TECHNISCHE MECHANIK, 30, 4, (2010), 354 – 363
submitted: October 19, 2009

Influence of the type of boundary conditions on the numerical properties of unit cell problems

F. Fritzen, T. Böhlke

Aspects of the numerical solution of the systems of equations resulting from the computational homogenization of unit cell problems using the finite element method are discussed. Different kinematic boundary conditions and solution techniques are examined and compared, both, theoretically and numerically. It is found that the combination of boundary conditions and solver significantly influences the computational cost in terms of memory and cpu time. Examples for model and real world problems are presented.

1 Introduction

The homogenization of microstructured materials is a subject of continuous interest for many years. A wide variety of semi-analytical and numerical methods has been developed (Nemat-Nasser and Hori, 1999; Kanoute et al., 2009). The computational homogenization of the properties of microheterogeneous materials has become an indispensible tool (Barbe et al. (2001); Fish and Qing (2001); Fritzen et al. (2009); Böhlke et al. (2009)). Often the finite element method (e.g., Zienkiewicz et al. (2006)) is used to compute the linear or non-linear properties of materials with microstructure applying the concept of volume elements (e.g., Ostoja-Starzewski (2006)). It has been found by many authors (e.g., Miehe (2002); Kanit (2003); Ostoja-Starzewski (2006)) that periodic displacement and antiperiodic traction boundary conditions are often preferable with respect to the size of the unit cell problem, which can then be chosen to be smaller. Unfortunately one is restricted to non-periodic materials in many cases, e.g., when experimental (usually non-periodic) data is used, so that periodic displacement fluctuations cannot be applied.

After choosing the type of boundary conditions some sort of numerical approximation of the exact solution is computed. When looking at the individual contributions to the total computational cost it is found that the solution of large, sparse and (often) symmetric linear systems of equations accounts for most of the overall solution time. The solution of the linear equations can be conducted using different methods where a subdivision into direct, iterative and domain decomposition algorithms makes sense.

In this paper the effects induced by different kinematic boundary conditions on the solution time of the linear system with respect to the applied solution method are examined. Section 2 is devoted to a classification of the considered kinematic boundary conditions. In section 3 two-dimensional model problems are examined in order to motivate some of the findings for the three-dimensional examples presented in section 4. In the closing section a brief summary and a guide for the selection of the appropriate solver is presented.

2 Boundary conditions

2.1 Classification of kinematic boundary conditions

By Ω we denote the domain of the unit cell and by $\Gamma = \partial\Omega$ its boundary. In this paper we focus on mechanical problems in the displacement field $\boldsymbol{u}$ with kinematic boundary conditions. This is equivalent to strain driven processes, where for a given macroscopic strain tensor $\bar{\boldsymbol{\varepsilon}}$ the local displacements $\boldsymbol{u}$, stresses $\boldsymbol{\sigma}$ and internal variables $\boldsymbol{\xi}$ have to be computed.

When kinematic boundary conditions are to be classified, it makes sense to introduce the additive decomposition

$$\boldsymbol{u} = \bar{\boldsymbol{u}} + \tilde{\boldsymbol{u}} \tag{1}$$

into a homogeneous deformation and a fluctuation field $\tilde{\boldsymbol{u}}$ which has to satisfy

$$\frac{1}{|\Omega|} \int_{\Gamma} (\tilde{\boldsymbol{u}} \otimes \boldsymbol{n} + \boldsymbol{n} \otimes \tilde{\boldsymbol{u}}) \, \mathrm{d}A = \boldsymbol{0}, \tag{2}$$

with $\boldsymbol{n}$ the outward normal to Γ. Then it is possible to classify the type of kinematic boundary conditions in terms of the function space for the fluctuation part. Here, the function spaces allowing for a solution of the weak form of the boundary value problem are considered as a subspace of the Sobolev space $\mathcal{W}^{1,2}$. A typical classification with descending restrictiveness is as follows:

- uniform kinematic boundary conditions UKBC
  The displacement on the entire boundary of the unit cell $\Gamma_{\mathrm{u}} = \Gamma$ is prescribed to be homogeneous, i.e. no fluctuations are feasible

$$\tilde{\boldsymbol{u}} = \boldsymbol{0} \quad (\text{on } \Gamma), \qquad \tilde{\boldsymbol{u}} \in V_{UKBC} = \{\boldsymbol{v} \in \mathcal{W}^{1,2} : \boldsymbol{v} = \boldsymbol{0} \text{ on } \Gamma\} \tag{3}$$

