# Two Preconditioners For Voxel $\mu$FEM Simulation

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Abstract

*Two parallel iterative solvers for large-scale linear systems related to $\mu$FEM simulation of human bones were developed. The considered benchmark problems represent the strongly heterogeneous structure of real bone specimens. The voxel data are obtained by a high resolution computer tomography. Non-conforming Rannacher-Turek finite elements are used for discretization of the considered problem of linear elasticity.*

*Here the preconditioned conjugate gradient method is used. The performance of two parallel preconditioners is studied. Both are based on displacement decomposition. The first one uses modified incomplete Cholesky factorization MIC(0) and the other – algebraic multigrid.*

## 1 Introduction

This work is devoted to the development and tuning of robust iterative solution methods, algorithms and software tools for $\mu$FE (micro finite element) simulation of human bones. A voxel representation of the bone structure based on micro computer tomography (CT) images is used to formulate the problem. The computational domain is a strongly heterogeneous composition of solid and fluid phases, see Figure 1. The considered isotropic linear elasticity model is a current brick in the development of a toolkit for $\mu$FE simulation of the bone microstructure. The implementation of a poroelasticity model is the next step in this project.

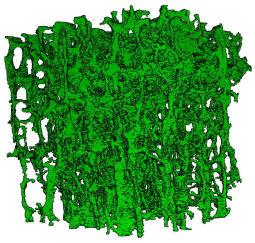

Figure 1: Bone microstructure.

Non-conforming Rannacher-Turek FEs are used for discretization of the problem. The obtained linear system is large, with a sparse, symmetric and positive definite matrix. This implies the use of iterative solvers based on the preconditioned conjugate gradient (PCG) method [1]. The elasticity stiffness matrix has a coupled block

structure corresponding to a separable displacement ordering of the unknowns. Here, the performance of the following two basic preconditioning codes, incorporated to a displacement decomposition framework, is studied. The first one is the modified incomplete factorization, MIC(0), and the second is the algebraic multigrid, AMG. The MIC(0) code is developed in IPP-BAS, Sofia, while the AMG one is the BoomerAMG module of the software system Hypre developed at LLNL, Livermore. The comparative analysis is focused on the number of iterations and the related computing times for real-life large-scale problems.

# 2 Non-conforming FEM formulation of the problem

We consider the weak formulation of the linear elasticity problem in the form: find $\mathbf{u} \in [H^1_E(\Omega)]^3 = \{\mathbf{v} \in [H^1(\Omega)]^3 : \mathbf{v}_{\Gamma_D} = \mathbf{u}_S\}$ such that

$$\int_\Omega [2\mu\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{v}) + \lambda\, div\ \mathbf{u}\, div\ \mathbf{v}]d\Omega = \int_\Omega \mathbf{f}^t\mathbf{v}d\Omega + \int_{\Gamma_N} \mathbf{g}^t\mathbf{v}d\Gamma, \tag{1}$$

$\forall \mathbf{v} \in [H^1_0(\Omega)]^3 = \{\mathbf{v} = [H^1(\Omega)]^3 : \mathbf{v}_{\Gamma_D} = 0\}$, with the positive constants $\lambda$ and $\mu$ of Lamé, the symmetric strains $\varepsilon(\mathbf{u}) := 0.5(\nabla\mathbf{u} + (\nabla\mathbf{u})^t)$, the volume forces $\mathbf{f}$, and the boundary tractions $\mathbf{g}$, $\Gamma_N \cup \Gamma_D = \partial\Omega$, $|\Gamma_D| \neq \emptyset$. The Lamé coefficients are given by $\lambda = \dfrac{\nu E}{(1+\nu)(1-2\nu)}$, $\mu = \dfrac{E}{2(1+\nu)}$, where $E$ stands for the modulus of elasticity, and $\nu \in (0, \frac{1}{2})$ is the Poisson ratio.

To obtain a stable saddle-point system one usually uses a mixed formulation for $\mathbf{u}$ and $div\ \mathbf{u}$. By the choice of piece-wise constant finite elements for the dual variable, it can be eliminated at the macroelement level, and thereafter we get a symmetric positive definite FEM system in primal unknowns (displacement). This approach is known as *reduced and selective integration* (RSI) technique, see [2]. For the discretization of (1) we use nonconforming rotated trilinear elements of Rannacher-Turek [3].

After the RSI discretization, the following system of linear equations is obtained

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} \begin{bmatrix} \mathbf{u}_h^1 \\ \mathbf{u}_h^2 \\ \mathbf{u}_h^3 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_h^1 \\ \mathbf{f}_h^2 \\ \mathbf{f}_h^3 \end{bmatrix}. \tag{2}$$

Here the stiffness matrix $K$ is written in block form corresponding to a separate displacements components ordering of the vector of nodal unknowns. Since $K$ is sparse, symmetric and positive definite, we use the PCG method to solve the system (2).

