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COMPUTATIONAL METHODS FOR EVALUATION OF OVERALL RESPONSE OF COMPOSITE MATERIALS

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Summary: *The purpose of this contribution is to introduce a comparison of two Finite Element-based methods for computing the mechanical response to (thermo)mechanical loading of composites on micro-scale. Namely, the classical homogenization method based either on the Hashin-Shtrikman method or on the existence of a suitable periodic unit cell, and the reduced substructuring approach, where the number of condensed nodes varies are studied in this work.*

1. Introduction

It was recognized long ago that a successful prediction of the macroscopic behavior of complex layered composite structures calls for modeling on various size scales. Multi-scale or hierarchical modeling now offers means to bridge length scale differences ranging from the size scale of microns to large composite structures (see [1], [2], [5]). In context of the present paper, the large macroscopic structural part is represented by the wound composite tube, Fig. 1, while the smallest scale considered herein is of the size of graphite fiber diameter, which is about 10 microns.

While the periodic nature of a fiber-tows arrangement reduces the basic geometrical model on meso-scale to a certain periodic unit cell, the distribution of fibers within individual tows (micro-scale) shows random character, see Fig. 1. Analysis of material systems with periodic fields is now well understood and the interested reader may consult works [6] and [7], among others, for more details. Analysis of material systems with disordered microstructures, however, is still a subject of ongoing research.

Since fibers are randomly distributed within the bundle and since this distribution is likely affected by the initial fiber pre-stress it is advisable to treat analysis on this level from the point of view of probabilistic methods. To provide for the lack of periodicity, one may incorporate various types of *n*-point statistical descriptors in the analysis of disordered media. Such statistical descriptors introduce information beyond that contained in the volume

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fractions. It turns out that the two-point correlation function S_{rs}, which gives the probability of finding two points $\mathbf{x}_1$, $\mathbf{x}_2$ randomly thrown into the media located in the phases r, s, is sufficient for determining the effective properties of the composite.

Once this function is known we may generally proceed in two different ways. The first approach draws on the extended Hashin-Shtrikman (H-S) variational principle. The material properties obtained by homogenization based on the H-S variational principle can be used directly in the classical version of the Finite Element Method.