- periodic displacement fluctuation boundary conditions PKBC
  The fluctuation field has the same value on opposing points $\boldsymbol{X}_+, \boldsymbol{X}_-$ of the unit cell

$$\tilde{\boldsymbol{u}}_+ = \tilde{\boldsymbol{u}}_- \quad (\text{on } \Gamma), \qquad \tilde{\boldsymbol{u}} \in V_{PKBC} = \{\boldsymbol{v} \in \mathcal{W}^{1,2} : \boldsymbol{v}(\boldsymbol{X}_+) = \boldsymbol{v}(\boldsymbol{X}_-) \text{ on } \Gamma\} \supsetneq V_{UKBC} \tag{4}$$

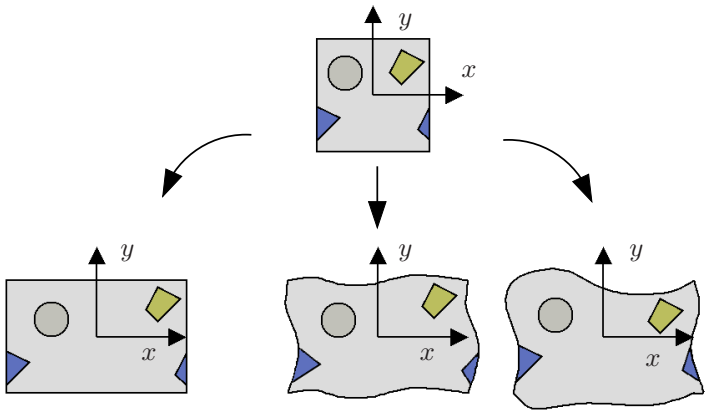


Figure 1: Uniform/periodic/weakly imposed boundary conditions (from left to right)

2.2 Numerical enforcement of boundary conditions

The linear systems of equations resulting from the finite element analysis are assumed to be of the form

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{f}, \tag{5}$$

with real, sparse, symmetric and semi-positive definite $\boldsymbol{K}$. The right hand side vector $\boldsymbol{f}$ denotes the nodal forces prescribed by external loading, e.g., due to a gravitational field. By the incorporation of kinematic boundary conditions the semi-positive definiteness of the system is replaced by the favorable positive definiteness. There exist various ways for the numerical implementation of boundary conditions. In this paper a method based on an *exact* enforcement of the boundary conditions by modification of the system of equations is used. More precisely, if the degree of freedom (DOF) with index i is prescribed, then the i-th column and row of the initial stiffness matrix are removed and a reduced vector of free variables is considered. If the boundary condition for the considered DOF is non-zero then the right-hand side has to be updated accordingly. For UKBC the described procedure is used in order to impose the boundary conditions and, thus, positive definiteness of the resulting matrix $\boldsymbol{K}_{\mathrm{u}}$ is attained.

For periodic displacement fluctuation conditions the following method is used: Let $\boldsymbol{u}_\mathrm{m}, \boldsymbol{u}_\mathrm{s}, \boldsymbol{u}_\mathrm{i}$ denote the vectors of unknowns associated with master/slave/internal[1] degrees of freedom and assume the entries of $\boldsymbol{u}_\mathrm{m}$ and $\boldsymbol{u}_\mathrm{s}$ are related by

$$\boldsymbol{u}_\mathrm{s} = \boldsymbol{u}_\mathrm{m} + \boldsymbol{y}, \tag{6}$$

for a constant vector $\boldsymbol{y}$. Then the vector of unknowns can be written as

$$\begin{pmatrix} \boldsymbol{u}_\mathrm{m} \\ \boldsymbol{u}_\mathrm{i} \\ \boldsymbol{u}_\mathrm{s} \end{pmatrix} = \underbrace{\begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{I} & \boldsymbol{0} \end{pmatrix}}_{\boldsymbol{P}} \underbrace{\begin{pmatrix} \boldsymbol{u}_\mathrm{m} \\ \boldsymbol{u}_\mathrm{i} \end{pmatrix}}_{\boldsymbol{v}} + \underbrace{\begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \\ \boldsymbol{y} \end{pmatrix}}_{=\boldsymbol{z}} = \boldsymbol{P}\boldsymbol{v} + \boldsymbol{z}. \tag{7}$$

Assuming the same ordering for the stiffness matrix yields the stiffness matrix of the periodic system

$$\begin{aligned} \boldsymbol{K}_{\mathrm{p},0} = \boldsymbol{P}^\mathsf{T}\boldsymbol{K}\boldsymbol{P} &= \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{0} & \boldsymbol{I} & \boldsymbol{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{K}_\mathrm{mm} & \boldsymbol{K}_\mathrm{mi} & \boldsymbol{K}_\mathrm{ms} \\ \boldsymbol{K}_\mathrm{mi}^\mathsf{T} & \boldsymbol{K}_\mathrm{ii} & \boldsymbol{K}_\mathrm{is} \\ \boldsymbol{K}_\mathrm{ms}^\mathsf{T} & \boldsymbol{K}_\mathrm{is}^\mathsf{T} & \boldsymbol{K}_\mathrm{ss} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{I} & \boldsymbol{0} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{K}_\mathrm{mm} + \boldsymbol{K}_\mathrm{ms} + \boldsymbol{K}_\mathrm{ms}^\mathsf{T} + \boldsymbol{K}_\mathrm{ss} & \boldsymbol{K}_\mathrm{mi} + \boldsymbol{K}_\mathrm{is}^\mathsf{T} \\ \boldsymbol{K}_\mathrm{mi}^\mathsf{T} + \boldsymbol{K}_\mathrm{is} & \boldsymbol{K}_\mathrm{ii} \end{pmatrix}. \end{aligned} \tag{8}$$

