

PARALLEL COMPUTATION OF MICROSTRUCTURAL FIELDS BASED ON EXTENDED WANG TILE SETS

L. Zrůbek¹, J. Kruis¹, J. Novák² and A. Kučerová¹

Summary: *This contribution addresses the method of Wang tilings used to reproduce fluctuating stresses, strains and displacements in materials with random microstructure subject to uniform strain excitation. Using small sets of Wang tiles allows to avoid an abrupt evaluation of fluctuating fields in a large macro-scopic domain, carrying a complete number of non-local solutions to desired mechanical quantities and synthesized by means of stochastic tiling algorithm. Assuming each tile discretized by the same regular finite element mesh, all admissible micro-scale problems can be obtained effectively by the Schur complement method.*

Keywords: *microstructure, Wang tilings, stress field synthesis, Schur complement method*

1. Introduction

In engineering applications we are witnessing a steadily increasing pressure to the utmost materials performance. It can be achieved, provided a detailed understanding of characteristic mechanical processes taking place on microstructural level. To that end, we draw our attention in high performance analysis of micro-scopic fluctuation fields in random particulate composites subject to uniform strain excitation that can be used as microstructure-sensitive enrichment functions in Partition of Unity (Melenk & Babuška (1996)) and Hybrid Finite Element methods (Freitas (1998); Novák, Kaczmarczyk, Grassl, Zeman, Pearce (2012)). The proposed technique rests on Wang tilings, known from computer graphics and materials science, where it has been applied to synthesis of random, statistically consistent, microstructural patterns on open planar domains. A synthesized domain is composed of tiles, statistical volume elements (Fulwood, Niezgoda, Adams, Kalidindi (2010)), gathered in sets. All distinct tiles together must involve complete morphological information of the texture quantity. If so, the set corresponds to representative volume element.

In real world applications, thousands of tile copies may be required to cover up a structural scale domain. In addition, and contrary to a purely microstructural information synthesized so far (presented by Novák, Kučerová, Zeman (2012)), the sought enrichment fields are nonlocal.

¹ Ing. Lukáš Zrůbek; Doc. Ing. Jaroslav Kruis, Ph.D.; Ing. Anna Kučerová, Ph.D.; Department of Mechanics, Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, 166 09, Prague 6

² Ing. Jan Novák, Ph.D.; Department of Mechanics, Faculty of Civil Engineering, Czech Technical University in Prague, Thákurova 7, 166 09 Prague 6 and Institute of Structural Mechanics, Faculty of Civil Engineering, Brno University of Technology, Antonínská 548/1, 601 90, Brno

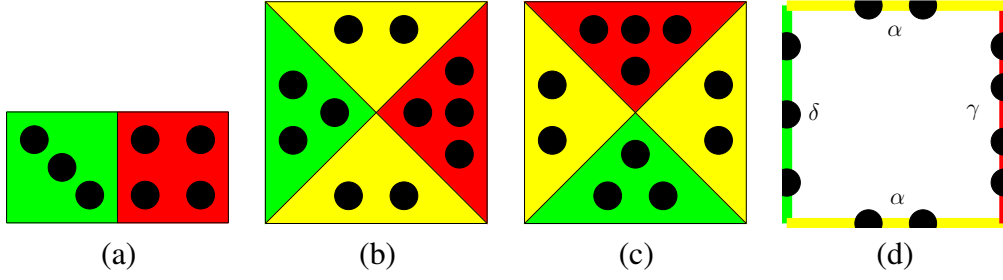


Figure 1: Wang tile, a) ancient domino piece, b) Wang tile with three different codes on four edges, c) another Wang tile obtained by rotating tile (b) by $\pi/4$ clockwise, d) tile (b) with edge regions concentrated to edges.

In other words, the neighbours of a certain distance from each individual tile are responsible for the fields inside the tile, and must be therefore taken into account in order to arrive at equilibrated traction fluctuations or compatible displacements on tile interfaces. It yields, thousands of micro-scale problems, square tilings of optional neighbourhood extent $m \times m$, Tabs. 2 and 3, with imposed periodic boundary conditions have to be solved. Recently, structured discretizations arising from raster image representations of microstructures have been resolved by Moulinec-Suquet Fast Fourier Transform based algorithm (Moulinec & Suquet (1994)). However, strongly heterogeneous materials with a significant contrast in material parameters of individual phases, e.g. high porosity foams or reinforced plastics, have caused serious convergence difficulty, thereby, turning our attention to conventional finite element method (FEM) and high performance computing (HPC).

