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ALIGNED WEAKLY PERIODIC BOUNDARY CONDITIONS ON REPRESENTATIVE VOLUME ELEMENTS

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Summary. In computational homogenization, periodic Boundary Conditions (BCs) are often imposed on the Representative Volume Element (RVE). However, it is well known that such BCs are inaccurate if cracks are present in the RVE and these cracks are not aligned with the periodicity directions. To overcome this problem, we propose aligned periodic BCs on weak form.

1 INTRODUCTION

In computational homogenization[1,2], the effective response of the microstructure is evaluated by computing the homogenized response of a Representative Volume Element (RVE). A key step in this computation is the imposition of suitable Boundary Conditions (BCs) on the RVE. Periodic boundary conditions are often used[3], even though it is well known that such boundary conditions lead to inaccurate results if localization bands or large cracks in the RVE are not aligned with the periodicity directions. In particular, artificial crack closure occurs on the RVE boundary in such cases, leading to overstiff response of the RVE. A previously proposed remedy is to use modified strong periodic boundary conditions, called Percolation Path Aligned Boundary Conditions (PPABC)[4,5], that are aligned with the dominating localization direction in the RVE. However, strong periodic boundary conditions require a periodic mesh in the RVE. To overcome this limitation, we here start from a previously proposed format for weakly periodic boundary conditions[6,7] and show that these BCs can conveniently be aligned with an identified localization direction. It turns out that this alignment can be achieved by only modifying the mapping (mirror function) between the associated parts of the RVE boundary. In the present work, we therefore propose a modified mirror function, corresponding to a shifted stacking of RVEs, that allows alignment with an identified localization direction.

2 THEORY

We consider the solution of a small strain elasticity problem in an RVE containing cracks, see for example[7,8]. To impose (strong or weak) periodic boundary conditions on the RVE, we divide the RVE boundary into an image part $\Gamma_{\square}^{+}$ and a mirror part $\Gamma_{\square}^{-}$ as shown in Figure 1. Next, we introduce a mapping (mirror function) $\boldsymbol{\varphi}_{per} : \Gamma_{\square}^{+} \rightarrow \Gamma_{\square}^{-}$, that relates points on $\Gamma_{\square}^{+}$ and $\Gamma_{\square}^{-}$ to each other according to $\boldsymbol{x}^{-} = \boldsymbol{\varphi}_{per}(\boldsymbol{x}^{+})$, and define the jump between $\Gamma_{\square}^{+}$ and $\Gamma_{\square}^{-}$ as $[\![\boldsymbol{u}]\!]_{\square} \stackrel{\text{def}}{=} \boldsymbol{u}^{+} - \boldsymbol{u}^{-}$. Letting $\bar{\boldsymbol{\epsilon}}$ denote the macroscopic strain on the RVE, strong periodicity would then be obtained by enforcing $[\![\boldsymbol{u}]\!]_{\square} = \bar{\boldsymbol{\epsilon}} \cdot [\![\boldsymbol{x} - \bar{\boldsymbol{x}}]\!]_{\square}$ pointwise on $\Gamma_{\square}^{+}$. Here, we will instead consider weakly periodic boundary conditions, whereby the periodicity constraint only needs to be fulfilled in a weak sense. The resulting mixed RVE problem is then to find $\boldsymbol{u} \in \mathbb{U}_{\square}$ and $\boldsymbol{t}_{\lambda} \in \mathbb{T}_{\square}$ such that

$$
\begin{aligned}
\frac{1}{|\Omega_{\square}|}\left[\int_{\Omega_{\square}} \boldsymbol{\sigma} : \boldsymbol{\epsilon}\left[\delta \boldsymbol{u}\right] \mathrm{d}\Omega - \int_{\Gamma_{\square,int}^{+}} \boldsymbol{t} \cdot [\![\delta \boldsymbol{u}]\!] \,\mathrm{d}\Gamma\right] - \frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \boldsymbol{t}_{\lambda} \cdot [\![\delta \boldsymbol{u}]\!]_{\square} \,\mathrm{d}\Gamma = 0 \;\forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}, \\
-\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \delta\, \boldsymbol{t}_{\lambda} \cdot [\![\boldsymbol{u}]\!]_{\square} \,\mathrm{d}\Gamma = -\frac{1}{|\Omega_{\square}|}\int_{\Gamma_{\square}^{+}} \delta\, \boldsymbol{t}_{\lambda} \cdot [\![\bar{\boldsymbol{\epsilon}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}]]\!]_{\square} \,\mathrm{d}\Gamma \;\forall \delta \boldsymbol{t}_{\lambda} \in \mathbb{T}_{\square},
\end{aligned}
\tag{1}
$$

where $\mathbb{U}_{\square}$ and $\mathbb{T}_{\square}$ are the spaces pertinent to $\boldsymbol{u}$ and $\boldsymbol{t}_{\lambda}$, respectively. In the equations above, we also introduced the displacement jump $[\![\boldsymbol{u}]\!]$ over the faces of a crack inside the domain $\Omega_{\square}$, and $\Gamma_{\square,int}^{+} = \Gamma_{int}^{+} \cap \Omega_{\square}$, representing the part of the internal boundary located inside the RVE $\Omega_{\square}$. Furthermore, $\boldsymbol{\epsilon} = \left[\boldsymbol{u} \otimes \boldsymbol{\nabla}\right]^{sym}$ is the engineering strain, $\boldsymbol{\sigma} = \boldsymbol{\sigma}\left(\boldsymbol{\epsilon}\right)$ is the Cauchy stress, $\boldsymbol{t} = \boldsymbol{t}\left([\![\boldsymbol{u}]\!]\right)$ is the traction on crack faces in the material, and $\boldsymbol{t}_{\lambda}$ is the traction on the RVE boundary. See[7] for further details.

