Efficient Solvers for 3-D Homogenized Elasticity Model

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Abstract. The optimization of the macroscopic behavior of microstructured materials using microscopic quantities as design variables is a well established discipline in materials science. The paper deals with recently produced microcellular biomorphic ceramics. The mechanical macromodel corresponding to these composite materials is obtained by homogenization. The homogenized elasticity tensor and its dependence on the design variables are computed numerically involving adaptive finite element approximations of elasticity problems in the 3-D periodicity cell. Efficient iterative solvers based on incomplete Cholesky (IC) decomposition and algebraic multigrid method (AMG) as preconditioners of the stiffness matrix are proposed in the application of PCG method.

1 Introduction

The production of microcellular biomorphic ceramics by biotemplating processes is a particular area within biomimetics which has emerged as a perspective new technology in materials science during the past decade (cf., e.g., [11]). The biological object under consideration in this paper is naturally grown wood which is known to be highly porous and to possess excellent mechanical properties. The wood morphologies are characterized by an open porous system of tracheidal cells which provide the transportation path for water and minerals in the living plants. The biotemplating process uses wooden specimen to produce graphite-like carbon preforms by high temperature pyrolysis followed by an infiltration by liquid-phase or gaseous-phase materials such as silicon (Si) or titanium (Ti) to come up with SiC- or TiC-ceramics (see, e.g., [6] for details). An important feature of the biotemplating process is that it preserves the high porosity of the wooden specimen and results in a final ceramics with excellent structural-mechanical and thermomechanical properties which can be used as heat insulators, particle filters, catalyst carriers, automotive tools, and medical implants.

The macroscopic mechanical behavior of the microcellular biomorphic ceramics depends on microscopic geometrical quantities such as the size of the voids and the lengths and widths of the different layers forming the cell walls. While the size of the voids is determined by the growth of the wood itself (early/late wood), the other quantities can be influenced by tuning the parameters of the biotemplating process. Therefore, an optimal structural design of the ceramics can be performed where the state equation is given by linear elasticity and the design variables are chosen as the microstructural geometrical quantities (cf., e.g., [8]). The objective functional depends on the mode

of loading. Since the resolution of the microstructures is cost prohibitive with respect to computational work, the idea is to derive a homogenized macromodel featuring the dependence on the microstructural design variables and to apply the optimization process to the homogenized model.

2 Computation of Homogenized Elasticity Tensor

For the structural optimization of the microcellular biomorphic SiC ceramics modern optimization techniques (see, [7]) are applied to the mechanical macromodel obtained by the homogenization approach (cf., e.g., [3,9]).

We assume the workpiece of macroscopic length L to consist of periodically distributed constituents with a cubic periodicity cell Y of microscopic characteristic length ℓ consisting of an interior void channel (V) surrounded by layers of silicon carbide (SiC) and carbon (C) (cf. Fig.1).

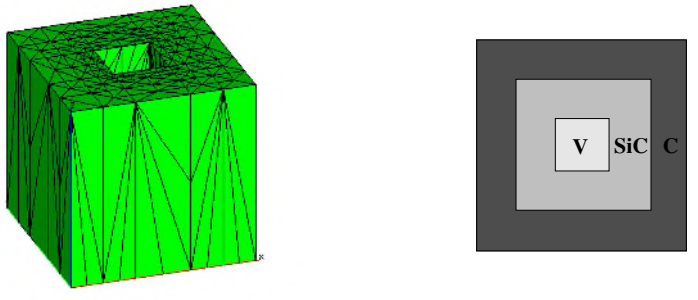

Fig. 1. a) Periodicity cell $Y = [0, \ell]^3$, b) Cross section of $Y = V \cup SiC \cup C$

Assuming linear elasticity and denoting by $\mathbf{u}$ the displacements vector, the stress tensor $\boldsymbol{\sigma}$ is related to the linearized strain tensor $\mathbf{e} = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$ by Hooke's law $\boldsymbol{\sigma} = \mathbf{E}\mathbf{e}$, where $\mathbf{E} = \mathbf{E}(X) = (E_{ijk\ell}(X))$ stands for the elasticity tensor whose components attain different values in the regions V, SiC, and C:

$$\mathbf{E} = \begin{pmatrix} E_{1111} & E_{1122} & E_{1133} & E_{1112} & E_{1123} & E_{1113} \\ & E_{2222} & E_{2233} & E_{2212} & E_{2223} & E_{2213} \\ & & E_{3333} & E_{3312} & E_{3323} & E_{3313} \\ & & & E_{1212} & E_{1223} & E_{1213} \\ & & & & E_{2323} & E_{2313} \\ \text{SYM} & & & & & E_{1313} \end{pmatrix} \tag{2.1}$$

