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MICROSTRUCTURE-INFORMED ENRICHMENT FUNCTIONS IN EXTENDED FINITE ELEMENT METHOD

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Abstract: *The present contribution reports on preliminary results of enhancing the approximation space of the Finite Element Method by means of pre-generated displacement fluctuation fields. The formulation builds on the Wang tile based compression of investigated microstructures and expands the application potential of the tiling compression into numerical methods. Enrichment functions are precomputed as responses of the compressed system to a set of load cases and synthesized analogously to the synthesis of the microstructure. The performance is illustrated with a two-dimensional linear diffusion problem.*

Keywords: Wang tiles, heterogeneous materials, fluctuation field synthesis, microstructure-informed enrichment functions, eXtended Finite Element Method.

1. Introduction

The issue of incorporating knowledge of a material microstructure into coarser scale analyses remains a vivid topic in Computational Mechanics. In the case of separation of scales, i.e., when the characteristic microstructural length is by orders of magnitude smaller than the size of a macro-scale task, the material can be treated as homogeneous from the macro-scale viewpoint. The microstructural characteristics are then propagated into upper scales by means of homogenization when either parameters of a given constitutive model are identified from numerical tests performed on a Representative Volume Element or the macroscopic constitutive model is obtained in an incremental form arising from the solution of a boundary value problem for each integration point of the macroscopic discretization, see (Geers et al., 2010) and reference therein.

In this work, we aim at tasks in which the separation of scales is not valid. In such a case, the standard Finite Element Method requires detailed resolution of the underlying microstructural geometry. As a result, the complexity of the macro-scale model significantly increases. The second disadvantage of such an approach stems from its dependence on a specific microstructure realization, which is stochastic in the majority of real-world materials. Therefore, Monte Carlo-like simulations are necessary to assess the model response under different realizations of the microstructure in an attempt to account for unfavorable compositions.

We have recently demonstrated, e.g., in (Novák et al., 2012; Doškář et al., 2014), that the representation based on Wang tiles is particularly appealing when multiple stochastic realizations of a microstructure should be efficiently generated, featuring spatial statistics similar to that of the reference sample. In the present contribution, we exploit the compressed form of a microstructure in the framework of eXtended Finite Element Method (XFEM), which allows to circumvent the requirement of the detailed resolution by enhancing the approximation space with specifically designed enrichment functions. In particular, we construct the enrichment functions as responses of the compressed system to prescribed loadings while preserving continuity of the functions across the corresponding edges of individual tiles. The global enrichment functions for a macro-scale analysis are then assembled in the same way the microstructure

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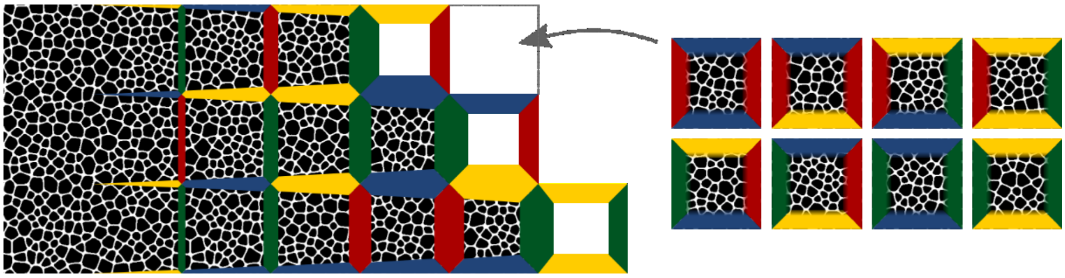

Fig. 1: Illustration of a reconstructed microstructure with the highlighted Wang tile codes defining the compatibility constraint during an assembly (left) and a set of Wang tiles (right).

realization is generated. We illustrate the proposed methodology with a preliminary results for the two-dimensional diffusion problem.