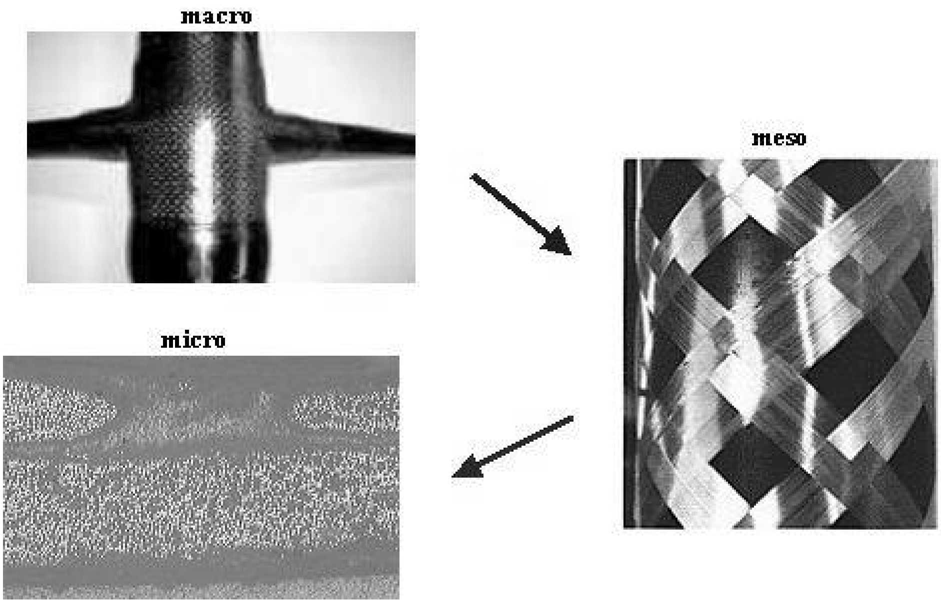

Fig. 1: Multi-level modeling of woven tubes

The second approach relies on the existence of a suitable periodic unit cell, where the reduced substructuring technique is employed. In our case, where the scale difference between micro scale and meso scale is large, such a method may seem as ineffective comparing to classical homogenization technics. On the contrary this approach appears to be more suitable for the analysis of meso-macro transition, but a study of this technic on meso scale is difficult due to the complicated three-dimensional geometry of a periodic unit cell.

Moreover, it naturally results in a certain “meso finite element” with stiffness matrix that can be directly introduced in the standard finite element analysis on meso-scale level and so such a strategy is very well suited for computational parallelization, where individual unit cells are computed separately and then included into the mesoscopic mesh. In the case of inelastic analysis, however, a suitable operator, which extends fields of deformation and stresses from the boundary of a periodic unit cell into its interior, must be developed. Clearly, such a mapping can be efficiently defined in the framework of the finite element method analysis and is consistent with the parallel strategy.

The paper is organized as follows. First, theoretical background for reduced substructuring and homogenization based on the Hashin-Shtrikman principle is given. Next, some numerical experiments at micro level are shown to explain and provide solution to the problems encountered in the three-dimensional analysis.

2. Reduced substructuring

Recently, problem-specific continuum elements have been developed to account for a textile and woven type mesostructure within a single element; see [12], [9] for more details. The elements introduced in these references are based on a single assumed displacement field throughout the entire mesostructure. A more flexible element formulation, based on general reduced substructuring theory [11], is presented herein. Note that this approach incorporates a single field approximation as a degenerated state.

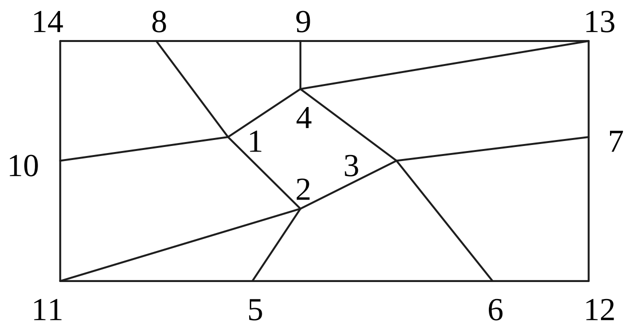

Fig. 2: Example of finite element mesh for micro-scale periodic unit

In brief, the implementation begins with the development of a standard finite element mesh for the periodic unit cell on the meso-scale (an example of such a mesh can be seen in Fig. 2). Then, interior degrees of freedom (dofs #1—4 in Fig. 2) are statically condensed out. Next, the number and location of the desired boundary degrees of freedom is selected. Finally, the remaining boundary degrees of freedom are expressed in terms of the desired boundary degrees of freedom. To describe this procedure in more formal way, assume that the governing equations resulting from the finite element discretization are partitioned as follows

$$\begin{pmatrix} \mathrm{K}_{AA} & \mathrm{K}_{AB} \\ \mathrm{K}_{BA} & \mathrm{K}_{BB} \end{pmatrix} \begin{pmatrix} q_A \\ q_B \end{pmatrix} = \begin{pmatrix} F_A \\ F_B \end{pmatrix}, \tag{1}$$

where K_{XX} are submatrices of the global stiffness matrix, F_X are nodal forces, q_A is the list of unknowns to be condensed out and q_B are unknowns, which will remain. Before imposing the multipoint constrains on the excess boundary degrees of freedom (dofs), the reduced stiffness matrix and load vector can be expressed as

$$\overline{\mathrm{K}}_{BB} = \mathrm{K}_{BB} - \mathrm{K}_{BA}\mathrm{K}_{AA}^{-1}\mathrm{K}_{AB}, \tag{2}$$