Introducing $x := X/L$ and $y := X/\ell$ as the macroscopic and microscopic variables and $\varepsilon := \ell/L$ as the scale parameter, homogenization based on the standard double scale asymptotic expansion results in the homogenized elasticity tensor $\mathbf{E}^H = (E^H_{ijk\ell})$ whose components are given by

$$E^H_{ijk\ell} \;=\; \frac{1}{|Y|}\int\limits_Y \big(E_{ijkl}(y) - E_{ijpq}(y)\frac{\partial \xi^{k\ell}_p}{\partial y_q}\big)dy\;. \tag{2.2}$$

The tensor $\boldsymbol{\xi}$=$(\xi^{k\ell}_p),\ k,l,p=1,2,3$, with periodic components $\xi^{k\ell}_p \in H^1_{per}(Y)$ has to be computed via the solution of the elasticity problems

$$\int_Y \left(E_{ijpq}(y)\frac{\partial \xi^{kl}_p}{\partial y_q}\right)\frac{\partial \phi_i}{\partial y_j}\,dy = \int_Y E_{ijkl}(y)\frac{\partial \phi_i}{\partial y_j}\,dy \tag{2.3}$$

for an arbitrary $Y-$periodic variational function $\boldsymbol{\phi} \in \mathbf{H}^1(Y)$. We note that explicit formulas for the homogenized elasticity tensor are only available in case of laminated or checkerboard structures (cf., e.g., [2,9]). Therefore, (2.3) has to be solved numerically which has been done by using continuous, piecewise linear finite elements with respect to adaptively generated locally quasi-uniform and shape regular simplicial tetrahedral partitionings of the periodicity cell Y.

3 Mesh Adaptivity by a Posteriori Error Estimation

The computation of the homogenized elasticity coefficients requires the solution of linear elastic boundary value problems with the periodicity cell Y as the computational domain. Due to the composite character of the cell there are material interfaces where the solution changes significantly. Hence, local refinement of the underlying finite element mesh is strongly advised. In contrast to previous work in structural optimization (cf., e.g., [1,2]) where local refinement is done by manual remeshing, we have used an automatic grid refinement based on a posteriori error estimator of Zienkiewicz-Zhu type [13] obtained by local averaging of the computed stress tensor.

Using an approximation of the components of the displacements vector by continuous, piecewise linear finite elements with respect to a simplicial tetrahedrization $\mathcal{T}_h$ of the periodicity cell Y, we denote by $\hat{\sigma}$ the discontinuous finite element stress. A continuous recovered stress σ^* is obtained at each nodal point p by local averaging: Denoting by $Y_p \subset Y$ the union of all elements $K \in \mathcal{T}_h$ sharing p as a vertex, we compute

$$\sigma^*(p) \;=\; \sum_{K\in Y_p} \omega_K\,\hat{\sigma}|_K \quad,\quad \omega_K \;:=\; \frac{|K|}{|Y_p|}\;,\; K \in Y_p\;. \tag{3.4}$$

Based on (3.4), we have chosen

$$\eta \;:=\; \left(\sum_{K\in\mathcal{T}_h} \eta_K^2\right)^{1/2} \quad,\quad \eta_K \;:=\; \|\sigma^* - \hat{\sigma}\|_{0,K}\;,\; K \in \mathcal{T}_h \tag{3.5}$$

as a global estimator whose local contributions η_K are cheaply computable.

Note that such an estimator has been studied and analyzed in [10] for linear second order elliptic boundary value problems where it was shown that η is asymptotically exact. Moreover, general averaging techniques for low order finite element approximations of linear elasticity problems have been considered in [5] and efficiency and reliability of Zienkiewicz-Zhu type estimators have been established.

4 Iterative Solution Techniques

After finite element discretization of the domain Y the elasticity equation (2.3) used to compute the effective coefficients results in the following system of linear equations

$$A\,\mathbf{u} = \mathbf{f}, \tag{4.6}$$

where $\mathbf{u}$ is the vector of unknown displacements and $\mathbf{f}$ is the discrete right–hand side. The stiffness matrix A is symmetric and positive definite but not an M-matrix. Two typical orderings of the unknowns are often used in practice, namely

$$\left(u_1^{(x)}, u_1^{(y)}, u_1^{(z)}, u_2^{(x)}, u_2^{(y)}, u_2^{(z)}, \ldots, u_n^{(x)}, u_n^{(y)}, u_n^{(z)}\right), \tag{4.7}$$

referred to as a *pointwise displacements ordering* and

$$\left(u_1^{(x)}, u_2^{(x)}, \ldots, u_n^{(x)}, u_1^{(y)}, u_2^{(y)}, \ldots, u_n^{(y)}, u_1^{(z)}, u_2^{(z)}, \ldots, u_n^{(z)}\right), \tag{4.8}$$

called the *separate displacements ordering*. Here, $u_k^{(x)}$, $u_k^{(y)}$, and $u_k^{(z)}$ are the corresponding x, y-, and z- displacement components.