The right hand side of the system transforms according to

$$\boldsymbol{f}_{\mathrm{p},0} = \boldsymbol{P}^\mathsf{T}\left(\boldsymbol{f} - \boldsymbol{K}\boldsymbol{z}\right). \tag{9}$$

Finally, the resulting system of equations becomes

$$\boldsymbol{K}_{\mathrm{p},0}\boldsymbol{v} = \boldsymbol{f}_{\mathrm{p},0}. \tag{10}$$

The matrix $\boldsymbol{K}_{\mathrm{p},0}$ is still only semi-positive definite. In order to get positive definiteness, the motion of the corner points of the unit cell is prescribed by using the previously described row and column elimination which eventually yields the positive matrix $\boldsymbol{K}_\mathrm{p}$ and the right hand side vector $\boldsymbol{f}_\mathrm{p}$.

3 Model problem

3.1 Problem setting

Before three-dimensional mechanical problems are considered, the influence of the boundary conditions onto two-dimensional model problems is investigated. The domain examined in the following is assumed to consist of a regular partitioning of the domain $[0,1] \times [0,1]$ (Fig. 2). For simplicity the following considerations are based on row-wise increasing ordering of the nodes and linear nodal basis functions. The different material parameters were considered at the integration points of the element only.

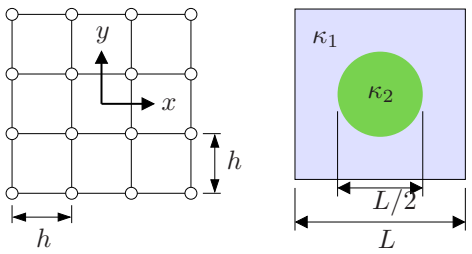


Figure 2: Discretization of the model problem

A homogeneous Poisson-like problem in a scalar field variable $u(\boldsymbol{x})$ is considered

$$\mathrm{div}\left(\boldsymbol{\kappa}(\boldsymbol{x})\,\mathrm{grad}(u(\boldsymbol{x}))\right) = 0 \qquad (\text{in } \Omega), \tag{11}$$

[1] Master nodes are assumed at $\boldsymbol{X}_+ \in \Gamma$, slave nodes at the opposing point $\boldsymbol{X}_-$. All remaining nodes are referred to as internal. The corner points of the unit cell are treated seperately by imposing Dirichlet conditions (see below).

where the heterogeneity of the material is introduced by the non-constant symmetric positive definite tensor $\boldsymbol{\kappa}(\boldsymbol{x}) = \kappa(\boldsymbol{x})\boldsymbol{I}$. An example for (11) is given by heat conductivity obeying Fourier's law. While the problem is not equivalent to mechanical problems, it can, however, serve to yield predictions on the numerical performance of these. It is noteworthy that (11) and all convex elasto-plastic problems denote elliptic partial differential equations, i.e., belong to the same problem class. The stiffness matrix of the resulting finite element system then has the penta-diagonal structure illustrated in Fig. 3. Below we examine the mathematical properties of the system matrices resulting from the two different kinematic boundary conditions. Different solution techniques are applied in order to investigate the numerical performance in dependency of the number of nodes and the chosen constraints.

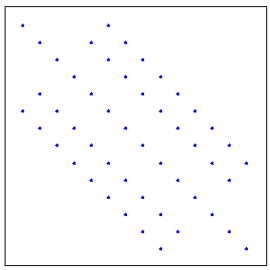
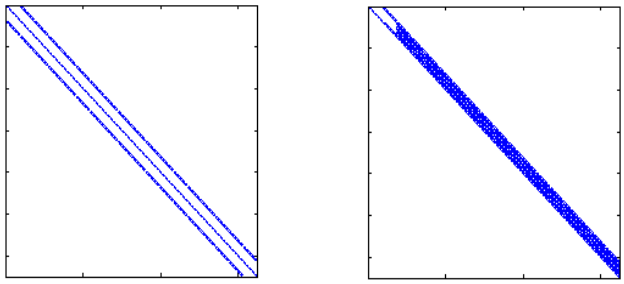