$$\overline{F}_B = F_B - \mathrm{K}_{BA}\mathrm{K}_{AA}^{-1}F_A. \tag{3}$$

This procedure is often not very efficient because of matrix inversion, which destroys sparsity pattern of K_{AA}, and expensive matrix-matrix multiplications. The elimination of internal dofs can also be accomplished using the Gaussian elimination if the dofs to be eliminated are grouped together either at the beginning or the end of the list of unknowns. In such a case assume that the n_A dofs to be eliminated are stored at the beginning of the list of unknowns. Then a direct Gaussian elimination procedure is carried out on n_A columns (i.e. eliminating n_A columns). Iteratively, this procedure is expressed as follows:

1. For i=1 to n_A begin
2. For j= i to n begin
3. For s= i to n begin
4. $\overline{\mathrm{K}}_{js} = \mathrm{K}_{ii}\mathrm{K}_{js} - \mathrm{K}_{is}\mathrm{K}_{ji}$
5. $\overline{F}_s = \mathrm{K}_{ii}F_s - \mathrm{K}_{ji}F_i$
6. End of loop.

Of course, pivoting can be integrated into this process as well. After that, the reduced stiffness matrix appears in the right bottom corner of the matrix. When the interior dofs are condensed out the multipoint constraints can be applied to the remaining dofs to eliminate unwanted boundary dofs. This can be expressed in the matrix form as $q_B = \mathrm{T}q_{micro}$. The transformation matrix T determines how the excess boundary dofs are slaved to the meso element dofs. It should be noted that if the internal dofs are also slaved to the meso-element dofs (rather than statically condensed), a single field approximation (i.e. field of translation is constant on the condensed element) is obtained. Further, it is not always efficient to order the dofs such that the Gaussian elimination can be used to obtain the reduced stiffness matrix and load vector, since such ordering might result in a large bandwidth when the standard skyline storage scheme is used.

An alternative procedure relies on the formal definition of the stiffness coefficients K_{ij},

K_{ij} = force at dof i due to unit displacement at dof j.

Using this definition, we would simply solve a series of problems in which one dof is set equal to one and the rest of the boundary dofs would be constrained to zero. The reaction forces at all the boundary dofs constitute one column of the reduced stiffness matrix. This process is repeated for each boundary dof to obtain the entire reduced stiffness matrix. The reduced load vector is determined by solving one additional problem in which all boundary dofs are constrained to zero and the internal loads are applied. The negative of the boundary reaction forces constitute the reduced load vector contribution for the internal loads. Once the reduced set of equations is obtained, the multipoint constraints can be imposed to eliminate unwanted boundary dofs.

The Lagrange polynomials, the Hermite polynomials, splines or any other approximation functions can be used as a basis for multipoint constraints. For example basic linear interpolation can be involved on micro-scale periodic unit cell (see Fig. 3). It yields only four nodes (nodes #11,12,13,14) will be preserved for meso finite element. One standard base function is shown in Fig. 3. In this case the dimension of the matrix T will be 28×8.

Alternative, more efficient, methods were developed to decrease the amount of operations in reducing the stiffness matrix. See, for example, [10] for more details.