2. Wang tiles, sets and tilings

The method of Wang tilings, introduced by Hao Wang (see Wang (1961)), is a fresh subject to computational mechanics community. In general, it can be viewed as a planar domino game or a jigsaw puzzle³. This study proceeds from the recent observation (Novák, Kučerová, Zeman (2012)) that the Wang tile sets represent a generalization to the periodic unit cell concept (PUC), common in multiscale simulations. However, contrary to PUC framework, the appealing feature of tilings consist of the ability to reproduce non-periodic microstructural patterns. A brief specification of Wang tiling features follows.

A single Wang *tile* can be referred to as a piece of square polyomino (tetromino or say doubled domino) which is not allowed to rotate when brought together with other pieces through congruent edges (green, red, yellow triangular sub-regions in figure Fig. 1(b)). This means, that two tiles with identical sequence of edges, mutually rotated by $k\pi/4$ are considered as different, Fig. 1(b,c). In practical applications, the triangular edge regions are concentrated to edges denoted either by colors (see e.g. Wang (1965)), alphabetical codes (in paper by Novák, Kučerová, Zeman (2012)) or enumerated by integers (Culik (1996); Aristoff & Radin (2011)), Fig. 1(d). A collection of unique tiles that enable to cover up open planar domains aperiodically is called *tile set*, Fig. 2(a). It is referred to as $Wn^t/n_1^c - n_2^c$, where W stands for “Wang” initial, n^t is the number of tiles in the set and n_i^c denotes the number of edge codes in i th spatial direction. The number of edge codes n^c in the i th spatial direction can be chosen

³ Here we recall the ETERNITY I and II game, see e.g. http://en.wikipedia.org/wiki/Eternity_II_puzzle

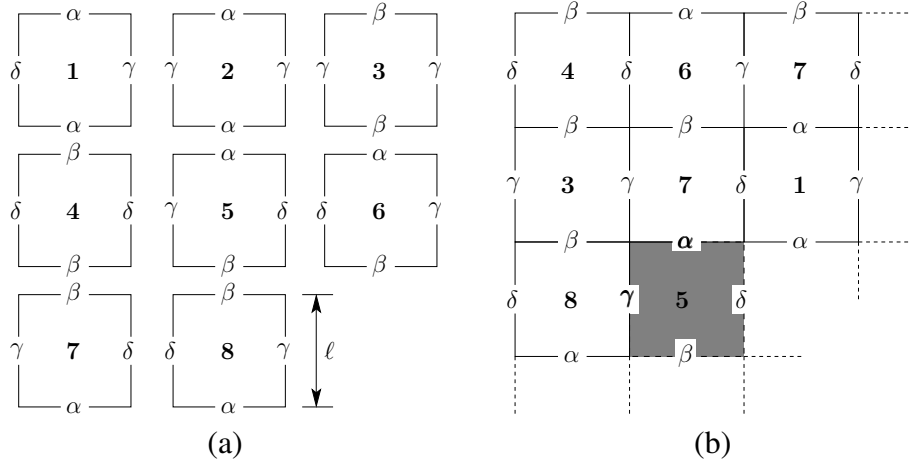


Figure 2: (a) Wang tile set W8/2-2, (b) example of valid tiling.

n_i^c		n^{cs}	n^{NW}	n^t	Tile set
n_1^c	n_2^c				
2	2	16	2	8	W8/2-2
3	3	81	2	18	W18/3-3
4	4	256	2	32	W32/4-4
5	5	625	2	50	W50/5-5
...	...				

Table 1: Number of tiles in Wang tile sets with respect to n_i^c , n^{cs} and n^{NW} .

arbitrarily, however, the number of tiles n^t must satisfy, Tab. 1,

$$n^t = n^{NW} \sqrt{n^{cs}}, \quad (1)$$

where $n^{cs} = (n_1^c n_2^c)^2$ is the number of tiles in the so called complete set and $n^{NW} \in \{2, \dots, \sqrt{n^{cs}}\}$ stands for the optional number of tiles with an identical arrangement of northwestern (NW) edge codes, α, γ adjacent to shaded tile $t = 5$ in Fig. 2(a). The complete set of n^{cs} tiles is obtained by permuting the chosen codes c_i , see Novák, Kučerová, Zeman (2012, 2013) for further details.

