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## Computational homogenization of microfractured continua using weakly periodic boundary conditions

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#### Highlights

- Computational homogenization of elastic media with stationary cracks is studied.
- A mixed variational format is used to impose periodic SVE boundary conditions weakly.
- A particular BC suitable for non-matching meshes and boundary cracks is proposed.
- Fulfillment of the LBB (inf-sup) condition for this BC is analytically proven.
- Superior convergence compared to conventional BCs is shown in the examples.

### Abstract

Computational homogenization of elastic media with stationary cracks is considered, whereby the macroscale stress is obtained by solving a boundary value problem on a Statistical Volume Element (SVE) and the cracks are represented by means of the eXtended Finite Element Method (XFEM). With the presence of cracks on the microscale, conventional BCs (Dirichlet, Neumann, strong periodic) perform poorly, in particular when cracks intersect the SVE boundary. As a remedy, we herein propose to use a mixed variational format to impose periodic boundary conditions in a weak sense on the SVE. Within this framework, we develop a novel traction approximation that is suitable when cracks intersect the SVE boundary. Our main result is the proposition of a stable traction approximation that is piecewise constant between crack–boundary intersections. In particular, we prove analytically that the proposed approximation is stable in terms of the LBB (inf–sup) condition and illustrate the stability properties with a numerical example. We emphasize that the stability analysis is carried out within the setting of weakly periodic boundary conditions, but it also applies to other mixed problems with similar structure, e.g. contact problems. The numerical examples show that the proposed traction approximation is more efficient than conventional boundary conditions (Dirichlet, Neumann, strong periodic) in terms of convergence with increasing SVE size.

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*Keywords:* XFEM; Multiscale modeling; Microcracks; LBB (inf–sup); Computational homogenization; Weak periodicity

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Fig. 1. SVE used for illustration of the problems associated to conventional BCs.

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Fig. 2. SVE subject to a macroscopic strain of  $\bar{\epsilon}_{xx} = 0.1$ ,  $\bar{\epsilon}_{yy} = 0.1$ ,  $\bar{\epsilon}_{xy} = 0$ : Qualitative comparison of Dirichlet BCs (left), Strong periodic BCs (center) and Neumann BCs (right).

### 1. Introduction

Computational homogenization [\[1](#page--1-0)[,2\]](#page--1-1) offers the possibility to model the effective response of microheterogeneous materials in numerical simulations. The standard approach is to homogenize the response of a Statistical Volume Element  $(SVE)$ ,<sup>[1](#page-1-0)</sup> whereby the choice of suitable boundary conditions (BCs) on the SVE is critical. It should be noted that conventional BCs (Neumann, Dirichlet and strong periodic [\[4,](#page--1-2)[5\]](#page--1-3)) are inaccurate if cracks are present in the microstructure. In particular, Neumann BCs result in severe underestimation of the effective stiffness if cracks cause a piece of the microstructure to be "cut loose" close to the SVE boundary. On the other hand, Dirichlet BCs as well as strong periodic BCs suppress crack opening at the SVE boundary, leading to overstiff predictions. To illustrate these deficiencies, consider the SVE shown in [Fig. 1,](#page-1-1) with traction free cracks and linear elastic bulk material. Applying a macroscopic strain of  $\bar{\epsilon}_{xx} = 0.1$ ,  $\bar{\epsilon}_{yy} = 0.1$ ,  $\bar{\epsilon}_{xy} = 0$  using Dirichlet, Strong periodic and Neumann boundary conditions gives the qualitative behavior shown in [Fig. 2.](#page-1-2) We note that Dirichlet BCs as well as strong periodic BCs enforce crack closure on the SVE boundary, leading to overstiff predictions. Neumann BCs predict very low stresses, leading to severe underprediction of the stiffness.

In the present work, we aim to alleviate the deficiencies illustrated above by proposing boundary conditions that are free of artificial crack closure on the SVE boundary without severely underestimating the effective stiffness. We recognize that the so-called window method, initially proposed by Babuška et al. [[6\]](#page--1-4), could be a suitable alternative to be investigated for our purposes. This since the window method has indicated to show faster convergence than Dirichlet and Neumann BCs and since it is readily applicable when voids (or cracks) are present at the boundary, in contrast to strong periodic boundary conditions in their standard form [\[7\]](#page--1-5). In this method, the SVE is embedded into a frame of a homogeneous material with a stiffness (updated iteratively) that matches the homogenized response of the SVE. This could potentially overcome some of the overstiffening effects obtained when enforcing crack closure at the boundaries using Dirichlet or strong periodic BCs.

However, in order to avoid the add-ons from the window method (iterative update of the stiffness of the frame material and an enlarged SVE), we instead develop a weak format of microperiodicity in the spirit of [\[6\]](#page--1-4), restricting

<span id="page-1-0"></span><sup>&</sup>lt;sup>1</sup> We prefer the notation SVE over Representative Volume Element (RVE), since a volume element of finite size will, in general, not be truly representative, cf. Ostoja-Starzewski [\[3\]](#page--1-6).

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