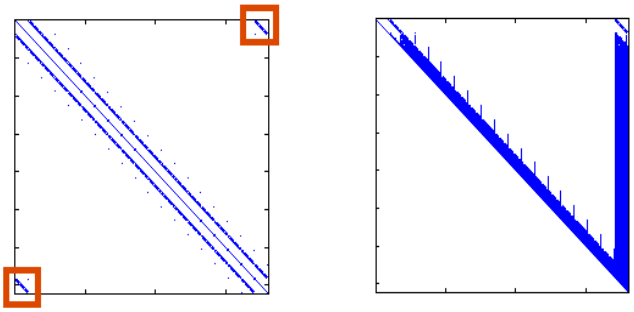
Figure 3: Schematic band structure of the global stiffness matrix of the system for the two-dimensional model problem

3.2 Properties of the global stiffness matrix

Based on the initial semi-positive definite stiffness matrix, uniform displacement boundary conditions UKBC ($\boldsymbol{K}_{\mathrm{u}}$) and periodic displacement fluctuation boundary conditions PKBC ($\boldsymbol{K}_{\mathrm{p}}$) are considered. The phase contrast $\kappa_2/\kappa_1 = 2$ was chosen. The structure of the resulting system matrices and of their Cholesky factorizations $\boldsymbol{L}_{\mathrm{u/p}}$ with $\boldsymbol{K}_{\mathrm{u/p}} = \boldsymbol{L}_{\mathrm{u/p}}\boldsymbol{L}^{\mathsf{T}}\mathrm{u/p}$ are illustrated in Fig. 4. The major difference in the periodic stiffness matrix is highlighted for better visibility.



(a) uniform kinematic boundary conditions



(b) periodic discplacement fluctuation boundary conditions

Figure 4: Comparison of modified stiffness matrix (left) and Cholesky factorization (right) (20×20=400 nodes)

Despite the small differences in the structures of the stiffness matrix, the fill-in of the Cholesky factorization induced by the periodicity condition is massive. The number of non-zero entries n_{nz} in the stiffness matrix and its factorization and an estimate of the condition number k are given in Tab. 1 for different resolutions of the spatial discretization. All values are normalized to those of the matrix obtained for UKBC . As the number of boundary

nodes decreases with respect to the total number of nodes, the number of unknowns in the problem with full boundary data and periodic fluctuation field is comparable for finer discretizations (columns two and three in Tab. 1). While the number of non-zero entries in the corresponding linear system is almost identical, the number of non-zero entries in the Cholesky factorization is approximately four times as large leading to a significant reduction of the spatial resolution that can be considered for a given amount of memory.

In order to reduce the fill-in, a permutation of the system matrices is advisable. The `amd` (approximate minimum degree) ordering algorithm was applied to $\boldsymbol{K}_{\mathrm{p}}$ and $\boldsymbol{K}_{\mathrm{u}}$. A significant reduction of the number of non-zero entries n^*_{nz} in the resulting (permuted) Cholesky factorization could be observed. Interestingly, the reduction is more pronounced for PKBC (last column in Tab. 1). It can be concluded that for the considered model problem on very fine discretizations, the number of non-zero entries in the factorization will be independent of the type of boundary condition. It can, however, rarely be realized in practice to achieve such fine discretizations due to the excessive memory requirement when three-dimensional unit cell problems are considered.

total #nodes	$\#\mathrm{DOF}_{\mathrm{ukbc}}$	$\#\mathrm{DOF}_{\mathrm{pkbc}}$	$\frac{n_{\mathrm{nz}}(\boldsymbol{K}_{\mathrm{p}})}{n_{\mathrm{nz}}(\boldsymbol{K})}$	$\frac{n_{\mathrm{nz}}(\boldsymbol{L}_{\mathrm{p}})}{n_{\mathrm{nz}}(\boldsymbol{L})}$	$\frac{k_{\mathrm{pkbc}}}{k_{\mathrm{ukbc}}}$	$\frac{n^*_{\mathrm{nz}}(\boldsymbol{L}_{\mathrm{p}})}{n^*_{\mathrm{nz}}(\boldsymbol{L})}$
10^2=100	$9.604\ 10^3$	$9.800\ 10^3$	1.523	4.228	14.064	2.917
20^2=400	$1.584\ 10^5$	$1.592\ 10^5$	1.214	4.132	17.179	2.283
50^2=2500	$6.240\ 10^6$	$6.245\ 10^6$	1.077	4.057	21.879	1.760
200^2=40000	$1.600\ 10^9$	$1.600\ 10^9$	1.018	4.015	28.602	1.524
300^2=90000	$8.100\ 10^9$	$8.100\ 10^9$	1.012	4.010	30.057	1.323
400^2=160000	$2.560\ 10^{10}$	$2.560\ 10^{10}$	1.009	4.007	31.960	1.142

Table 1: Comparison of the properties of the system matrices ($\kappa_2/\kappa_1 = 2$; $*$: with preordering)

