Challenges of Finite Element Discretization of Wang Cubes

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Abstract

The recently introduced concept of Wang tiling is an efficient technique for modelling real-world microstructures that supersedes the classical microstructure representation based on a periodic unit cell (PUC). Microstructure characteristics are attributed to a small set of mutually compatible cells – Wang tiles – such that the internal structure of cells matches across the corresponding interfaces. As a result, arbitrarily large, stochastic realizations of the compressed microstructure can be efficiently generated. The assembly is applicable also to a finite element (FE) discretization, accelerating generation of numerical microstructure models even further. This paper addresses specific requirements related to the generalized periodic boundary conditions, arising in the FE discretization of Wang tiles, and illustrates their handling with processing a 3D microstructure with ellipsoidal inclusions.

Keywords: Wang tiles, Wang cubes, RVE synthesis, generalized periodic boundary conditions, finite element discretization

1. Introduction

Advances in numerical multi-scale methods [1] require an efficient and representative description of the underlying material microstructure. Nowadays, the commonly adopted approach to characterization of a material microstructure is based on a PUC [2, 3]. An appealing extension of PUC has been introduced recently in [4], employing an abstract concept of Wang tiling [5]. In this extension, the material microstructure is described with a set of small cells (squares/cubes in 2D/3D) which can be assembled into larger blocks serving as a continuous representation of the compressed microstructure. The assembly process must comply with the boundary constraints so that the internal structure of adjacent cells matches across the shared boundary. This is demonstrated in Fig. 1, where the constraints are indicated with color codes of cell edges. From this point of view, the PUC approach is a trivial instance of Wang tiling set containing a single cell with the same code on the opposite pairs of sides. In order to make the assembly process stochastic, there must exist always at least two tiles satisfying the constraints at current position in the tiling at any given assembly stage. The most attractive feature of the Wang tiling concept is the efficiency with which stochastic (or aperiodic), arbitrarily large realizations of compressed microstructure can be generated while reducing spurious artefacts, otherwise inherent to the PUC. The standard ways

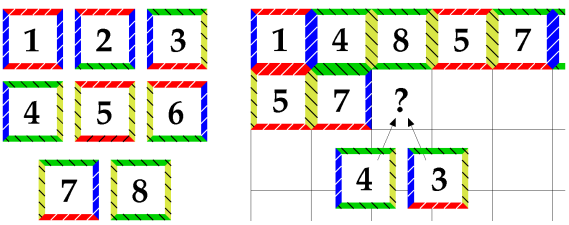

Figure 1: Wang tiling concept: set of 8 Wang tiles (left), assembly process (right). Different black and white hatching is used to distinguish color codes on black and white prints.

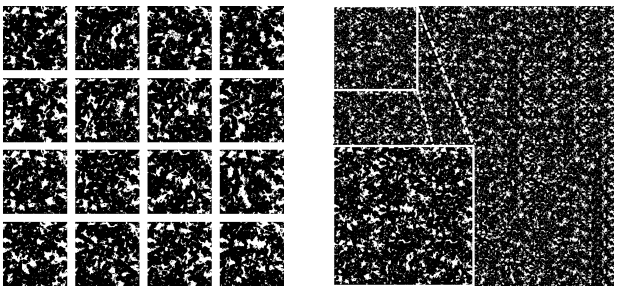

Figure 2: Real microstructure: compression using set of 16 Wang tiles (left), reconstruction using 10×10 tiles (right).

of PUC design, typically based on an optimization approach, e.g., [3], can be straightforwardly modified to incorporate the generalized boundary conditions of Wang tiles. Alternatively, the Wang tiles can be designed using pattern generation techniques developed in computational graphics [6]. These techniques, however, need to be appropriately modified to account for spatial description widely used in statistical physics [7]. An example of a compression of a real microstructure and its realizations based on that compression is depicted in Fig 2.

The reconstruction of the microstructure using the concept of Wang tiling can be applied on various levels – from the level of the CT scan images of given material microstructure up to the level of its FE discretization, the last being focus of this abstract. In the illustrative problem of the RVE size determination, two factors come into play [8]: size of the investigated microstructure specimen, which can differ for various physical phenomena [6], and accuracy of numerical solution to boundary value problem utilized either for determination of the homogenized properties or as a micro-scale model in FE^2 analyses [1]. Often many realizations of rather complex geometries of the microstructure are required, which makes a fast and robust discretization of the microstructure specimen into FE mesh indispensable. With the concept of Wang cubes at hand, it suffices to create discretizations of

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individual cells (see Fig. 3) of a particular Wang tiling set which satisfy the boundary constraints and that can be efficiently assembled into larger realizations without the need to explicitly search for pairs of nodes that have to be merged together.

