Parallel Performance Evaluation of MIC(0) Preconditioning Algorithm for Voxel μFE Simulation

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Abstract. Numerical homogenization is used for up-scaling of a linear elasticity tensor of strongly heterogeneous micro-structures. Utilized approach assumes presence of a periodic micro-structure and thus periodic boundary conditions. Rotated trilinear Rannacher-Turek finite elements are used for the discretization, while a parallel PCG method is used to solve arising large-scale systems with sparse, symmetric, positive semidefinite matrices. Applied preconditioner is based on modified incomplete Cholesky factorization MIC(0).

The test problem represents a trabecular bone tissue, and takes into account only the elastic response of the solid phase. The voxel micro-structure of the bone is extracted from a high resolution computer tomography image. Numerical tests performed on parallel computers demonstrate the efficiency of the developed algorithm.

Keywords: micro finite element simulation, modeling of human bone tissue, parallel algorithms, PCG method, preconditioner, MIC(0) factorization, parallel performance.

1 Introduction

Many, seemingly different materials, such as human bone tissue, geocomposites, filtering media in industrial applications have very complex hierarchical organization spanning multiple length scales and involve complex multi-physical processes at some of these scales. However, their overall mechanical response and ability to conduct fluids can be described using multilevel techniques that are built upon basic conservation principles at the micro or nano levels.

In our work, we consider modeling of human bone tissue which is based on the recently developed morphology of bones. In general, model used here has a multilevel structure according to the specific material dimensions (and as such

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generalizes to other problems mentioned above). At a length scale of about several hundred nanometers, oriented, highly organized collagen molecules, the minority of the hydroxy-apatite crystals (present in bone tissues) and water, build up (mineralized) fibrils. At the same length scale, but in the extra-fibrillar space, the majority of (largely disordered) hydroxy-apatite crystals build up a mineral foam (polycrystalline), with water filling the inter-crystalline (nano)space. At a length scale of several micrometers, the fibrils and the extra-fibrillar space builds up solid bone matrix or ultrastructure. Finally, at a length scale of several millimeters, macroscopic bone material (cortical or trabecular bone) comprises solid bone matrix and the micro-porous space. This four-level model has been validated by statistically and physically independent experiments, see e.g. [11,13,15]. Having in mind that the aforementioned dosages (concentrations, volume fractions) are dependent on complex biochemical control cycles (defining the metabolism of the organism), the purely mechanical theory can be linked to biology, biochemistry, and, on the applied side, to clinical practice.

Many problems in bone modeling result in need to solve large- and very large-scale linear systems. This, in turn, requires application of parallel computers. Furthermore, even though recent advances in direct solvers for large-scale sparse linear systems has to be acknowledged (see, [7,17], for an interesting comparison), the method of choice for the problem at hand has to be iterative.

In this context, this study concerns development and tuning of solution methods, algorithms, and software tools for micro finite element (μFE) simulation of human bones (e.g. [1,2]). Furthermore, the isotropic linear elasticity model considered here is a brick in the development of a generalized toolkit for μFE simulation of the bone micro-structure.

A boundary value problem can be discretized in various ways. Among the most popular are: the finite volume method, the Galerkin finite element method (FEM), and the mixed FEM. Many engineering problems need very accurate velocity (flux) determinations in the presence of heterogeneities and large jumps in the coefficient. This can be achieved through the mixed FEM. However, this technique usually leads to an algebraic saddle point problem that is more difficult and more expensive to solve. An important discovery of Arnold and Brezzi [4] is that the Schur system for the Lagrange multipliers can be obtained also as a discretization by a Galerkin method using nonconforming elements. The application of rotated trilinear hexahedral FEs is studied in this paper.

The resulting linear system is large, with a sparse, symmetric and positive definite matrix. This implies use of preconditioned conjugate gradient (PCG) solvers [5], while choice of preconditioning is crucial for the PCG performance. It is also known that the PCG method converges for semidefinite matrices in the orthogonal to the kernel subspace.

The elasticity stiffness matrix has a coupled block structure corresponding to separable displacement ordering of the unknowns. Until now, the displacement decomposition (see, [6,10]) remains one of the most robust approaches for preconditioning of such matrices. Here, one of the most popular and the most successful class of preconditioners is the class of incomplete LU (ILU) factorizations (see,

e.g. [5,12]). However, one potential problem with the ILU preconditioners is that they exhibit a limited degree of parallelism. To alleviate this problem we have developed a preconditioning algorithm based on a parallel MIC(0) (Modified Incomplete Cholesky) elasticity solver [20]. Suitable modification of the MIC(0) algorithm allows efficient parallelization of the preconditioning.