A *tiling* is the assembly of multiple copies of tiles from the set, Fig. 2(b). If there are no missing tiles in the tiling lattice and a morphological information across congruent edges is compatible everywhere we say the tiling is *valid* (so called ground state, see Aristoff & Radin (2011)). Since, invalid tilings are meaningless from the viewpoint of microstructure synthesis, the abbreviation *tiling* is used instead of valid tiling (Novák, Kučerová, Zeman (2012)).

When tiling a domain, we use stochastic algorithm created by Cohen, Shade, Hiller, Deussen (2003) (CSHD). The tiles are randomly selected from a set and successively placed one by one from the top-left corner towards bottom-right, so that the edge codes of newly placed tiles must comply with those of their neighbours placed previously. Owing to the rectangular nature of Wang tiles, it is sufficient to control the north-western pair of edges. The index of a new tile to be placed is selected randomly. In order to keep the procedure random, there must be always at least two of such tiles associated with each north-western edge-code combination. Aperiodicity of resulting tilings is thus guaranteed when assuming that the random generator never returns a periodic sequence of numbers (see Cohen, Shade, Hiller, Deussen (2003) for further details).

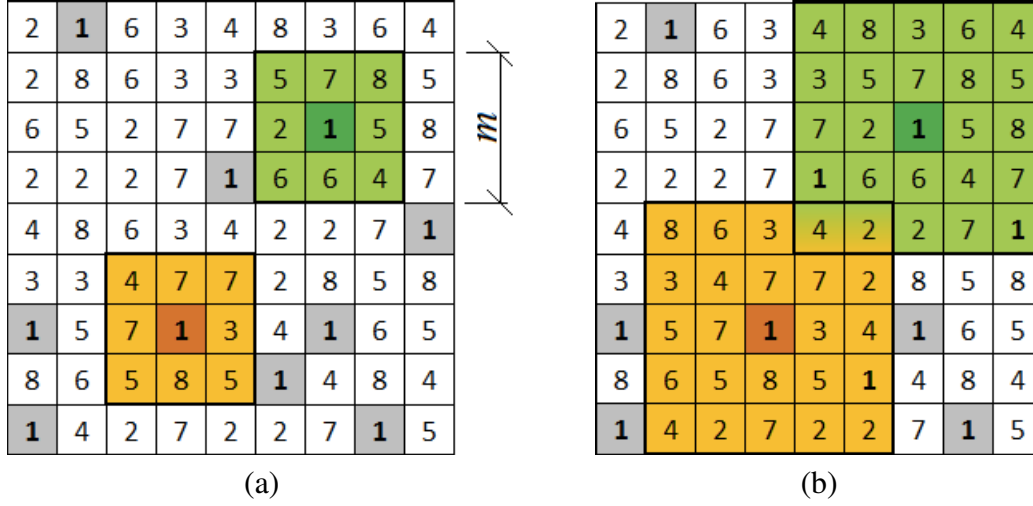


Figure 3: Tiling map, with highlighted neighbours of the first tile from $W8 \ 2 \ 2$, a) nearest, adjacent neighbours, b) first and second layer of neighbour tiles.

3. Tiles with nonlocal stress fluctuation patterns

Contrary to the synthesis of purely microstructural data, as reported e.g. in Novák, Kučerová, Zeman (2012), the subject of this contribution is more difficult as it aims at synthesis of non-local field patterns. In what follows, we limit our exposition to stress fluctuations due to the uniform strain excitation⁴. Regarding the non-local character of stresses, we do not last with the same number of tiles as it is normally used for microstructural data, see eg. Zrůbek, Kučerová, Novák (2012). The distribution of all components σ_{ij} in each tile depends, at least, on their distribution in adjacent tiles.

To simplify the exposition, let us assume the highlighted tiles $t = 1$ in Fig. 3(a). The stresses in each of the tiles are the functions of the interior microstructure and stress distribution in eight tiles placed around. It yields that, despite the fact that all tiles “one” have identical microstructure, the σ_{ij} components will differ for distinct combinations of surrounding tiles. It is also obvious that those differences will be further pronounced by decreasing ratio of the tile edge dimension ℓ , Fig. 2(a), and characteristic microstructural length(s), disk diameters and/or typical distances among the disks in Fig. 4(a).

