21st International Conference ENGINEERING MECHANICS 2015
Svratka, Czech Republic, May 11 –14, 2015
Paper #142, pp. 50–51

Wang Tilings in Numerical Homogenization

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Keywords: Wang tilings, heterogeneous materials, numerical homogenization, RVE determination

Abstract: Wang tilings have been recently shown to bring novel insights to microstructure representation efforts generalizing the conventional unit-cell approach. It allows to reconstruct stochastic realizations of the compressed medium without prior periodic assumptions on microstructural patterns. Moreover, once the microstructure is compressed, realizations of various sizes can be generated at almost negligible cost. We follow the standard numerical homogenization procedure and utilize the Wang tiles-based microstructure representation to generate computational domains. In order to alleviate computational cost, ideas of domain decomposition are adopted benefiting from the repetitive patterns in the computational domains.

Introduction

Homogenization is a standard method of incorporating knowledge of microstructure composition into macro-scale models providing that the characteristic lengths of the microstructure, l, and the macroscopic model, L, are well separated, i.e. $l/L \rightarrow 0$. For standard microstructure geometries, analytical homogenization methods provide accurate estimates of the effective properties. However, in the case of high contrast in microstructure constituents' properties, the influence of actual microstructure geometry is significantly pronounced. As a result, the general guaranteed bounds on the effective properties become unacceptably loose and a numerical homogenization technique is usually employed to determine the sought overall parameters. Besides, the latter enables to determine the size of the Representative Volume Element (RVE) and thus to validate the condition of scale-separation.

Modelling heterogeneous materials with Wang tilings

The abstract concept of Wang tilings, originally introduced in [1] in 1961 as a mean of proving certain logical statements, eventually drew attention of researchers from various branches of science, see e.g. [2] and references therein. The concept itself resembles a game of jigsaw puzzle up to some distinctions. The basic element of the concept is a square cell, a Wang tile, with codes attributed to its edges. The codes take a role of constraints during an assembly of tiles in a larger patch, a tiling, since only the tiles with the corresponding codes on the congruent edges can be placed side by side. However, unlike in jigsaw puzzles, there are infinitely many copies of each tile in the tile set allowing so generating arbitrarily large and random tilings.

First shown in Computer Graphics [3], once a visual pattern is attributed to the interior of each tile such that the pattern remains continuous across the edges sharing the same code, one can produce naturally looking patterns without visible periodicity. Benefiting from this features, Novák et al. demonstrated that the Wang tiling-based representation of material microstructure surpasses the conventional Periodic Unit Cell (PUC) approach to modelling of heterogeneous materials, namely in reducing long range order artefacts [2].They also showed that the standard procedures developed for generating PUC, e.g. optimization-based approaches, can be straightforwardly altered to account for the edge continuity requirement. As an alternative, a method making use of reference microstructure samples has been introduced in [3] and augmented with spatial statistics for purposes of material modelling in [4]. Once the tiles are designed to incorporate a part of microstructural information continuous across the corresponding edge, stochastic microstructure realizations of any size can be instantaneously generated using the stochastic tiling algorithm [3].

Numerical homogenization and RVE determination

One of the main concerns in numerical homogenization is the issue of representativeness of the computational domain. In order to render the effective properties, the domain is required to be large enough to incorporate all the microstructural features and yet remain small to be considered a material point from the perspective of the macro-scale task. Such a domain is referred to as Representative Volume Element [5]. In the standard numerical homogenization analysis, computational domains, called Statistical Volume Elements (SVE), of increasing size are generated with multiple realizations for each size. For each realisation two boundary value problems are solved rendering so the apparent properties [6]. Using the Partition theorem [7], we construct confidence intervals of the upper and lower bounds on the sought effective property for each SVE size. Taking advantage of nearly no additional cost related to generating microstructure realizations with Wang tilings, the number of realizations of each SVE size is not given a priori and adapts on-the-fly in order to accurately determine the bounds. Ideally, the SVE size is kept sequentially increasing until the bounds coincide defining so the effective property and the size of RVE. However, this holds only for an infinitely large domain. Therefore we stop the procedure when a given threshold for the bounds proximity is reached.

The above described approach leads to many calculations. Due to the tiling-based microstructure representation, computational domains are composed of non-periodic yet repeating patterns. thus, we advantageously adopt ideas of domain decomposition, the Schur complements method in particular, to mitigate the computational cost. For linear problems, each tile can be converted to a macro-element by eliminating the internal degrees of freedom (DOFs). As a result, a significantly reduced number of DOFs is necessary for each SVE's calculation.

Acknowledgements: The support by the Czech Science Foundation through project No. 1324027S is gratefully acknowledged. We would also like to thank the Grant Agency of the Czech Technical University in Prague, grant No. SGS15/030/OHK1/1T/11, and the European Social Fund endowment under Grant No. CZ.1.07/2.3.00/30.0005 of Brno University of Technology (Support for the creation of excellent interdisciplinary research teams at Brno University of Technology).

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