2 Homogenization Technique

Let Ω be a hexagonal domain representing our reference volume element (RVE) and $\mathbf{u} = (u_1, u_2, u_3)$ be the displacements vector in Ω. Here, components of the small strain tensor are:

$$\varepsilon_{ij}\left(\mathbf{u}\left(\mathbf{x}\right)\right) = \frac{1}{2}\left(\frac{\partial u_i(\mathbf{x})}{\partial x_j} + \frac{\partial u_j(\mathbf{x})}{\partial x_i}\right) \tag{1}$$

We assume that Hooke's law holds:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix} c_{1111} & c_{1122} & c_{1133} & c_{1123} & c_{1113} & c_{1112}\\ c_{2211} & c_{2222} & c_{2233} & c_{2223} & c_{2213} & c_{2212}\\ c_{3311} & c_{3322} & c_{3333} & c_{3323} & c_{3313} & c_{3312}\\ c_{2311} & c_{2322} & c_{2333} & c_{2323} & c_{2313} & c_{2312}\\ c_{1311} & c_{1322} & c_{1333} & c_{1323} & c_{1313} & c_{1312}\\ c_{1211} & c_{1222} & c_{1233} & c_{1223} & c_{1213} & c_{1212}\end{bmatrix} \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ 2\varepsilon_{23}\\ 2\varepsilon_{13}\\ 2\varepsilon_{12}\end{bmatrix}. \tag{2}$$

Here, tensor c is called the stiffness tensor, while σ is the stress tensor.

The symmetric 6×6 matrix C is called the stiffness matrix. For an isotropic material C has only two independent degrees of freedom. For materials containing three orthogonal planes of symmetry, matrix C has nine independent degrees of freedom: three Young's moduli E_1, E_2, E_3, three Poisson's ratios $\nu_{12}, \nu_{23}, \nu_{31}$ and three shear moduli $\mu_{12}, \mu_{23}, \mu_{31}$.

$$C = \delta \begin{bmatrix} \frac{1-\nu_{23}\nu_{32}}{E_1} & \frac{\nu_{12}+\nu_{31}\nu_{23}}{E_1} & \frac{\nu_{31}+\nu_{21}\nu_{32}}{E_1} & & & \\ \frac{\nu_{12}+\nu_{13}\nu_{32}}{E_2} & \frac{1-\nu_{31}\nu_{13}}{E_2} & \frac{\nu_{32}+\nu_{31}\nu_{12}}{E_2} & & & \\ \frac{\nu_{13}+\nu_{12}\nu_{23}}{E_3} & \frac{\nu_{23}+\nu_{13}\nu_{21}}{E_3} & \frac{1-\nu_{12}\nu_{21}}{E_3} & & & \\ & & & \frac{\mu_{23}}{\delta} & & \\ & & & & \frac{\mu_{31}}{\delta} & \\ & & & & & \frac{\mu_{12}}{\delta} \end{bmatrix}, \tag{3}$$

where

$$\delta = 1 - \nu_{12}\nu_{21} - \nu_{13}\nu_{31} - \nu_{23}\nu_{32} - 2\nu_{12}\nu_{23}\nu_{31},$$

$$\frac{\nu_{12}}{E_1} = \frac{\nu_{21}}{E_2}, \qquad \frac{\nu_{23}}{E_2} = \frac{\nu_{32}}{E_3}, \qquad \frac{\nu_{31}}{E_3} = \frac{\nu_{13}}{E_1}.$$

Our goal was to obtain homogenized material properties of the trabecular bone tissue. In other words, to find the stiffness tensor of a homogeneous material, with the same macro-level properties as our RVE. In the proposed approach, we follow the numerical up-scaling method from [14] (see also [9]). The homogenization scheme requires finding functions $\boldsymbol{\xi}^{kl} = (\xi_1^{kl}, \xi_2^{kl}, \xi_3^{kl})$, $k, l = 1, 2, 3$, satisfying the following problem in a week formulation:

$$\int_{\Omega} \left(c_{ijpq}(x) \frac{\partial \xi_p^{kl}}{\partial x_q} \right) \frac{\partial \phi_i}{\partial x_j} d\Omega = \int_{\Omega} c_{ijkl}(x) \frac{\partial \phi_i}{\partial x_j} d\Omega, \tag{4}$$

for an arbitrary Ω-periodic variational function $\boldsymbol{\phi} \in H^1(\Omega)$. After computing the characteristic displacements $\boldsymbol{\xi}^{kl}$, from (4) we can compute the homogenized elasticity tensor c^H using the following formula:

$$c_{ijkl}^H = \frac{1}{|\Omega|} \int_{\Omega} \left(c_{ijkl}(x) - c_{ijpq}(x) \frac{\partial \xi_p^{kl}}{\partial x_q} \right) d\Omega. \tag{5}$$

Due to symmetry of the stiffness tensor c, we have the relation $\boldsymbol{\xi}^{kl} = \boldsymbol{\xi}^{lk}$ and it is enough to solve only six problems (4) to obtain the homogenized stiffness tensor.