2. Wang tiles

Originally developed as a decidability procedure in Mathematical Logic (Wang, 1961), Wang tiles are currently a well-established tool for efficient synthesis of naturally looking textures in Computer Graphics (Cohen et al., 2003). The direct correspondence between goals of texture synthesis and representation of heterogeneous materials motivated our current effort and allowed us to introduce the concept of Wang tiles as a promising generalization of the Statistically Equivalent Periodic Unit Cell (SEPUC) approach to modelling of heterogeneous materials (Novák et al., 2012). We replace the single cell with a set of piecewise compatible domains—Wang Tiles—and employ the formalism of the original tiling concept in order to formulate the compatibility constraint during the assembly of tiles into a realization of the compressed microstructure, see Fig. 1. Microstructural information can be compressed into the tile set by making use of the methods developed for SEPUC generation, modified in order to account for the generalized periodic boundary conditions arising in the tiling concept (Novák et al., 2012). In order to alleviate computation cost of the optimization approach, we have proposed an alternative method, see (Doškář et al., 2014), that was inspired by the approach of Computer Graphics (Cohen et al., 2013), and employs a provided sample of the microstructure. The major merit of Wang tiles is their ability to reconstruct instantly stochastic realizations of arbitrary size with suppressed artificial periodicity inherent to PUC. Therefore, the concept is appealing for a wide range of tasks in which multiple statistically coherent realizations of the investigated microstructure are needed, for instance in numerical homogenization (Doškář & Novák, 2016). With the present contribution, we expand its application potential into enrichment based numerical methods.

3. Methodology

The standard formulation of Finite Element Method (FEM) builds on the weak form of the governing equations which in general reads as

$$Find\ u \in V: a(u, v) = b(v),\ \forall v \in V_0. \quad (1)$$

The quality of the solution directly follows from the finite-dimensional approximation space $V^h \subset V$, which in the case of FEM is constructed from element-wise polynomials. As mentioned above, this construction requires a mesh refinement in order to properly account for microstructural details. The eXtended Finite Element Method (XFEM), also called the Generalized Finite Element Method[1], supplements the approximation space with a priori knowledge of a (local) character of the solution. As a result, significantly smaller number of degrees of freedom (DOFs) is necessary.

In mechanics of solids and modelling of materials in particular, XFEM is usually used to capture crack propagation, shear bands, or complex microstructural geometries, see (Belytschko et al., 2009; Fries & Belytschko, 2010) for a comprehensive review. Usually, analytical enrichment functions derived for a single microstructural feature are used to enhance the approximation space, e.g., (Strouboulis et al., 2001). However, numerical "handbook" functions have been already introduced by Strouboulis et al. (2003) for the case of multiple closely packed inclusions. A similar approach has been recently proposed by Plews and Duarte (2014). The both approaches rely on computing Boundary Value Problems on subdomains of

[1] Description of etymology of the names can be found in (Belytschko et al., 2009).

the original task and extracting the dominant response of the microstructure. In this perspective, our approach can be understood as their off-line counterpart. The original idea of employing the Wang tiles for a synthesis of enrichment functions dates back to (Novák et al., 2013), where the constraint of stress compatibility among congruent tile edges was incorporated into the objective function of the optimization algorithm used to design tile morphology. However, this condition led to a nearly periodic arrangement of particles. In this work, we generate enrichment functions separately after a microstructure is compressed in the tile set. Each tile is discretized with an FE mesh that is compatible across the congruent edges. Inspired by the first-order numerical homogenization, we consider the decomposition of the displacement field into the fluctuation part and the part corresponding to a prescribed macroscopic gradient tensor. We assemble a stiffness matrix for each tile, condensate out inner fluctuation DOFs, and localize the remaining unknowns according to the edge codes into the stiffness matrix for the whole tile set. The resulting system is then solved for a prescribed unit macroscopic gradient and the edge fluctuation unknowns are obtained. The fluctuation fields inside each tile are then reconstructed from the edge DOFs. This treatment ensures continuity of the enrichment fields across the corresponding tile edges.

With the displacement fluctuation fields pre-computed for each tile, we can define n_j enrichment functions for every microstructure reconstructed with the Wang tile set as an assembly of the fluctuation fields derived from n_j loading cases. The approximate solution of Eq. (1) then takes the form

$$u^h(x) = \sum_{i=1}^{n_i} N_i(x) u_i + \sum_{i=1}^{n_i} \sum_{j=1}^{n_j} N_i(x) \left(\psi_j(x) - \psi_j(x_i)\right) u_i^j, \qquad (2)$$

where $N_i(x)$ and u_i are the standard polynomial shape functions and DOFs while $\psi_j(x)$ denotes an enrichment function (in our case global) with the corresponding DOF u_i^j. The enrichment function is (i) shifted by $\psi_j(x_i)$ and (ii) multiplied by the shape functions $N_i(x)$ in order to (i) restore the Kronecker delta property $u^h(x_i) = u_i$ and (ii) preserve the banded structure of the resulting algebraic system.