3.3 Implications for iterative solution techniques

In addition to the large number of non-zero entries in the factorization, the condition number of the periodic problem was found to be significantly higher than the one of the problem with uniform boundary data. An increased condition number usually leads to increased computational costs when using numerical solution methods such as the conjugate gradient (CG) method (e.g., Shewchuk (1994)). For the latter, the a priori estimate for the residual $\boldsymbol{e}^{(i)}$ of the i-th iteration

$$\|\boldsymbol{e}^{(i)}\| < \left(\frac{\sqrt{k}-1}{\sqrt{k}+1}\right)^i \|\boldsymbol{e}^{(0)}\| \tag{12}$$

holds. However, not only the condition number but also the clustering of the eigenvalues has a strong impact on the convergence of the CG method. In order to evaluate the effect of the boundary conditions onto the approximate solution, a series of random right hand side vectors was generated and a diagonally preconditioned CG algorithm was used for solving the resulting linear system. A selection of the obtained results is listed in Tab. 2 for a problem containing 40000 nodes and for the two different phase contrasts $\kappa_2/\kappa_1 = 2$ and 10, respectively. Here, $N_{\mathrm{CG,ukbc}}$ and $N_{\mathrm{CG,pkbc}}$ denote the number of iterations required until convergence and N_{FLOP} is an estimate of the total number of floating point operations in the solution process. The phase contrast was varied since the condition number of the stiffness matrix does strongly depend on it. No investigations with respect to the size or shape of the inclusion were performed for the model problem.

From further numerical testing it was found that the computational effort for the solution of the system of equations is almost independent of the number of nodes and, thus, of the number of boundary nodes (Fig. 5) since

$$n_{\mathrm{bc-nodes}} \approx 4\sqrt{n_{\mathrm{nodes}}}. \tag{13}$$

Only for problems involving few internal degrees of freedom the increase in the number of floating point operations of the periodic problem is more pronounced.

3.4 Discussion of the results for the model problem

The results presented in Tab. 1 show that the memory required for a full Cholesky factorization of the stiffness matrix of the model problem shows a strong dependency on the type of kinematic boundary condition. In particular,

# test vector	$\kappa_2/\kappa_1 = 2$			$\kappa_2/\kappa_1 = 10$		
	$N_{\mathrm{CG,ukbc}}$	$N_{\mathrm{CG,pkbc}}$	$\frac{N_{\mathrm{FLOP,pkbc}}}{N_{\mathrm{FLOP,ukbc}}}$	$N_{\mathrm{CG,ukbc}}$	$N_{\mathrm{CG,pkbc}}$	$\frac{N_{\mathrm{FLOP,pkbc}}}{N_{\mathrm{FLOP,ukbc}}}$
1	452	798	1.798	467	851	1.856
2	453	797	1.792	452	851	1.917
3	454	797	1.788	467	850	1.853
4	452	798	1.798	467	850	1.853
5	452	794	1.789	478	838	1.785
6	452	800	1.802	468	847	1.843
7	456	805	1.798	471	856	1.851
8	451	762	1.720	475	857	1.837
9	453	795	1.787	471	859	1.857
10	450	802	1.815	450	854	1.932

Table 2: Comparison of the numerical performance of the CG method (200^2=40000 nodes, $\kappa_2/\kappa_1 = 2$ and 10)

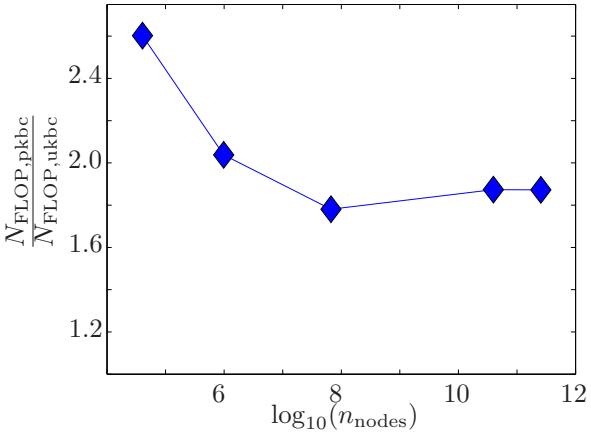


Figure 5: Relative computational cost of PKBC over UKBC for the preconditioned CG method ($\kappa_2/\kappa_1 = 10$)

the ratio of the number of boundary associated degrees of freedom with respect to the number of internal degrees of freedom influences the memory requirements. It was found that a preordering algorithm is basically inevitable for large scale periodic problems in order to achieve acceptable computational efficiency, particularly with respect to memory requirements. If rectangular unit cells are to be considered this ratio is optimal for quadratic unit cells (in two dimensions) and for a cube (in three dimensions). The `amd` algorithm (Amestoy et al., 2004, 1996) showed a good performance and helped to dramatically reduce the observed fill-in. However, the number of non-zero entries in the factorization is still larger for PKBC than for UKBC.