In order to eliminate the traction jumps in a synthesized enrichment function, larger neighbourhoods should be considered, see Fig. 3(b). A particular number of distinct stress pattern patches in all tiles $1 \leq t \leq n^t$, with respect to the particular extent of neighbours $m \leq m$ is given by disjunctive colligation of admissible patches in each tile as, Tab. 2,

$$n_{m \ m}^{\text{comb}} = n^t (2n_i^c)^{2(m-1)} (n^{NW})^{(m-1)^2} \quad (2)$$

⁴ The stress fluctuations in a microstructured domain, arising from uniform excitations in normal and shear directions, simply called “stresses”.

Tile set	No. of all possible tilings $\mathcal{O}_{m \ m}$ for increasing extent $m \ m$							
	1 1	3 3	5 5	7 7	9 9	11 11	11 11	11 11
W8/2-2	8 0 10 ⁰	3 3 10 ⁴	3 4 10 ¹⁰	9 2 10 ¹⁸	6 3 10 ²⁹	1 1 10 ⁴³		
W18/3-3	1 8 10 ¹	3 7 10 ⁵	2 0 10 ¹²	2 7 10 ²¹	9 4 10 ³²	8 3 10 ⁴⁶		
W32/4-4	3 2 10 ¹	2 1 10 ⁶	3 5 10 ¹³	1 5 10 ²³	1 7 10 ³⁵	4 7 10 ⁴⁹		
W50/5-5	5 0 10 ¹	8 0 10 ⁶	3 3 10 ¹⁴	3 4 10 ²⁴	9 2 10 ³⁶	6 3 10 ⁵¹		

Table 2: Number of tilings to be solved in order to obtain all possible combinations of stress patterns for tiles $t = 1 \dots n^t$.

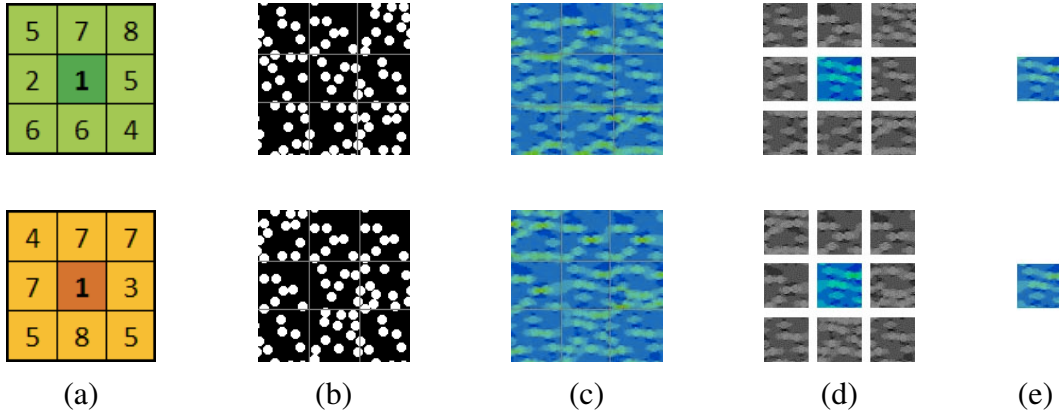


Figure 4: Stress patch flowchart, a) map of two distinct tilings $\mathcal{O}_{m \ m} = \mathcal{O}_{3 \ 3}$, b) microstructure of tiling $\mathcal{O}_{3 \ 3}$, c) stress fluctuations σ_x in $\mathcal{O}_{3 \ 3}$, d) $\mathcal{O}_{3 \ 3}$ decomposition, e) distinct stress fluctuation patterns (patches) in tile $t = 1$ as functions of different neighbourhoods.

3.1. Designing tile set morphology

As mentioned above, to create open domain tilings of self-equilibrated stress fluctuations (balanced traction fluctuations in the tiling lattice), it is necessary to store a number of copies of each tile $t = 1 \dots n^t$. This is given by all possible combinations of tiles that can arise around each tile t , when preserving the edge matching rules Tabs.(2, 3). An example of the genesis of two distinct copies of tile $t = 1$, embedded in the smallest neighbourhood $m = 3$, is represented by flowcharts in Fig. 4.