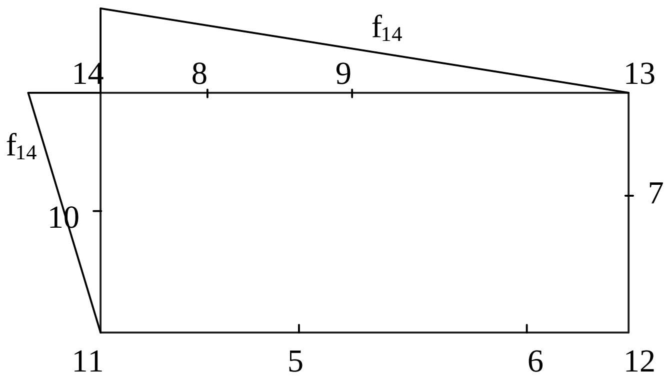

Fig. 3: Standard base function for multipoint constraints

3. Homogenization on micro scale

As already suggested in [14] the computational modeling on this level of sophistication calls for numerical procedures allowing investigation of random, non-periodic systems. In what follows we assume that such a system can be characterized by statistically homogeneous distribution of reinforcements. Then, an efficient and reliable solution procedure for evaluation of both local and overall response of a tow *F* (a bundle of fibers *f*) on micro-scale can be developed on the basis of Hashin-Shtrikman variational principles for elastic media. See [13], [14] for further discussion on this subject. This section reviews just a few basic steps.

With reference to combined meso-micro analysis we consider only the primary principle and write the two equivalent representations of local stresses in the form

$$\sigma(\mathbf{x}) = \mathbf{L}(\mathbf{x})\varepsilon(\mathbf{x}) + \lambda(\mathbf{x}) \qquad \sigma(\mathbf{x}) = \mathbf{L}_0(\mathbf{x})\varepsilon(\mathbf{x}) + \tau(\mathbf{x}), \tag{4}$$

where $\mathbf{L}(\mathbf{x})$ is the local stiffness matrix and $\mathbf{L}_0$ is the stiffness matrix of a certain homogeneous reference medium. Recall that the Hashin-Shtrikman functional written as

$$U_\tau = \frac{1}{2}\int_{\Omega_F} (\mathbf{E}^{\mathrm{T}}\Sigma - (\tau-\lambda)^{\mathrm{T}}(\mathbf{L}-\mathbf{L}_0)^{-1}(\tau-\lambda) - 2\tau^{\mathrm{T}}\mathbf{E} - \varepsilon'^{\mathrm{T}}\tau - \lambda^{\mathrm{T}}\mathbf{L}^{-1}\lambda)\mathrm{d}\Omega, \tag{5}$$

where $\mathbf{E}$ and Σ are the overall strains and stresses supplied to the medium from the analysis on meso-scale. The fluctuation part ε' of the local strain ε is provided by (see [8])

$$\varepsilon'(\mathbf{x}) = \varepsilon(\mathbf{x}) - \mathbf{E}. \tag{6}$$

To facilitate the solution we further restrict our attention to a piecewise uniform distribution of polarization stress $\tau_r(\mathbf{x}) = \tau_r$ and the eigenstress vector $\lambda_r(\mathbf{x}) = \lambda_r$ within a given phase *r=f,m* (fiber, matrix). The eigenstress vector λ_r can be attributed to various physical sources such as thermal loading, plasticity, initial prestress, etc. Taking an ensemble average of functional (5) and performing its variation with respect to τ_r finally supplies a set of algebraic equations for unknown phase averages of polarization stress τ_r

$$\sum_{s=1}^{n}[\delta_{rs}(\mathbf{L}_r-\mathbf{L}_0)^{-1}c_r-\mathbf{A}_{rs}]\tau_s=\mathbf{E}c_r+(\mathbf{L}_r-\mathbf{L}_0)^{-1}\lambda_r c_r, \qquad r=1,\ldots,n, \tag{7}$$

where $\mathbf{A}_{rs}$ are certain microstructure-dependent matrices. Formal inversion of (7) yields the mesoscopic constitutive equation for a tow

$$\sigma_{meso}=\mathbf{L}_{meso}\varepsilon_{meso}+\lambda_{meso}, \tag{8}$$

where $\varepsilon_{meso}=\mathbf{E}$. The overall stiffness matrix $\mathbf{L}_{meso}$ (effective stiffness matrix of a fiber tow) and the macroscopic eigenstress vector λ_{meso} (initial stress vector prescribed on meso-scale that results from an initial fiber prestress λ_f) are provided by

$$\begin{aligned}\mathbf{L}_{meso}&=\mathbf{L}_0+\sum_{r=1}^{n}\sum_{s=1}^{n}c_r\mathbf{T}_{rs}c_s\\ \lambda_{meso}&=\sum_{r=1}^{n}\sum_{s=1}^{n}c_r\mathbf{T}_{rs}c_s(\mathbf{L}_s-\mathbf{L}_0)^{-1}\lambda_s.\end{aligned} \tag{9}$$

$\mathbf{T}_{rs}$ then represent individual blocks of the inverse matrix to the left hand side of system (7).

