cell with multiple fibers

A quadruple packed fiber-reinforced composite volume as shown in Fig. 2(b) is considered. The volume contains four center positioned fiber-reinforced matrix cells. All fibers have same material properties. This is equivalent to a combination of four single cell example shown in Fig. 2(a).

\[
\begin{bmatrix}
2.6626945 \times 10^9 & 9.0064065 \times 10^8 & -9.1916712 \times 10^{-6} \\
9.0064065 \times 10^8 & 2.6626945 \times 10^9 & -8.1497381 \times 10^{-6} \\
-9.1916712 \times 10^{-6} & -8.1497381 \times 10^{-6} & 8.7405017 \times 10^8
\end{bmatrix} \text{ Pa}
\]

(16)

The effective material properties obtained are compared with single cell results as given in Table 4.
3.3. Cell with microscopic void

A defected matrix cell with a circular shaped void positioned in the center is considered as shown in Fig. 3(a).

![Fig. 3](image)

Fig. 3. (a) matrix cell with single void; (b) matrix cell with quadruple voids.

Properties of such cell are given in Table 5.

<table>
<thead>
<tr>
<th>Material name</th>
<th>Elastic modulus $E$ (Pa)</th>
<th>Poison Ratio $\nu$</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>$2 \times 10^9$</td>
<td>0.3</td>
<td>0.9685841</td>
</tr>
<tr>
<td>Void</td>
<td>-</td>
<td>-</td>
<td>0.0314159</td>
</tr>
</tbody>
</table>

The 2-dimensional effective stiffness tensor is then obtained as

$$
\mathbf{C}^* = \begin{bmatrix}
2.1279947 \times 10^9 & 6.3912176 \times 10^8 & -1.3652028 \times 10^{-7} \\
6.3912176 \times 10^8 & 2.1279947 \times 10^9 & -2.9960819 \times 10^{-6} \\
-1.3652028 \times 10^{-7} & -2.9960819 \times 10^{-6} & 7.4401262 \times 10^8
\end{bmatrix} \text{ Pa}
$$

(17)

The effective material properties are given in Table 6.
3.4. Cell with multiple microscopic voids

A defected matrix cell with four microscopic voids positioned under a repetitive pattern as shown in the Fig. 3(b) is considered. Properties of such cell is given in Table 7.

<table>
<thead>
<tr>
<th>Material name</th>
<th>Elastic modulus $E$ (Pa)</th>
<th>Poison Ratio $\nu$</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>$2 \times 10^9$</td>
<td>0.3</td>
<td>0.8743363</td>
</tr>
<tr>
<td>Void</td>
<td>-</td>
<td>-</td>
<td>0.0314159 x 4</td>
</tr>
</tbody>
</table>

The 2D effective stiffness tensor is obtained as

$$C^* = \begin{bmatrix}
1.9152877 \times 10^9 & 5.7728186 \times 10^8 & -9.1710183 \times 10^{-6} \\
5.7728186 \times 10^8 & 1.9152877 \times 10^9 & -5.9270207 \times 10^{-6} \\
-9.1710183 \times 10^{-6} & -5.9270207 \times 10^{-6} & 6.6818474 \times 10^8 \\
\end{bmatrix} \text{ Pa}$$ (18)

The effective material properties are then evaluated as given in Table 8.

<table>
<thead>
<tr>
<th></th>
<th>$E_2$ (Pa)</th>
<th>$E_3$ (Pa)</th>
<th>$G_{23}$ (Pa)</th>
<th>$\nu_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Four voids</td>
<td>$1.7412907 \times 10^9$</td>
<td>$1.7412907 \times 10^9$</td>
<td>$6.68184743 \times 10^8$</td>
<td>0.30033991</td>
</tr>
</tbody>
</table>

4. Conclusion

Present study illustrates the feasibility of performing RVE homogenization on composite cells containing fibers and defect such as voids using ordinary state based peridynamics. The enforcement of periodic boundary condition in peridynamics homogenization is also being demonstrated. The homogenization result for fiber-reinforced composite using peridynamics RVE homogenization shows good agreement with finite element homogenization method.

References