Having all the $\mathcal{O}_{m \ m}$ at hand, we solve $n_{m \ m}^{\text{comb}}$ of periodic boundary value problems where $\mathcal{O}_{m \ m}$ are the subject to uniform strain loadcases as in classical homogenization framework.

Tile set	Cardinal i -th and ordinal ij -th directions									No. combinations $n_{3 \ 3}^{\text{comb}}$
	n^t	N	S	E	W	NW	NE	SW	SE	
W8/2-2	8	4	4	4	4	2	2	2	2	32 768
W18/3-3	18	6	6	6	6	2	2	2	2	373 248
W32/4-4	32	8	8	8	8	2	2	2	2	2 097 152
W50/5-5	50	10	10	10	10	2	2	2	2	8 000 000

Table 3: No. combinations of tiles on neighbour positions in cardinal i -th and ordinal ij -th directions for minimal Wang tile sets, with extending to 3×3 tiles.

In two dimensions, we set the loading strain vector component successively to one, while the remaining two equal to zero. Despite the domain $\mathcal{O}_{m \times m}$ is not periodic on external boundary, the periodic boundary conditions are acceptable considering the very local character of stress fluctuations and their negligible action to the solution in the central tile (see Terada, Hori, Kyoya, Kikuchi (2000)). For example, instead of eight tiles (recall that $n^t = 8$ for $W8/2 - 2$) necessary to reconstruct either microstructural or stress patterns according to the methodology reported in Novák, Kučerová, Zeman (2013), this number increases to 32,768 when using the proposed strategy, see the first row of Tab. 3.

4. Evaluation of stress fluctuation patterns in tiles

4.1. Moulinec-Suquet FFT based solver

As mentioned above, the periodic boundary conditions are applied to tilings $\mathcal{O}_{m \times m}$, despite the microstructure does not need to necessarily exhibit periodicity. The periodic boundary conditions allow as to use the solution to elastic fields by means of the fast Fourier transform (FFT) based Moulinec-Suquet solver (Moulinec & Suquet (1994)). It is characterised by a well-known Lippman-Schwinger type equation. The periodic kernel of the integral formulation admits a compact closed-form expression in the Fourier space, so that its action to sought stresses can be effectively evaluated by FFT algorithms (Frigo & Johnson (2005)). The complexity of such solution proceeds from recent observations by Zeman, Vondřejc, Novák, Marek (2010), where the original iterative scheme is replaced by the solution to the linear system of equations of the size $N = d \times m \times \ell$, where d denotes the number of degrees of freedom (DOF) in a single discretization node (pixel). Each iteration thus measures $O(N \log N)$ operations. Although the computational overhead of this numerical strategy is imperceptible, it has several demerits as Gibbs effects, problems with infinite contrast of phases to cite a few.

4.2. Schur complement method

Assuming now the situation, when each tile is discretized by the finite element method. It has to be emphasized that all tiles of the same type are discretized by identical finite element mesh. Optionally, each pixel is a single element. A conventional approach of solving the full system would be thus extremely demanding. In order to speed up the computation, the Schur complement method can be used. For each type of tile, the Schur complement is evaluated. It means, all DOFs defined inside the tile are eliminated out to the edges, therefore, the tile is represented by its boundary DOFs only. Now, the tile resembles a generalized finite element or a subdomain in the domain decomposition methods. For simplicity, we illustrate the complexity on the following example. Let each tile be covered by a FE discretization of 200×200 finite elements, i.e. $\ell = 200$ px, yielding approximately 40,000 nodes per tile. However, the Schur complement method reduces the nodes to boundaries, resulting the total number of nodes to 800. The smallest admissible tiling $\mathcal{O}_{3 \times 3}$ is composed of 9 tiles and contains 360×10^3 nodes, which must be solved in the case of conventional approach. Contrary, the Schur complement method requires approximately 5×10^3 nodes.