Using (4.8), for instance, the matrix A admits the following 3×3 block decomposition

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}. \tag{4.9}$$

In case of isotropic materials, the diagonal blocks A_{jj}, $j = 1, 2, 3$, in (4.9) are discrete analogs of the following anisotropic Laplacian operators

$$\tilde{D}_1 = a\frac{\partial^2}{\partial x^2} + b\frac{\partial^2}{\partial y^2} + b\frac{\partial^2}{\partial z^2},\ \tilde{D}_2 = b\frac{\partial^2}{\partial x^2} + a\frac{\partial^2}{\partial y^2} + b\frac{\partial^2}{\partial z^2},\ \tilde{D}_3 = b\frac{\partial^2}{\partial x^2} + b\frac{\partial^2}{\partial y^2} + a\frac{\partial^2}{\partial z^2}$$

with coefficients $a = E(1-\nu)/((1+\nu)(1-2\nu))$ and $b = 0.5E/(1+\nu)$ where E is the Young modulus and ν is the Poisson ratio of the corresponding material. This anisotropy requires a special care to construct an efficient preconditioner for the iterative solution method. Based on Korn's inequality, it can be shown that A and its block diagonal part are spectrally equivalent. The condition number of the preconditioned system depends on the Poisson ratio ν of the materials and the constant in the Korn inequality. For the background of the spectral equivalence approach using block diagonal displacement decomposition preconditioners in linear elasticity problems we refer to [4]. Note that the spectral equivalence estimate will deteriorate for ν close to 0.5 which is not the case in our particular applications.

The PCG method is applied to solve the linear system (4.6). We propose two approaches to construct a preconditioner for A:

(i) construct a preconditioner for the global matrix A

(ii) construct a preconditioner for A of the type

$$M = \begin{bmatrix} M_{11} & 0 & 0 \\ 0 & M_{22} & 0 \\ 0 & 0 & M_{33} \end{bmatrix}, \tag{4.10}$$

where $M_{jj} \sim A_{jj},\ j = 1, 2, 3$, are "good" approximations to the diagonal blocks of A. In case (i) we have chosen the incomplete Cholesky (IC) factorization of A with an appropriate stopping criterion.

An efficient preconditioner for A_{jj} in case (ii) turns out to be a matrix M_{jj} corresponding to a Laplacian operator $(-\mathrm{div}\,(c\,\mathrm{grad}\,u))$ with a fixed scale factor c. In our case we use, for instance, $c = b/2$ for all three diagonal blocks. *Algebraic multigrid* (AMG) method is applied as a "plug-in" solver for A (see [12] for details). This method is a purely matrix–based version of the algebraic multilevel approach and has shown in the last decade numerous efficient implementations in solving large sparse unstructured linear systems of equations without any geometric background.

5 Numerical Experiments

In this section, we present some computational results concerning the microscopic problem to find the homogenized elasticity coefficients. The elasticity equation (2.3) is solved numerically using initial decomposition of the periodic microcell Y into hexahedra and then continuous, piecewise linear finite elements on tetrahedral shape regular meshes. Due to the equal solutions $\boldsymbol{\xi}^{12} = \boldsymbol{\xi}^{21}$, $\boldsymbol{\xi}^{23} = \boldsymbol{\xi}^{32}$, and $\boldsymbol{\xi}^{13} = \boldsymbol{\xi}^{31}$ one has to solve six problems in the period Y to find $\boldsymbol{\xi}^{11}$ (Problem 1), $\boldsymbol{\xi}^{22}$ (Problem 2), $\boldsymbol{\xi}^{33}$ (Problem 3), $\boldsymbol{\xi}^{12}$ (Problem 4), $\boldsymbol{\xi}^{23}$ (Problem 5), and $\boldsymbol{\xi}^{13}$ (Problem 6). The discretized problems have been solved by the iterative solvers discussed in Section 4 and the mesh adaptivity has been realized by means of a Zienkiewicz-Zhu type a posteriori error estimator [13].