Numerical tests based on the conjugate gradient method with diagonal preconditioning have shown that the increased condition number of the periodic system negatively influences the solution time. However, (almost) no additional memory was required in order to apply the CG method since the number of non-zero entries in the stiffness matrix is approximately independent of the type of boundary conditions. For many practical applications this observation can be exploited in order to treat large scale problems without having to account for the massive memory requirement of direct solution techniques.

4 Analysis of the stiffness matrices

4.1 Solvers

In this paper we compare the following four different solution techniques which are applied to three-dimensional elastic unit cell problems:

- ABAQUS/STANDARD: direct sparse solver,
- ABAQUS/STANDARD: domain decomposition solver (DDM) based on the FETI method (Finite Element Tearing Appart and Interconnecting),
- Sparse Cholesky factorization (CHOLMOD (Chen et al., 2008)),
- Preconditioned conjugate gradient (PCG) method (own implementation) (see, e.g., Shewchuk (1994)).

The displacements are approximated based on a nodal basis with quadratic ansatz function. This leads to an increase in the bandwith of the system matrix in comparison to linear displacement elements.

The commercial finite element program ABAQUS/STANDARD is used to compute results in an environment accessible to many people using the finite element method with the CPU time and the memory requirement being the measurable factors. The self-written implementation using either the CHOLMOD package or the conjugate gradient method helps to highlighten some specific aspects of direct and sparse solvers when used in combination with the different kinematic boundary conditions. The program uses the same shape functions as the commercial software and consistency of the results with ABAQUS/STANDARD has been validated. In ABAQUS/STANDARD the periodic boundary fluctuation conditions have been implemented using so-called `equation` constraints. This leads to matrix operations similar to the ones described in section 3.

4.2 Problem setting

The numerical properties of the stiffness matrix of a unit cell representing an aggregate of crystals are examined. A discretization technique developed by the authors (Fritzen et al., 2009) is used to discretize the periodic unit cell based on the Voronoi tessellation and using different mesh densities. In this study meshes containing 20 grains and 7173 to 119265 nodes are considered (Fig. 6). The constitutive behaviour of the material was modeled as linear elasticity with cubic material symmetry. The elastic constants of copper ($C_{1111} = 168\,\text{GPa}$, $C_{1122} = 121\,\text{GPa}$, $C_{1212} = 75\,\text{GPa}$) are used (Beran et al., 1996).

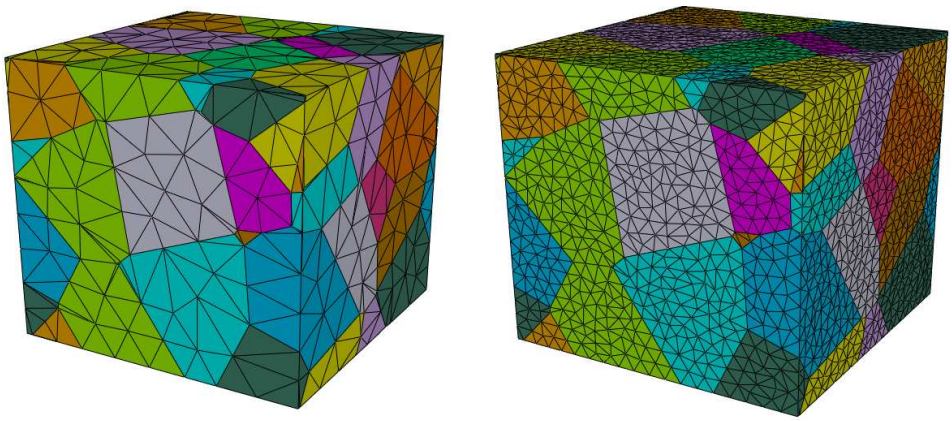


Figure 6: Finite element mesh of the crystalline structure: coarsest (left) and finest (right) discretization

The number of non-zero entries and an approximation of the memory required for the storage of the Cholesky factorization of the global stiffness matrix are presented in table 3 for our own implementation. The memory required for the storage of the stiffness matrices is almost identical for both problems. However, a Cholesky decomposition of the stiffness matrix requires significantly more memory for PKBC than for UKBC . Although an `amd` based preordering algorithm is employed, the periodicity of the field variables still implies a massive fill-in. Unfortunately the memory requirement for the factorization using the `cholmod` algorithm are not satisfying, i.e. the memory usage is prohibitively large.