Rotated trilinear (Rannacher-Turek) finite elements [18] are used for the numerical solution of (4). This choice is motivated by the additional stability of the nonconforming finite element discretization in the case of strongly heterogeneous materials [4]. Construction of a robust non-conforming finite element method is generally based on application of mixed formulation leading to a saddle-point system. By the choice of non continuous finite elements for the dual (pressure) variable, it can be eliminated at the (macro)element level. As a result we obtain a symmetric positive (semi-)definite finite element system in primal (displacements) variables. We utilize this approach, which is referred as the *reduced and selective integration* (RSI).

3 Parallel Displacement Decomposition MIC(0) Preconditioning

A preconditioning algorithm was developed using a parallel MIC(0) elasticity solver [20], based on a parallel MIC(0) solver for the scalar elliptic problem [3]. The preconditioner uses the isotropic variant of the displacement decomposition (DD) [6,10]. We write the DD auxiliary matrix in the form

$$M_{DD} = \begin{bmatrix} A & & \\ & A & \\ & & A \end{bmatrix} \tag{6}$$

where A is the stiffness matrix corresponding to the bilinear form

$$a(u^h, v^h) = \int_{\Omega} E(\mathbf{x}) \left(\sum_{i=1}^{3} \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_i} \right) d\mathbf{x}, \tag{7}$$

and u and v are Ω-periodic functions. Such approach is motivated by the second Korn's inequality, which holds for the RSI finite element discretization under consideration. This means that the estimate for the relative condition number of the preconditioned system

$$\kappa\left(M_{DD}^{-1}K\right) = \mathcal{O}\left((1-2\nu)^{-1}\right)$$

holds uniformly with respect to the mesh size parameter, while K is the stiffness matrix. Our preconditioner is obtained by the MIC(0) factorization of blocks in (6).

Remark 1. To satisfy conditions for the stable MIC(0) factorization in the case of a semi-definite matrix, we are using the perturbed version of the MIC(0) algorithm, where the incomplete factorization is applied to the matrix $\tilde{A} = A + \tilde{D}$. The diagonal perturbation $\tilde{D} = \tilde{D}(\xi) = diag(\tilde{d}_1, \ldots \tilde{d}_N)$ is defined as follows:

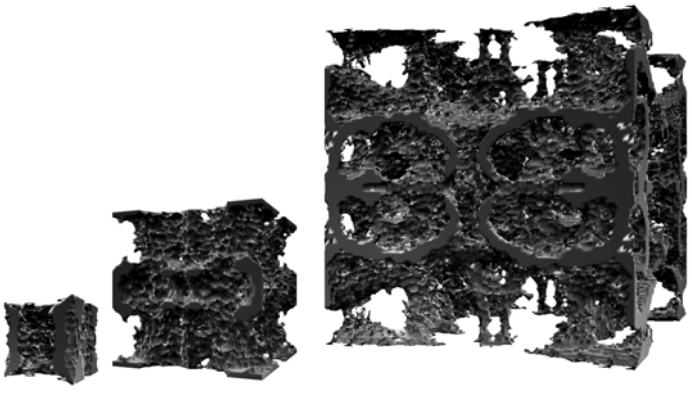
$$\tilde{d}_i = \begin{cases} \xi a_{ii} & \text{if } a_{ii} \geq 2w_i \\ \xi^{1/2} a_{ii} & \text{if } a_{ii} < 2w_i \end{cases}$$

where $0 < \xi < 1$ is a properly chosen parameter, and $w_i = \sum_{j>i} -a_{ij}$.