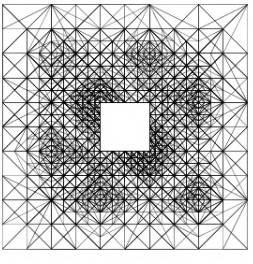

Fig. 2. Cross section of Y, density = 96%, Problem 3, $nt = 12395$, $nn = 2692$

The Young modulus E (in GPa) and the Poisson ratio ν of our two materials are, respectively, $E = 10,\ \nu = 0.22$ for carbon and $E = 410,\ \nu = 0.14$ for SiC. We denote by nt the number of tetrahedra and by nn the number of nodes on the corresponding refinement level. In Fig.2 the adaptive mesh refinement is visualized on the cross section of the period Y. Tables 1 and 2 contain information for the computed homogenized coefficients according to the refinement level.

Table 3 presents some convergence results for the proposed preconditioners within PCG method. For various values of the density μ of the periodicity microstructure we report the number of degrees of freedom d.o.f., the number of iterations iter, and the CPU–time in seconds for the first 11 adaptive refinement levels. One can see from the numerical results a better convergence of AMG–preconditioner compared to IC–factorization. We observe an essential efficiency of AMG for a larger number of unknowns.

Table 1. Homogenized coefficients w.r.t. adaptive refinement level, $\mu = 19\%$

level	E^H_{1111}	E^H_{2222}	E^H_{3333}	nt/nn (Prob.1)	nt/nn (Prob.2)	nt/nn (Prob.3)
1	160.82	174.34	204.39	288/126	288/126	288/126
2	175.60	207.65	214.79	334/137	332/136	332/136
3	159.18	170.78	206.73	443/166	457/169	441/165
4	174.07	166.79	213.77	637/222	593/208	595/211
5	168.97	163.26	214.10	982 /297	971/292	948/287
6	146.50	147.22	208.64	1641/433	1609/431	1684/443
7	160.25	147.90	211.11	2516/624	2422/604	2427/601
8	146.80	138.09	211.82	3761/896	3915/927	3881/920
9	137.10	134.55	210.36	5134/1171	7743/1722	5092/1160
10	133.22	131.84	210.91	10839/2259	13698/2869	11078/2289

Table 2. Homogenized coefficients for late wood, density $\mu = 91\%$

level	E^H_{1111}	E^H_{2222}	E^H_{3333}	E^H_{1212}	E^H_{2323}	E^H_{1313}
1	148.35	152.57	153.96	60.22	62.46	59.50
2	154.34	162.64	162.77	69.71	71.31	65.79
3	142.66	148.42	162.79	60.51	65.26	63.23
4	145.84	137.61	161.70	53.91	59.04	62.92
5	127.99	134.32	161.43	49.41	56.19	56.49
6	98.29	111.65	160.71	40.44	46.14	48.45
7	91.79	90.23	158.29	35.70	43.69	46.03
8	82.42	83.00	160.57	30.59	41.03	43.70
9	75.05	75.11	160.22	26.93	39.75	40.97
10	69.66	70.30	159.82	25.47	37.16	39.30

Table 3. Convergence results with IC and AMG preconditioners, density μ, Problem 1

prec.	level	1	2	3	4	5	6	7	8	9	10	11
$\mu = 51\%$	d.o.f.	78	90	126	225	336	579	1185	1908	3360	5598	9987
IC	iter	9	8	14	23	40	66	105	150	235	269	299
	CPU	e-16	e-16	e-16	0.1	0.2	0.2	0.9	2.4	8.2	20.9	59.1
AMG	iter	11	13	13	15	18	23	38	57	89	94	99
	CPU	e-16	e-16	e-16	0.2	0.3	0.5	1.5	3	7.6	14.8	23.5
$\mu = 84\%$	d.o.f.	78	93	150	261	510	1047	2103	3843	6537	10485	18459
IC	iter	10	11	16	21	44	78	117	171	226	273	301
	CPU	e-16	e-16	0.1	0.1	0.1	0.6	2.4	8.4	24.3	63.7	187.1
AMG	iter	12	14	14	14	18	31	43	73	69	74	75
	CPU	e-16	e-16	e-16	0.2	0.4	1.1	3	7.5	15.5	25.6	33.8

Acknowledgments

This work has been partially supported by the German National Science Foundation (DFG) under Grant No.HO877/5-3. The second author has also been supported in part by the Bulgarian NSF under Grant I1402/2004.

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