In ABAQUS/STANDARD the memory requirement for the periodic unit cell problem shows the same qualitative behaviour as in the implementation based on `cholmod`. However, the employed matrix storage and preordering algorithm seems to be very efficient. The total memory requirement is dramatically reduced compared to the

mesh #	1	2	3	4
# nodes	7173	13590	48237	119265
$n_{\mathrm{DOF,ukbc}}$	15873	31956	125001	322821
$n_{\mathrm{DOF,pkbc}}$	18519	36162	134559	339939
$n_{\mathrm{nz,ukbc}}$	$5.763\ 10^5$	$1.220\ 10^6$	$5.067\ 10^6$	$1.345\ 10^7$
$n_{\mathrm{nz,pkbc}}$	$8.127\ 10^5$	$1.591\ 10^6$	$5.931\ 10^6$	$1.500\ 10^7$
Cholmod $n_{\mathrm{nz,ukbc}}$	$5.637\ 10^6$	$2.203\ 10^7$	$2.047\ 10^8$	$9.958\ 10^8$
Cholmod $n_{\mathrm{nz,pkbc}}$	$1.766\ 10^7$	$6.168\ 10^7$	$5.927\ 10^8$	$2.533\ 10^9$
Memory estimate $\boldsymbol{L}_{\mathrm{ukbc}}$	64.6 MB	252 MB	2343 MB	11400 MB
Memory estimate $\boldsymbol{L}_{\mathrm{pkbc}}$	202 MB	706 MB	6783 MB	28990 MB

Table 3: Comparison of the different matrix properties

`cholmod` based approach.

In the sequel an elastic homogenization problem is considered, i.e., the effective stiffness matrix of the micro-heterogeneous material is computed. Therefore, six linear systems with the same stiffness matrix but different right hand sides have to be solved. Due to the unfortunate memory requirements, the `cholmod` based approach was not traced. The results of the numerical tests are summarized in Tab. 4. While the direct methods require only one factorization in order to solve the system for the six right hand sides, the CG based ansatz and the ABAQUS DDM solver, both, need to be run individually on each of the six right hand side vectors. Rows entitled 'max. DOF wavefront' represent the maximum bandwith of the reordered sparse stiffness matrix.

mesh density #	1	2	3	4
# nodes	7173	13590	48237	119265
precon. CG UKBC	8 s (34 MB)	15 s (54 MB)	109 s (155 MB)	346 s (367 MB)
precon. CG PKBC	21 s (37 MB)	41 s (59 MB)	208 s (167 MB)	764 s (384 MB)
ABAQUS direct UKBC	4 s (31 MB)	13 s (68 MB)	95 s (334 MB)	527 s (1040 MB)
max. DOF wavefront UKBC	1479	2496	6105	11577
ABAQUS direct PKBC	9 s (65.7 MB)	29 s (195 MB)	348 s (1002 MB)	2087 s (3540 MB)
max. DOF wavefront PKBC	2751	4977	12723	22920
ABAQUS DDM UKBC	36 s (129 MB)	41 s (219 MB)	171 s (781 MB)	415 s (1960 MB)
max. DOF wavefront UKBC	882	876	954	1068
ABAQUS DDM PKBC	72 s (206 MB)	138 s (340 MB)	401 s (986 MB)	1080 s (2260 MB)
max. DOF wavefront PKBC	1371	1365	1083	1116

Table 4: Comparison of the total solution time and memory required for the computation of the effective stiffness of the volume element

In Fig. 7 the solution time normalized with respect to the number of nodes is compared for UKBC (left) and PKBC (right). It can be observed from the linearity of $t_{\mathrm{sol.}}/\#n_{\mathrm{nodes}}$ with respect to n_{nodes} that the solution time of the direct solver in ABAQUS shows almost exactly quadratic dependency of the solution time with respect to the number of nodes. The ABAQUS DDM solver was found to have almost constant solution time per node. However, for a small number of nodes the solution of the interface equations between the different regions and the communication overhead is significant. It can thus be recommended to use the DDM solver for large scale problems only, particularly when UKBC are considered. The preconditioned CG method showed good performance for small and large systems. The solution time was smaller than for the DDM solver in all cases considered in this work. For many problems the solution time of the CG method was the same or smaller than for the direct solver.

5 Summary and conclusions

The numerical aspects of unit cell problems arising from computational homogenization are investigated. Two different sets of problems subjected to Dirichlet boundary conditions were examined. First, a two-dimensional heat conductivity type problem acting as a model problem to capture some of the important aspects of the different boundary conditions is considered. Second, a three-dimensional elastic homogenization problem is used to confirm the findings for mechanical real-world problems. An important outcome of the current investigation is the