The Schur complement method, also known as the substructuring method (Kruis (2004); Medek, Kruis, Tvrdík, Bittnar (2007)), is based on special ordering of DOFs. The DOFs defined in the internal nodes are ordered as first and the DOFs defined on the boundary are ordered as

last. With respect to this ordering of unknowns, the system of equations defined on a single tile can be written in the form

$$\begin{pmatrix} \mathbf{K}_{ii} & \mathbf{K}_{ib} \\ \mathbf{K}_{bi} & \mathbf{K}_{bb} \end{pmatrix} \begin{pmatrix} \mathbf{d}_i \\ \mathbf{d}_b \end{pmatrix} = \begin{pmatrix} \mathbf{f}_i \\ \mathbf{f}_b \end{pmatrix}, \quad (3)$$

where \mathbf{d}_i stands for the vector of internal unknowns, and \mathbf{d}_b represents its external (boundary) counterpart. By analogy, \mathbf{f}_i and \mathbf{f}_b , respectively, are associated with the part of the right hand side vector connected to tile interior and edges. Symbols \mathbf{K}_{ii} , \mathbf{K}_{ib} , \mathbf{K}_{bi} , \mathbf{K}_{bb} are the appropriate matrices. If the matrix \mathbf{K}_{ii} is non-singular, it further follows from Eq. 3, that the vector \mathbf{d}_i can be recasted as

$$\mathbf{d}_i = \mathbf{K}_{ii}^{-1}(\mathbf{f}_i - \mathbf{K}_{ib}\mathbf{d}_b), \quad (4)$$

and the original system of equations, Eq. 3, reduces to

$$(\mathbf{K}_{bb} - \mathbf{K}_{bi}\mathbf{K}_{ii}^{-1}\mathbf{K}_{ib})\mathbf{d}_b = \mathbf{f}_b - \mathbf{K}_{bi}\mathbf{K}_{ii}^{-1}\mathbf{f}_i. \quad (5)$$

Notice, that the above system of equations contains only the unknowns defined in the boundary nodes.

The Schur complement matrix $\mathbf{K}_{bb} - \mathbf{K}_{bi}\mathbf{K}_{ii}^{-1}\mathbf{K}_{ib}$ is the stiffness matrix of a tile and it resembles the stiffness matrix of a generalized element. In other words, for the tiling with 9 tiles, the problem of reconstruction of mechanical fields is assembled similarly to a problem with 9 finite elements.

5. Brief results

So far very simple numerical experiments have been executed to compare computing time needed by the FFT based solver and the Schur complement method. In the performed tests we changed a few variables to get an overview of how different variables affect the computation time. The first of the variables is the ratio of elastic modulus of phases, which influence on the time required for the calculation is shown in the Fig. 5(a), where capital 'S' is for the Schur complement method and capital 'F' denotes the FFT based solver. Lowercase 's' or 'b' stands for small (26px) or big (78px) tiles and numbers 4, 6 or 8 correspond to required accuracy 10^{-4} , 10^{-6} or 10^{-8} , respectively. Increasing the ratio of elastic modulus of phases increases slightly the calculation time of the Schur complement method but many times in case of the FFT method. The presented results confirm that high contrast in material stiffness leads to enormous computational time needed by FFT based solvers and the Schur complement method becomes much faster.

The second variable we change during the experiments is the required accuracy of results. The dependence of time on the required accuracy is shown in the Fig. 5(b), where the key is almost same as in Fig. 5(a) but with the difference that here the numbers 2, 10, 100 and 1000 indicate the ratio of elastic modulus of phases. One can notice that computational time is almost not affected by required accuracy in case of the Schur complement method, while it is significantly increased in case of the FFT based method.

The third altered variable is size of solved domains, i.e. size of the employed tiles. We used only two sizes, namely small tiles with the 26px edge and the large tiles with the 78px