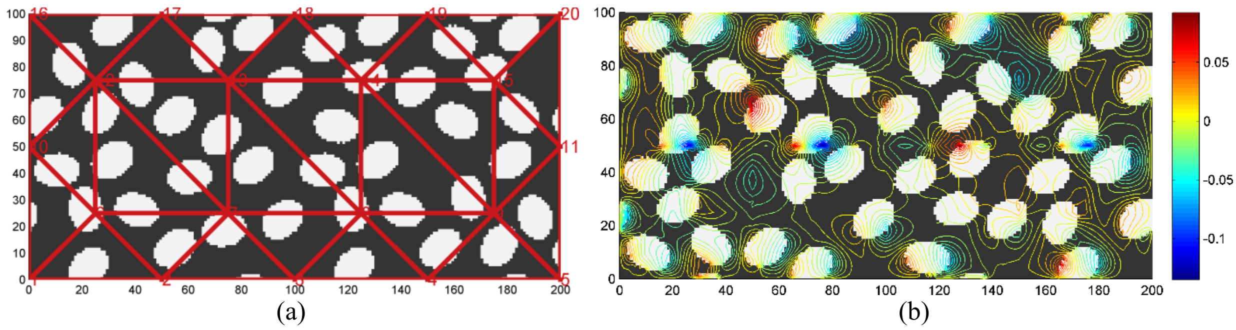

Fig. 2: The discretization and the microstructure of the considered task (a) and (b) contours of the discrepancy between the XFEM solution (24 DOFs) and the fully resolved FEM (nearly 20k DOFs).

4. Numerical example

As an illustrative example, we considered the Laplace equation for a simple rectangular domain with a microstructure generated from a tiling composed of 4×2 tiles. The loading of the domain was induced through Dirichlet boundary conditions prescribed with a macroscopic gradient in x direction (horizontal) of magnitude 0.02. At the tile level, the microstructure was discretized using a regular grid of quadrilateral linear elements corresponding to pixel representation of the tiles, the resolution of a tile was 50×50 px. Two global enrichment functions related to a unit gradient in each direction were provided to XFEM. At the macro-scale level, linear triangular elements were used. The discretization of the macro-scale task is depicted in red in Fig. 2a along with the considered microstructure, dimensions of the domain are given in px. The integration of the weak form (1) was performed employing the tile discretization and the 9 point Gauss quadrature rule. The obtained XFEM solution (24 DOFs) was compared to the reference solution of the fully resolved microstructure (nearly 20k DOFs). The absolute discrepancy between the two solutions is plotted in Fig. 2b. Note that the errors concentrate mainly along the tile edges and near the boundary of the domain which is due to the pre-computed nature of the enrichment functions. The boundary related errors can be compensated for by a finer discretization near the domain boundary whilst the discrepancies related to the tile edges would be reduced by taking more enrichment functions into account.

5. Conclusions

With a simple example, we have demonstrated that the proposed methodology can provide comparable results to the fully resolved FEM with a significantly smaller number of DOFs. The geometry of the macro-scale task is not restricted to rectangular shapes and can be arbitrary due to the multiplication of the enrichments functions by the standard shape functions in Eq. (2). On the other hand, our approach shares the main sore common to XFEM, namely the integration of the discretized weak form, which can in turn dissipate the computation savings arising from less DOFs. Moreover, the integration has to be carried out carefully in the regions where the macro-scale elements intersect the tile-level elements. Strouboulis et al. (2003) also showed that the XFEM solution is particularly sensitive to the accuracy of the provided enrichment, which is only approximate in our approach. Thus, our particular attention will be devoted to the question of an appropriate formulation of the enrichment functions and efficient integration. The method holds promise also for a non-linear regime. The assembled enrichment functions will address only the linear mode and will allow for identification of regions with onset of the non-linearity. Additional enrichment functions reflecting the non-linear mode will be supplemented on-the-fly only locally for the identified regions, similarly to the proposed strategy by Plews and Duarte (2014).

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