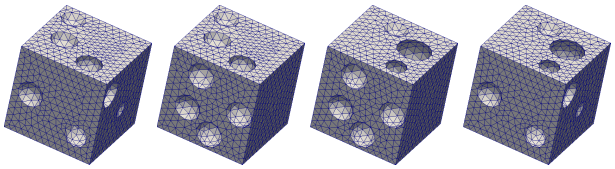

Figure 3: Discretization of several Wang cubes representing compressed microstructure with spherical inclusions.

The remainder of this paper examines issues which should be considered when generating FE grids over Wang cubes within the context of processing a 3D microstructure with ellipsoidal inclusions using the T3D mesh generator [9]. This mesh generator is capable to discretize models described by boundary representation into high quality tetrahedral meshes using an advancing front technique with octree based mesh density control.

2. Discretization of Wang Cubes

The crucial aspect of FE discretization of individual Wang cubes is to facilitate satisfaction of the assembly constraints trough the generalized periodic boundary conditions imposed on the discretization. This implies that 2D meshes over faces of Wang cubes marked with the same color code (thereafter called matching faces) should be discretized by geometrically (in the sense of coordinates of nodes) and topologically (in the sense of element connectivity) identical meshes. At the first glance, this requirement seems straightforward to achieve as the geometry of matching faces of the relevant Wang cubes should be identical. However, with respect to a particular meshing technique, the mesh may depend on the topology of the model (for example, on the ordering or orientation of curves bounding the face). Even if the meshing technique is not sensitive to the model topology, the meshes generated independently over geometrically identical faces can differ because the mesh spacing along the matching faces of separate cubes, generally influenced by the mesh density in the interior of these cubes, may differ. The only viable solution is to subject one of the matching faces to the discretization and replicate the mesh on the remaining faces. This more or less implies that individual cubes of a particular Wang set cannot be discretized independently but should be processes together within the same model.

The replication of meshes can be significantly simplified if the topology of the faces is identical. This can be achieved if the model of each Wang cube respects the global numbering of individual ellipsoidal inclusions used in the complete set of Wang cubes. Since each of the matching faces is intersected by the same set of inclusions (otherwise the faces would not match each other), the processing of inclusions according to their global numbering results in topologically identical representation of matching faces. Moreover, if the meshing is performed hierarchically, e.g., from vertices, to curves, surfaces and volumes, and if the output of nodes on individual model entities follows this hierarchical ordering, then processing of inclusions according to their global numbering makes the relative ordering of mesh nodes on matching faces in the output file identical irrespectively whether treating the face on which the mesh was really generated or the face on which the mesh was replicated. This is essential for an efficient assembly of FE meshes of individual Wang cubes into RVE of required size.

The simple replication of a 2D mesh over matching faces of Wang cubes may cause, however, discrepancies in the mesh spacing between the replicated mesh and the mesh density control space. This may significantly deteriorate the quality of a volume mesh inside cubes bounded by faces on which the mesh was replicated. It is therefore desirable to "synchronize" the mesh density control space(s) along the matching faces before the actual mesh generation takes place. The synchronization should be usually done in several passes, as modification of mesh density control space along a particular face may partially amend the mesh spacing along other (possibly also matching) face. Note also that the synchronization should not be scrupulously strict to avoid undesirable refinement of the mesh.

When using a separate mesh density control space for each cube, the individual cubes can occupy the same position (overlapping each other) within a common model, provided that the adopted meshing technique can handle such setup. Otherwise, the cubes must be arranged on a regular 2D or 3D grid, for example, with a mutual spacing that will guarantee that the cubes do not overlap each other and, if a single common mesh density control space is used, that parts of this space corresponding to individual cubes do not interfere with each other. Apparently, meshes generated over shifted cubes must be translated back to a reference position to make the later FE mesh assembly process straightforward.

3. Conclusions

This paper examines specific issues related to the FE mesh generation over individual cells of Wang tiling set in the context of efficient RVE synthesis on the level of FE computational grids. Namely the procedures needed to comply with the generalized periodic boundary conditions are discussed. The presented concept of RVE synthesis is very appealing as it can naturally deliver high quality discretization of virtually unlimited number of microstructure realizations in an extremely economic manner. For example, nearly 85 % saving in mesh generation time is observed already for two realizations of $4\times4\times4$ tiles specimen built using a basic Wang set composed of 16 cubes.

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