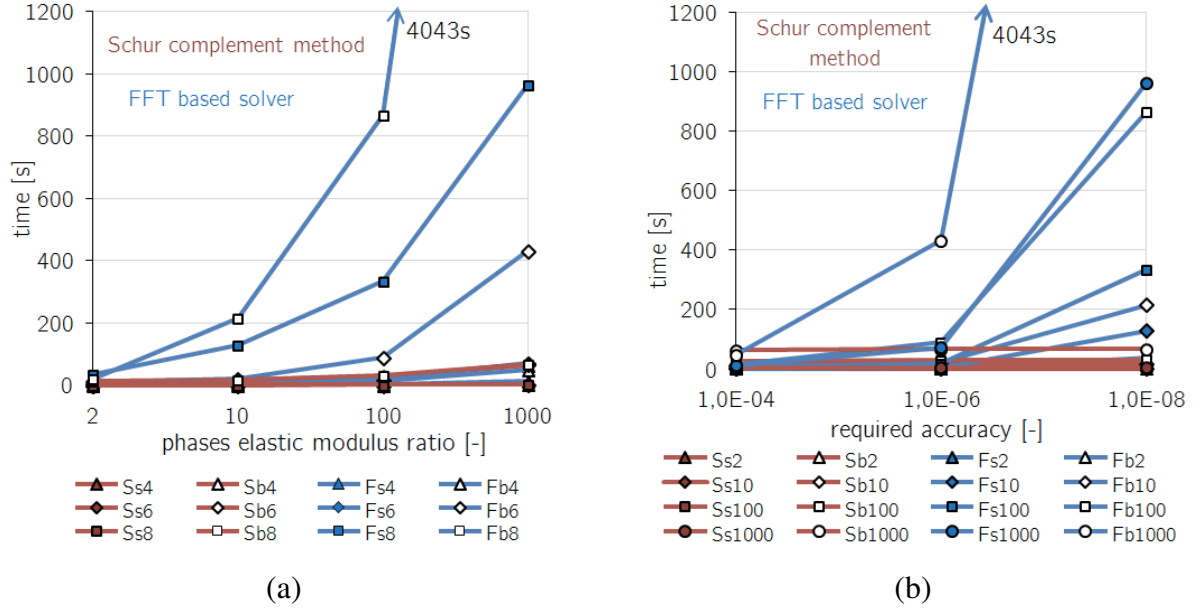


Figure 5: Brief results, a) dependence of computation time on ratio of elastic modulus of phases, b) dependence of computation time on required accuracy.

edge. As it turned out, the solved domain size significantly affects the time required to solve a Schur complements on individual tiles, because the number of DOF's on whole tile increases quadratically. Nevertheless, Schur complements need to be solved only once at the beginning and further calculations are affected only with a linear increase of DOF's on the tile boundary.

6. Discussion and future work

The results thus show that using the Schur complement method we can count with high or even infinite elastic modulus ratios (in the case of porous materials) of phases, which is not possible using the FFT based solver and furthermore, we are able to achieve high accuracy of calculations in a reasonable time.

Specific properties of the Wang tilings lead to special implementation in parallel environment which results in substantial speedup with respect to other methods. First step is devoted to the elimination of the internal DOFs on tiles. It means, the Schur complement matrices K_{bb} , $K_{bi}K_{ii}^{-1}K_{ib}$ are evaluated for each tile $1 \leq i \leq n^t$. The smallest number of tiles is 8 ($W/8 \times 2$) and therefore the identical number of processors is used in this step. After the all Schur complements are computed, all of them are sent to remaining cluster processors which will be used for the reconstruction of mechanical fields only in central tile. While relatively small number of processors is used for the Schur complements (e.g. eight), the number of processors allocated for the reconstruction is assumed to be much larger, e.g. hundreds or thousands. Implementation of this broadcast is crucial. It will be studied whether computation of all Schur complements on all processors is not faster then the broadcasting.

Second step of the computation will be devoted to the reconstruction of the mechanical fields. As mentioned above, the number of all tilings is known in advance. Each processor used for the reconstruction is assumed to be loaded by $n_m^{\text{comb}} n_{\text{CPU}}$ tasks, where n_{CPU} denotes the number of processors. Regarding the Schur complements of $1 \leq i \leq n^t$ are known, the reconstruction is

performed only by means of the appropriate Schur complement matrix and boundary solution.

As mentioned in Section 1. we also plan to use the reconstructed fields in Partition of Unity and Hybrid finite element methods. This will require the integration of the field fluctuations. In particular, the solution of the hypothetical macro-level analysis is done on the master processor. The solution requires correct values of the mechanical fields obtained from the micro-level problems in integration points. In addition, it is known which tile contains the appropriate integration point. Therefore, the values in the integration point are obtained from the appropriate tile by reading the value from computer memory. However, a special attention has to be devoted to the implementation of the data exchange between slave processors which contain the tiles and the master processor. The number of integration points on the macro-level must be determined first.

In order to minimize the communication between processors, all requests to slave processors are aggregated and yielding the response is aggregated as well. Therefore, there will be only a single communication between the master processor and each slave. If all integration points receive their values, the macro-level problem can be finished.

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