The idea of the proposed parallel algorithm is to apply the MIC(0) factorization on an auxiliary matrix B, which approximates A. This matrix B has a special block structure, which facilitates implementation of a scalable parallel solver. Following the standard FEM assembling procedure we write A in the form $A = \sum_{e \in \omega_h} R_e^T A_e R_e$, where A_e is the element stiffness matrix, while R_e stands for the restriction mapping of the global vector of unknowns to the local one corresponding to the current element e. Let us consider the following approximation B_e of A_e:

$$A_e = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} \end{bmatrix} \qquad B_e = \begin{bmatrix} b_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ a_{21} & b_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ a_{31} & a_{32} & b_{33} & 0 & 0 & 0 \\ a_{41} & a_{42} & 0 & b_{44} & 0 & 0 \\ a_{51} & a_{52} & 0 & 0 & b_{55} & 0 \\ a_{61} & a_{62} & 0 & 0 & 0 & b_{66} \end{bmatrix}$$

Local numbering applied here follows the pairs of the opposite nodes of the reference element. Here, diagonal entries of B_e are modified to hold the row-sum criteria (for more details see [3]). Assembling the locally defined matrices B_e we obtain the global matrix $B = \sum_{e \in \omega_h} R_e^T B_e R_e$. The condition number estimate $\kappa(B^{-1}A) \leq 3$ holds uniformly with respect to the mesh parameter and to possible coefficient jumps (for the related analysis see discussion presented in [3]). After this modification we obtain matrix B with its diagonal blocks (corresponding to horizontal cross sections) being diagonal matrices. The solution of linear systems with the preconditioner can be performed in parallel. It is important to note that the use of periodic boundary conditions does not change diagonal blocks of the



(a) (b) (c)

Fig. 1. Structure of the solid phase: (a) $32 \times 32 \times 32$ voxels, (b) $64 \times 64 \times 64$ voxels, (c) $128 \times 128 \times 128$ voxels

stiffness matrix A, and thus the same parallel algorithm can be applied also here. The obtained preconditioner has the form.

$$M_{DDMIC(0)} = \begin{bmatrix} M_{MIC(0)}(B) & & \\ & M_{MIC(0)}(B) & \\ & & M_{MIC(0)}(B) \end{bmatrix}.$$

4 Experimental Results

Our test specimen is part of a trabecular bone tissue obtained from a high resolution computer tomography [8]. The trabecular bone tissue has a strongly heterogeneous micro-structure composed of solid and fluid phases and thus matches very well with the proposed approach. To obtain a periodic RVE the bone tissue specimen is mirrored three times, see Fig. 1. The voxel size is 37 μm.

In this paper we focus on the parallel performance of the proposed numerical up-scaling technique. Experiments to study the homogenized properties of the RVE with dimensions $n \times n \times n$ voxels were performed, where $n = 32, 64, 128$. The Young moduli $E^s = 14.7$ GPa for the solid phase, and $E^f = 1.323$ GPa for the fluid phase were used. The same Poisson ratio $\nu^s = \nu^f = 0.325$ was used for both phases. The iteration stopping criterion was $||\mathbf{r}^j||_{M^{-1}}/||\mathbf{r}^0||_{M^{-1}} < 10^{-3}$, where $\mathbf{r}^j$ stands for the residual at the j-th iteration step of the preconditioned conjugate gradient method.

To solve the above described problems, a portable parallel FEM code was designed and implemented in C++, while the parallelization has been facilitated using the MPI library [19,21]. The parallel code has been tested on cluster computer system located in the Oklahoma Supercomputing Center (OSCER) and the IBM Blue Gene/P machine at the Bulgarian Supercomputing Center. In our experiments, times have been collected using the MPI provided timer and

Table 1. Experimental results on Sooner

n	Problem size	p	Time	Speed-up	Efficiency
32	2 359 296	1	631.05		
		2	355.73	1.77	0.887
		4	243.61	2.59	0.648
		8	217.92	2.90	0.362
		16	133.24	4.74	0.296
		32	87.86	7.18	0.224
64	18 874 368	1	6317.35		
		2	3362.10	1.88	0.939
		4	2270.16	2.78	0.696
		8	1921.95	3.29	0.411
		16	1154.40	5.47	0.342
		32	774.10	8.16	0.255
		64	588.81	10.73	0.168
128	150 994 944	1	82468.90		
		2	44902.69	1.84	0.918
		4	28065.57	2.94	0.735
		8	23621.77	3.49	0.436
		16	12146.39	6.79	0.424
		32	7212.52	11.43	0.357
		64	4881.75	16.89	0.264
		128	3761.78	21.92	0.171

we report the best results from multiple runs. We report the elapsed time T_p in seconds on p processors, the parallel speed-up $S_p = T_1/T_p$, and the parallel efficiency $E_p = S_p/p$. The obtained up-scaled properties can be found in [16].