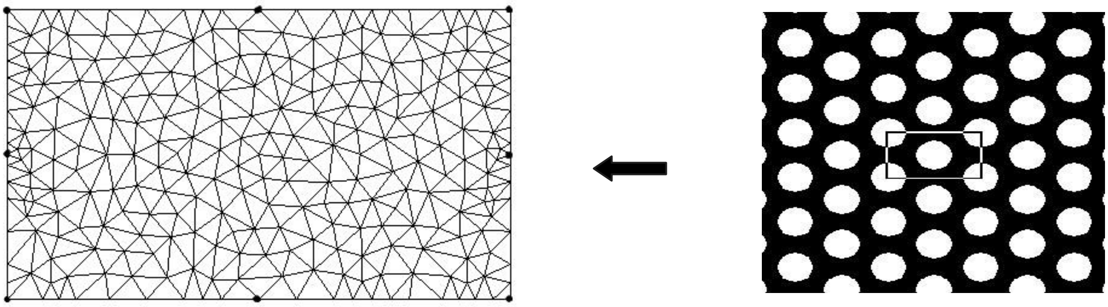

Fig. 4: 2D mesh of the periodic unit cell

4. Results of analysis on micro scale

This particular study (recall Section 2) is focused on the influence of the amount of the boundary nodes condensed out and on the suitability of using homogenized material properties derived in Section 3. A hexagonal packing of carbon fibers embedded in an epoxy matrix is used as testing two-dimensional example. Two numerical models are developed.

The first approach uses macro elements. The macro element employed for reduced substructuring (highlighted in the center) and the mesh of this periodic unit cell is depicted in Fig. 4. The full mesh has 72 boundary nodes. Five macro elements (i.e. elements with some nodes condensed out) with variable amount of boundary nodes are created. In particular, 72, 36, 18, 8 and 4 boundary nodes are preserved after the condensation. An example of a mesh created from elements with eight preserved nodes is depicted in Fig. 5.

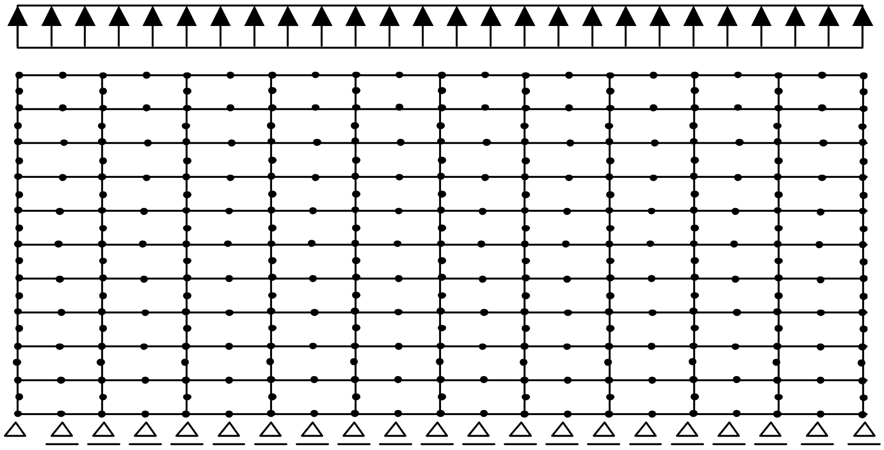

Fig. 5: Numerical model from macro elements with 8 nodes

The second model draws upon homogenized material properties. The effective material properties obtained by homogenization based on the primary Hashin-Shtrikman variational principle [14] are used for mesh composed of Constant Strain Triangles, where two triangles cover one macro element.

