

SYNTHESIZED MICROMECHANICAL FIELDS BASED ON THE SYNERGY OF WANG TILES AND FEM

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Abstract: *In this contribution, we present the concept of replacing periodic unit cell (PUC) with a set of specifically designed cells and their utilization for modeling of materials with heterogeneous microstructures and for reconstruction of micromechanical fields. The approach is based on the Wang tiles method that compresses the stochastic microstructure into a small set of statistical volume elements – tiles. Tiles are placed side by side according to matching edge codes like in a game domino. Using the stochastic tiling algorithms the microstructure of arbitrarily large domain is recreated and opposite to the repeating pattern of PUC it preserves its randomness. To obtain the mechanical response of whole domain, the micromechanical quantities are evaluated only on tiles and then synthesized back. But because of the non-local character of mechanical quantities the resulting field contains jumps between adjacent tiles. To prevent this phenomenon, the surrounding layers of tiles of each addressed tile are included into the evaluation. In our latest work, we are focused on how the characteristic microstructural lengths influence the convenient size of individual tiles and how the number of included layers of tiles affects the resulting error between the synthesized and reference micromechanical field.*

Keywords: Heterogeneous microstructures, Wang tiles, Synthesized Micromechanical Fields, Finite Element Method.

1. Introduction

With the increasing pressure to the utmost material performance, we need a detailed understanding of characteristic mechanical processes taking place on a microstructural level. But when we look closely at materials used in engineering applications the majority of them is heterogeneous with a stochastic microstructure layout.

Several methods can be used for modeling of such microstructures. One of the most widely used methods is numerical homogenization. For materials with periodic patterns are the heterogeneities modeled as periodic unit cells (PUC). A small part of the original microstructure is representing the cell and just by duplication in cardinal directions we obtain original microstructure. For non-periodic microstructures is used the statistically equivalent periodic unit cell (SEPUC) which shares the statistical description with the original microstructure. However, in both cases, only a single cell is describing the whole microstructure which brings periodicity in all further operations. If we are searching only for the effective parameters the periodicity plays no role but when we want to study mechanical response of the microstructure itself (e.g. stresses, strains or displacements) we need to preserve the stochastic microstructure.

In contrast, a different method that does not operate with only one cell, but represents the media through a set of cells can be used. These cells are mutually compatible on the edges and using specific algorithm they can create an infinitely large reconstructed microstructure which preserve stochastic distribution. This method is called Wang tiles.

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2. Wang tiles

The principle of the method of Wang tiles was introduced in the early sixties of the 20th century by Mr. Hao Wang (Wang. H., 1961; Wang H., 1965). It can be viewed as a game domino (Fig. 1a) where the goal is to place pieces side by side so they match in a number of dots on adjacent sides. The concept is nearly same for the Wang tiles, but in contrast to bilaterally coded rectangular domino pieces, the tiles are squares with four edge codes (Fig. 1b). Tiles are placed next to each other in cardinal directions according to matching codes on edges but cannot be rotated during the process. The created planar domain with no errors like incorrectly placed tiles or holes is called valid tiling.



Fig. 1: Principle of Wang tiles, a) domino game, b) Wang tiles.

2.1. Tile sets

As mentioned above, the Wang tiles compress the given structure into only a few small pieces, together called tile set, which holds the properties of the original structure. That means the tiles must be designed specifically.

One of the few approaches to design tiles is based on optimization of tile morphology according to statistical descriptors so the statistics of reconstructed microstructure corresponds to the original. But as shown in the paper from authors Novák J., Kučerová A., & Zeman J. (2012) with increasing pressure on optimization the tiles tends to become identical and the reconstructed microstructure show signs of periodicity. The second approach is called Automatic Tile Design (Cohen M. F. et al., 2003). Each tile is created as a cutout from a combination of four small samples of the original microstructure. This method is almost instantaneous if compared with first one which is much more time demanding because of the optimization. Another way of designing tiles is useful only for microstructures with individual particles that can be described by simple geometrical shapes. This method use the dynamics of each particle and by their movement and collisions the particles are distributed in tiles (Stránský J., 2014; Šedlbauer D. & Lepš M., 2013).

Whether we use any of these methods the created tiles must fulfill such conditions that we are able to create a stochastic valid tiling.