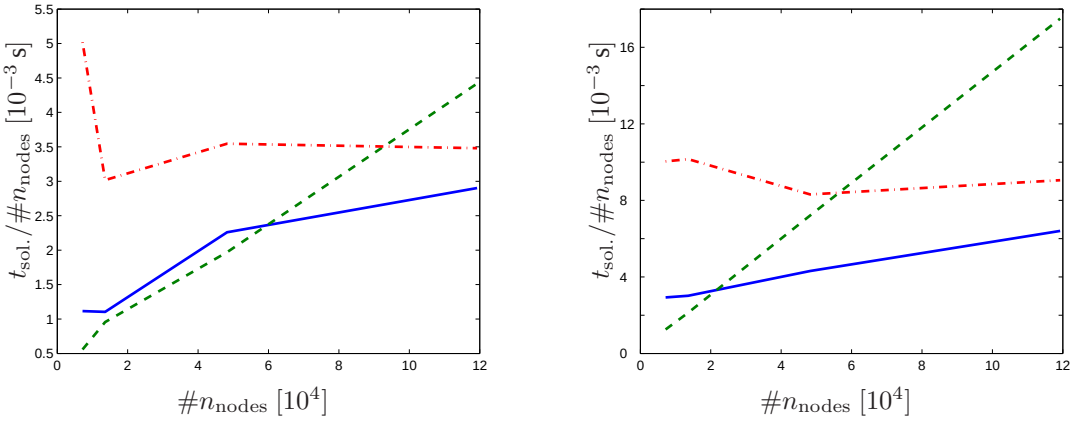


Figure 7: Comparison of normalized solution time for UKBC (left) and PKBC (right) (blue/solid: PCG, green/dashed: ABQ (direct), red/dash-dotted: ABQ (DDM)

considerable increase in the solution time induced by the use of periodic fluctuation boundary conditions which is independent of the applied solution technique. The reason for the increase in the solution time is (i) the large amount of fill-in mainly induced by the increased bandwith of the system matrix (for direct solvers) and (ii) the worse conditioning of the system matrix (for iterative solvers). Additionally, direct solvers suffer severly from an increase in the memory required for a full factorization of the occuring matrices. The amount of fill-in can be reduced by reordering of the system. However, the observed fill-in for the periodic problems was still larger than for UKBC.

Based on the current investigation the following conclusions are drawn:

- For materials with small/moderate phase contrast (e.g., less than one order of difference in the physical properties) the preconditioned CG method is recommended for medium or large problems independent of the type of kinematic boundary conditions. For small problems, it can however be sensible to use direct solution methods. This is particularly true, if the same linear system with a large number of different right hand sides has to be solved or if very large phase contrasts are considered (e.g., pairing of very soft and almost rigid materials).

- We recommend the use of a preconditioned CG (PCG) method or a domain decomposition technique (e.g., ABAQUS DDM solver) for problems containing a large number of degrees of freedom and containing materials with a large phase contrast, i.e., for inelastic materials. For inelasticity or pronounced phase contrasts the efficiency of the PCG method is largely depending on the quality of the preconditioner. Small or moderate numbers of degrees of freedom can efficiently be treated using sparse direct methods which have the advantage of being applicable to an arbitrary number of right hand sides with barely any additional computational cost. These methods are applicable for badly conditioned problems with barely any additional computational cost.

- For all problem sizes the preordering of the equations can yield a dramatic decrease of the amount of additional fill-in due to periodic boundary conditions (see, e.g., Tab. 1, last column). Then for very large problems the difference in the number of non-zeros in the Cholesky factor is (almost) identical for UKBC and PKBC. However, the absolute number of non-zeros and, thus, the memory required for the factorization are often inacceptable, if this large problems are considered (e.g., 400^3=64 Mio. nodes in 3d).

- For PKBC the resolution of the mesh is restricted for many methods due to excessive memory requirements (direct methods; ABAQUS DDM solver). For these methods the preconditioned CG method shows good performs without the need for additional memory over UKBC . The reduced memory requirement is particularly advantageous for problems involving very fine discretizations, which can otherwise not be solved due to limited amounts of memory or only by resorting to supercomputers.

- If the number of boundary nodes is large with respect to the number of inner nodes, i.e., for elongated cuboidal cells, direct solution techniques are not recommended for PKBC due to massive fill-in. The preconditioned CG method is expected to suffer from the bad conditioning of the system matrix, but can,

however, be used without particular consideration of memory requirements. The ABAQUS DDM solver is partially applicable to these problems, i.e. it is recommended, if two dimensions of the three-dimensional unit cell are small compared to the third.

- The results of section 3.3 are intended to give a first impression of the influence of the phase contrast on the CG method. Noteably, the choice of the preconditioner, the actual geometry and the physical properties form a complex ensemble. However, the results state that variations of the physical properties in the range of one magnitude lead to almost constant computational cost.

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Address: Felix Fritzen and Thomas Böhlke, Kontinuumsmechanik im Maschinenbau, Institut für Technische Mechanik, Karlsruhe Institut für Technologie, D-76133 Karlsruhe.
email: `fritzen@itm.uni-karlsruhe.de`, `boehlke@itm.uni-karlsruhe.de`