Tab. 1: Comparison of models using either homogenized material properties or reduced substructuring

	Displacement	**Time**	**Number of nodes**
Condensed 72	0.0073	146.39	3861
Condensed 36	0.0085	17.79	1881
Condensed 18	0.0121	1.69	891
Condensed 8	0.0244	0.17	341
Condensed 4	0.0657	0.07	121
Homogenization	0.0061	0.05	121

Finally a mesh from 10x10 macro elements (200 triangles) is formed. See Fig. 5 for the mesh composed of macro elements with 8 nodes. Such a structure is loaded at one side with prescribed normal tractions such that the overall sum of nodal forces remains constant for every type of meshing. The opposite side is fixed. Comparison of average displacement of loaded nodes with a computing time appears in Tab. 1 and Fig. 6. Note that the result obtained from 72-element boundary nodes is the exact one (the same as if we used ”’meso mesh” on

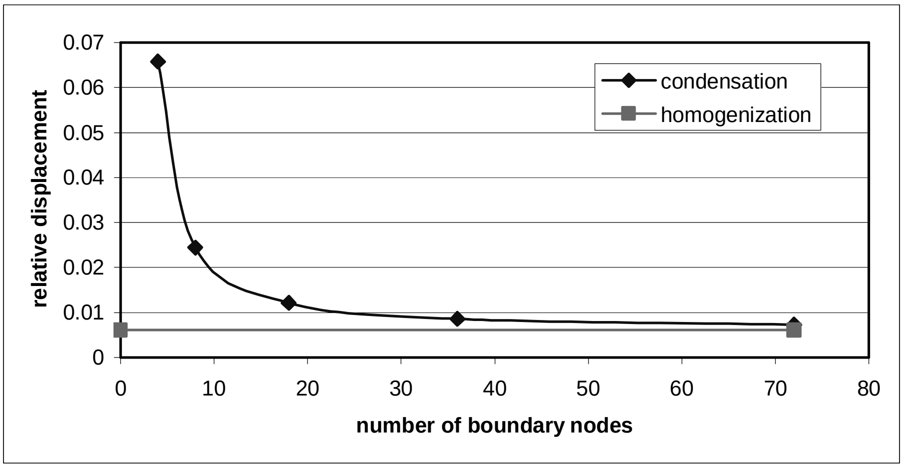

Fig. 6: Comparison of relative displacement

the entire structure). The results indicate that the reduction of the number of boundary nodes leads to a considerable error. Condensing out a half of boundary nodes gives approximately 25% error in displacement even for a uniform loading. As expected, the reduction of the number of boundary nodes in static condensation (reduced substructures) decreases rapidly computing time consumption. The error in displacements, however, increases rapidly as well, and so such a reduction does not appear to be very appropriate. The homogenized properties, on the other hand, predict the overall behavior with the reasonable precision (error is about 10%) with a substantially smaller computational time.

5. Conclusion

This article shows one possible way for computing the mechanical response of composites subjected to (thermo)mechanical loading. The approach is based on the static condensation and mesh of periodic unit cell on the micro-scale. The results of two-dimensional analysis reveal fundamental importance of a number of nodes to be condensed out. In particular, it directly follows from the presented analysis that only the internal nodes can be condensed out since the condensation of even a small subset of boundary nodes introduces large errors in the analysis and so some multi-point constraints to preserved boundary nodes must be involved. The homogenization method, on the other hand, seems to be a reasonable approach to the modeling of a given heterogeneous body as the uniform stress fields occur in this particular case. We expect, however, that for three-dimensional problems, the error of the homogenization method is not negligible and thus the static condensation approach, combined with parallel implementation, is inevitable. This topic will be considered in the future work.

Acknowledgement

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