2.2. Stochastic tiling

When creating a tiling we start with a single tile. In the next step we place another tile (with one corresponding edge code) next to the first one in four possible directions. Let's call these directions north (N), south (S), east (E) and west (W) (Fig. 2a). If we are not creating a long strip of tiles, we will at some point get in a situation where we need to place a tile in a position where two edge codes must correspond (Fig. 2b). To create the stochastic tiling and match the conditions of stochastic tiling algorithm (Cohen M. F. et al., 2003) we need at least two tiles that can be placed correctly in these corner positions. The smallest set that comply these requirements is set consisting of 8 tiles with two different vertical edge codes and two different horizontal edge codes. We call this set W8/2-2 and we use it in all following steps of our work.

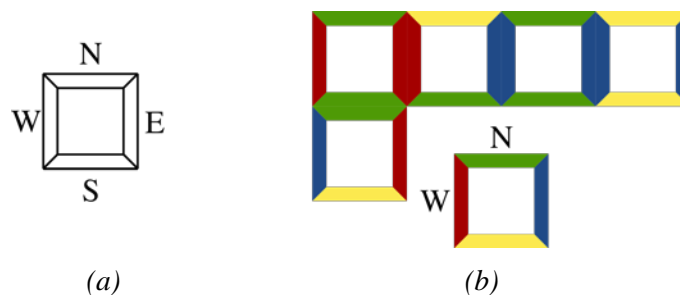


Fig. 2: Wang tiles edges and corner position, a) cardinal directions and b) the NW corner position.

3. Synthesis of micromechanical fields

The Wang tiles method can be used in numerous ways. One of the first applications of the Wang tiles method was modeling of quasicrystals and generating naturally looking textures for computer graphic (Cohen M. F. et al., 2003). In material modeling, the method can be considered as a substitution of the PUC and SEPUC concepts or as a microstructure sensitive enrichment functions in Partition Unity (Melenk J. M. & Babuška I., 1996) and Hybrid finite element method (Freitas J.T. de., 1998).

In this paper, we focus on the analysis of microscale quantities as stresses, strains and displacements solved by finite element method (FEM). Simply said, the micromechanical response is evaluated on tiles instead of time-consuming evaluation of whole discretized domain and then, using the results from individual tiles, synthesized back. But because of the non-local character of mechanical quantities the grid of underlying tiles is clearly visible in the reconstructed mechanical field. The evaluated response of adjacent tiles does not coincide on edges and therefore, the micromechanical field is not continuous. That is because the mechanical response of each tile is affected by its surrounding tiles.

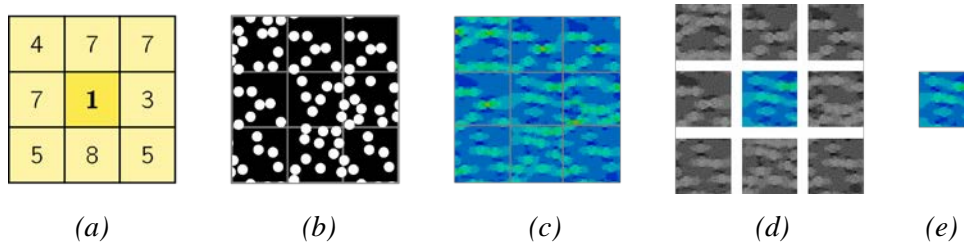


Fig. 3: Process of creating a tile from extended Wang tile set, a) center tile with one layer of surrounding tiles, b) small synthesized domain, c) solved small domain, d) cutting off included tiles and e) tile from extended Wang tile set.

One way to address this problem is to include the surrounding layers of tiles into the evaluation of the micromechanical response. For each tile from the tiling, we add the surrounding layers of tiles, in this case only one layer (Fig. 3a), synthesize small microstructural subdomain (Fig. 3b), solve the mechanical response for this subdomain (Fig. 3c) and cut off the included tiles from results (Fig. 3d). The outcome is the tile from so-called extended Wang tile set (Fig. 3e). After repeating this process for every tile from the tiling, the micromechanical field is synthesized using the tiles from the extended Wang tile set.

This technique gives us synthesized fields where the underlying grid is not so distinct and the jumps on edges of adjacent tiles are much smaller, as shown in paper Zrůbek, et al., (2012). However, this approach dramatically increases the number of small tasks that have to be evaluated. On top of that, as more than one layer of surrounding tiles can be included, the size m of the subdomain is increasing, which increase the evaluation time.