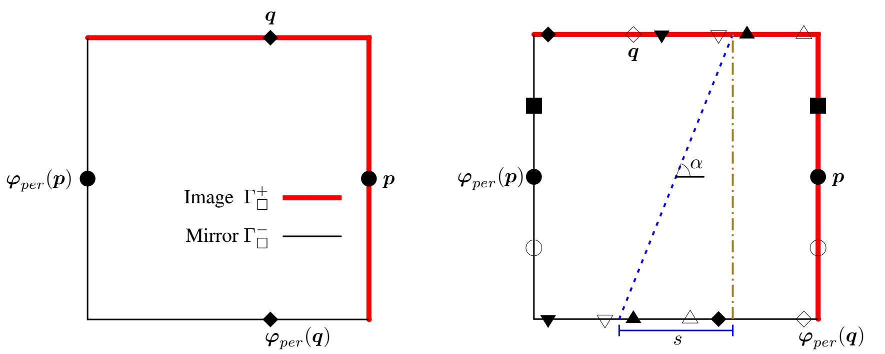
When solving Equation (1), different choices for the mirror function $\boldsymbol{\varphi}_{per}$ are possible. The standard choice, which is used by[6,7] among many others, is to map points along horizontal or vertical lines as shown in Figure 1a, so that $\boldsymbol{\varphi}_{per}$ is explicitly given by $\boldsymbol{\varphi}_{per}\left(l_{\square}, y\right) = (0, y)$ and $\boldsymbol{\varphi}_{per}\left(x, l_{\square}\right) = (x, 0)$, where $l_{\square}$ denotes the side length of the RVE. However, as pointed out by several researchers[4,9], this choice leads to inaccurate results due to artificial crack closure on the RVE boundary for cracks that are not aligned with these directions.

To develop an alternative mirror function, now assume that a dominating crack direction exists as indicated in Figure 1b. Then, we may modify $\boldsymbol{\varphi}_{per}$ such that the crack pattern is compatible over RVE boundaries, thereby preventing artificial crack closure on RVE boundaries[10]. The explicit alternative expression for $\boldsymbol{\varphi}_{per}$ as shown in Figure 1b (for $45^{\circ} < \alpha < 90^{\circ}$) is now given by

$$
\begin{aligned}
&\boldsymbol{\varphi}_{per}\left(l_{\square}, y\right) = (0, y), \\
&\boldsymbol{\varphi}_{per}\left(x, l_{\square}\right) = (l_{\square} - s + x, 0) \text{ if } 0 \leq x < s, \\
&\boldsymbol{\varphi}_{per}\left(x, l_{\square}\right) = (x - s, 0) \text{ if } s \leq x \leq l_{\square},
\end{aligned}
\tag{2}
$$

where the shifting distance is given by $s = l_\square/\tan\alpha$. Clearly, we may carry out the same procedure also for cracks with $\alpha < 45°$.

Using the expression given by Equation (2), we may obtain aligned periodic boundary conditions on weak form by only modifying the mirror function $\boldsymbol{\varphi}_{per}$. Since the shifting distance s depends only on α and $l_\square$, the shifting is valid also for cracks that do not pass through the center of the RVE.



(a) Standard mirror function.

(b) Shifted mirror function. The shifting distance s is given by $s = l_\square/\tan\alpha$.

Figure 1: RVE with boundary divided into image ($\Gamma_\square^+$) and mirror ($\Gamma_\square^-$) parts, with standard mirror function (a) and shifted mirror function (b). The symbols denote related points on $\Gamma_\square^+$ and $\Gamma_\square^-$.

3 RESULTS

To demonstrate the effect of aligning the boundary conditions, we consider an RVE consisting of hard bulk material and a curved band of softer material (Figure 2). The RVE is deformed in x-direction and the resulting effective stress is shown in Figure 2. As can be seen, severe stress concentrations occur when using unaligned BCs, whereas aligned BCs lead to a more uniform stress field.

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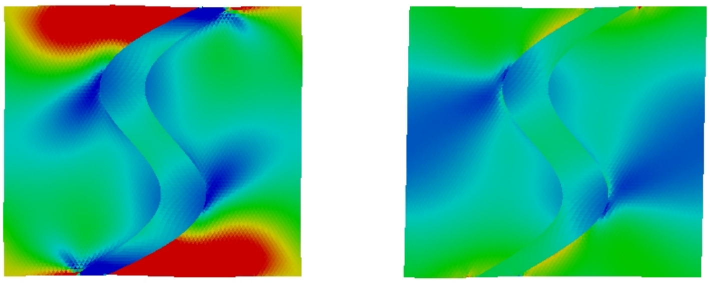

Figure 2: Effective stress in an RVE computed with unaligned (left) and aligned (right) weakly periodic boundary conditions. As can be seen, severe stress concentrations occur on the upper and lower boundaries when unaligned BCs are used.

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