Table 1 summarizes results collected on Sooner. It is a Dell Pentium4 Xeon E5405 ("Harpertown") quad core Linux cluster located in the Oklahoma Supercomputing Center (see `http://www.oscer.ou.edu/resources.php`). It has 486 Dell PowerEdge 1950 III nodes and two quad core processors per node. Each processor runs at 2 GHz. Processors within each node share 16 GB of memory, while nodes are interconnected with a high-speed InfiniBand network. We have used Intel C++ compiler and compiled the code with the following options: "-O3 -march=core2 -mtune=core2".

As expected, the parallel efficiency improves with the size of the discrete problems. The efficiency on 16 processors increases from 30% for the smallest problems to 42% for the largest problems in this set of experiments. Also, the execution times decrease with increasing number of processors which shows that the communications in our parallel algorithm are mainly local.

Table 2 shows execution times on IBM Blue Gene/P machine at the Bulgarian Supercomputing Center (see `http://www.scc.acad.bg/`). It consists of 2048 compute nodes with quad core PowerPC 450 processors (running at 850 MHz). Each node has 2 GB of RAM. For the point-to-point communications a 3.4 Gb 3D mesh network is used. Reduction operations are performed on a 6.8 Gb tree

Table 2. Experimental results on IBM Blue Gene/P

n	Problem size	p	Time	Speed-up	Efficiency
32	2 359 296	1	3442.29		
		2	1782.88	1.93	0.965
		4	954.90	3.61	0.901
		8	532.29	6.47	0.808
		16	322.62	10.67	0.667
		32	205.40	16.76	0.524
64	18 874 368	1	34166.01		
		2	17358.17	1.97	0.984
		4	8975.65	3.81	0.952
		8	4763.87	7.17	0.896
		16	2633.40	12.97	0.811
		32	1589.88	21.49	0.672
		64	1003.19	34.06	0.532
128	150 994 944	8	55413.21		
		16	29132.86		0.951
		32	15967.65		0.868
		64	9773.76		0.709
		128	6131.38		0.565

network. We have used IBM XL C++ compiler and compiled the code with the following options: "-O5 -qstrict -qarch=450d -qtune=450".

The memory available on a single node of Blue Gene/P is not sufficient to run experiments for the largest problem and we report execution times starting from eight processors located within different nodes. Therefore, for the largest problem, we report parallel efficiency related to results collected on eight processors. Execution times on Blue Gene/P are substantially larger than that on Sooner,

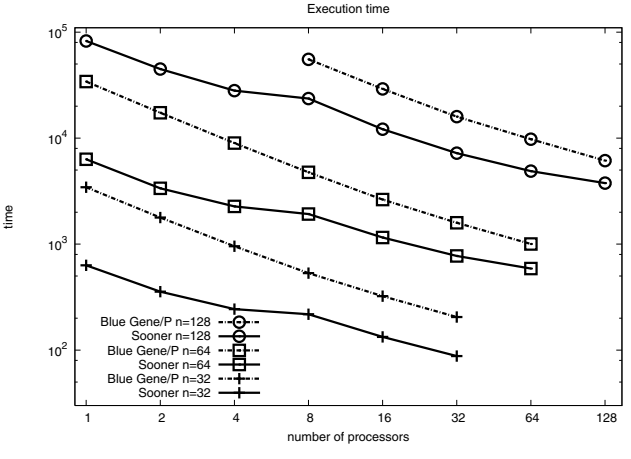


Fig. 2. Execution times for the test problems

but parallel efficiency obtained on the supercomputer is better. For instance, the execution on 64 processors on Sooner is only twice faster than on the Blue Gene/P, in comparison with five times faster performance on single processor.

To summarize, in Fig. 2 computing times on both parallel systems are shown. The somehow slower performance on Sooner using 8 processors is clearly visible. It can be stipulated that this effect is a result of limitations of memory subsystems and their hierarchical organization. One of them might be the limited bandwidth of the main memory bus. This causes processors to "starve" for data, thus, decreasing the overall performance. Note that L2 cache memory is shared among each pair of cores within the processors of Sooner. This boosts performance of programs utilizing only a single core within such pair. Conversely, this leads to somewhat decreased performance when all cores are used.

5 Conclusions and Future Work

We have studied the parallel performance of the recently developed numerical homogenization technique utilizing parallel MIC(0) factorization [16]. The performance was evaluated on two different parallel architectures. Satisfying parallel efficiency is obtained on the IBM Blue Gene/P. The efficiency on Sooner quickly deteriorates with the increase of the number of the processors. Despite of the worse efficiency, the faster CPUs on Sooner lead to shorter runtime, on the same number of processors. The network latency is crucial for the parallel performance of the algorithm. To hide some of the network latency, the computations were overlapped with the communications wherever possible. We plan to investigate the possibility to hide further the latency, solving simultaneously more than one of the six independent problems (4).

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