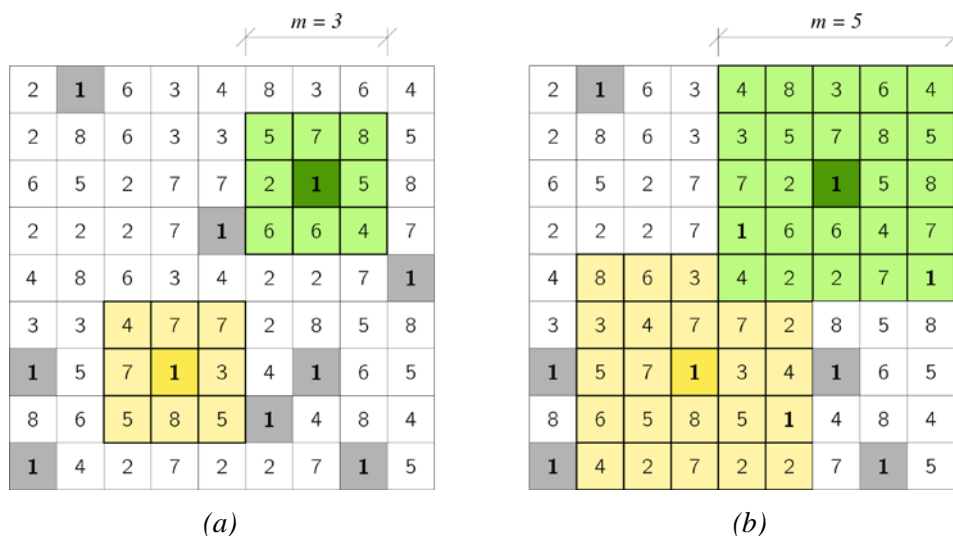


Fig. 4: Included surrounding layers of tiles and size m of the subdomain, a) single included layer ($m=3$), b) two included layers ($m=5$).

4. Future work and summary

At this stage, we are working on a sensitive analysis where we are focusing on two main topics. The first one is the evolution of error when including one, two or more layers of surrounding tiles. The error is obtained as difference between synthesized micromechanical field and reference solution. So far obtained results suggest that with increasing number of layers the error should have a decreasing tendency.

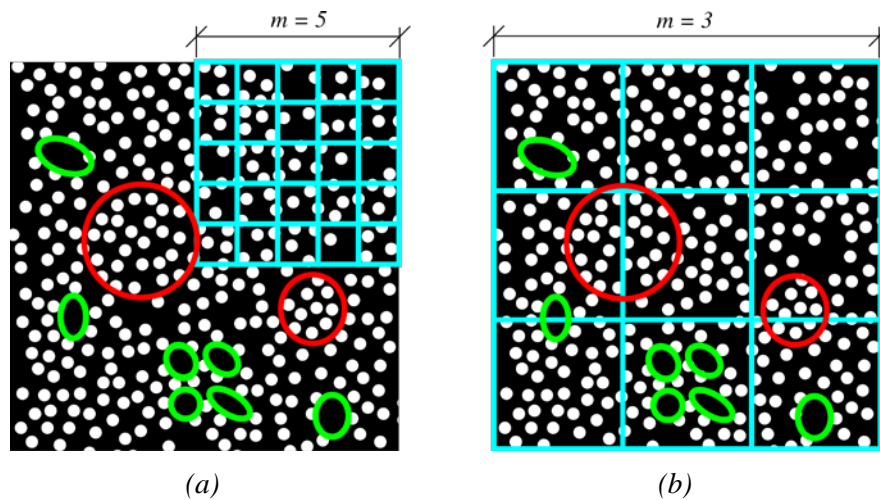


Fig. 5: Characteristic microstructural lengths, tile size and subdomain size.

In the second topic, which is closely tied with the first one, we are trying to analyze how the characteristic microstructural lengths are affecting the optimal size of tiles. As shown in the Fig. 5, the microstructure contains some sort of clusters of empty matrix (green) and even clusters of particles (red). In the Fig. 5a the size of clusters is bigger than the size of tiles which means that the influence of these clusters may act over several tiles (cyan squares) and we need to extend subdomains with more layers of surrounding tiles. In Fig. 5b are tiles (cyan squares) bigger than clusters so a subdomain with only one layer extension of surrounding tiles is sufficient. But as larger the tiles are the more time-consuming is the evaluation of individual subdomains. Therefore, we are trying to find optimal size of tiles with an optimal number of subdomain layer extensions, to minimize the error and required computer time.

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