# 3 Preconditioning algorithms

Crucial for the performance of the PCG algorithm is the preconditioning technique used. Here we present two preconditioners based on the isotropic variant of the displacement decomposition (DD)[4, 5]. We write the DD auxiliary matrix in the form

$$C_{DD} = \begin{bmatrix} A & & \\ & A & \\ & & A \end{bmatrix} \tag{3}$$

where $A$ is the stiffness matrix corresponding to the bilinear form

$$a(u^h, v^h) = \sum_{e \in \Omega^h} \int_e E \left( \sum_{i=1}^{3} \frac{\partial u^h}{\partial x_i} \frac{\partial v^h}{\partial x_i} \right) de. \quad (4)$$

Such approach is motivated by the second Korn's inequality, which holds for the RSI FEM discretization under consideration. This means that the estimate $\kappa(C_{DD}^{-1}K) = O((1-2\nu)^{-1})$ holds uniformly with respect to the mesh size parameter in the FEM discretization.

The first approach used is based on the recently developed parallel MIC(0) preconditioner for scalar elliptic problems [6]. Its basic idea is to apply MIC(0) factorization of an approximation $B$ of the stiffness matrix $A$. Matrix $B$ has a special block structure. Its diagonal blocks are diagonal matrices. This allows the solution of the preconditioning system to be performed in parallel. The condition number estimate $\kappa(B^{-1}A) \leq 3$ holds uniformly with respect to mesh parameter and possible coefficient jumps (see for the related analysis in [6]). This technique is applied three times - once for each diagonal block of (3).

In our second approach inner PCG iteration is used. BoomerAMG code from the Hypre package is used as a preconditioner. The Falgout coarsening was used in the presented tests. A V(1,1)-cycle with hybrid Gauss-Seidel smoothing was performed. The related AMG strength threshold was 0.5. Aggressive coarsening was used. The number of the inner iterations was fixed to 4.

# 4 Comparative numerical tests

## 4.1 Scalability tests

Numerical tests with the considered two parallel algorithms and codes are present and analyzed in this section. The tests are run on three parallel platforms, referred to further as C1, C2 and C3. Platform C1 is an "IBM SP Cluster 1600" consisting of 64 p5-575 nodes interconnected with a pair of connections to the Federation HPS (High Performance Switch). Each p5-575 node contains 8 Power5 SMP processors at 1.9GHz and 16GB of RAM. The network bandwidth is 16Gb/s. Platform C2 is an IBM Linux Cluster 1350, made of 512 dual-core IBM X335 nodes. Each node contains 2 Xeon Pentium IV processors and 2GB of RAM. Nodes are interconnected with a 1Gb Myrinet network. Platform C3 is a "Cray XD1" cabinet, fully equipped with 72 2-way nodes, totaling in 144 AMD Opteron processors at 2.4GHz. Each node has 4GB of memory. The CPUs are interconnected with the Cray RaidArray network with a bandwidth of 5.6Gb/s.

The computational domain is the cube $[0,1]^3$, where homogeneous Dirichlet boundary conditions are assumed at the bottom. The force $||g|| = 1$ is acting on the top. The mesh is uniform. Here $n$ stands for the number of subintervals in the fine grid of the RSI FEM discretization in each direction. The mechanical characteristics of the model problem are $E = 1$ and $\nu = 0.3$. The size of the resulting nonconforming FEM system is $N = 9n^2(n+1)$. The number of processors $p$ is increased proportionally with the problem size $N$. The stopping criterion in all considered tests is $(C^{-1}r^{N_{it}}, r^{N_{it}})/(C^{-1}r^0, r^0) < 10^{-6}$, where $r^i$ is the current residual and $C$ stands for the used preconditioner. Table 1 presents the time $T$ in seconds, the number of iterations $It$ (the outer ones for the AMG code), varying the preconditioners, the problem sizes and the platforms.

Table 1: Parallel Tests I

| | | | C1 | | | | C2 | | | | C3 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | MIC(0) | | AMG | | MIC(0) | | AMG | | MIC(0) | | AMG | |
| $n$ | N | $p$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ |
| 64 | 2 396 160 | 1 | 136.6 | 115 | 150.1 | 9 | 83.7 | 115 | 84.0 | 9 | 83.9 | 115 | 115.1 | 9 |
| 128 | 19 021 824 | 8 | 202.0 | 163 | 195.6 | 10 | 172.1 | 163 | 229.8 | 10 | 127.8 | 163 | 152.6 | 10 |
| 256 | 151 584 768 | 64 | 355.6 | 230 | 261.4 | 10 | 464.1 | 230 | 430.0 | 10 | 328.2 | 230 | 307.1 | 10 |

## 4.2 Voxel analysis tests

The bone microstructure is a typical example of strongly heterogeneous media. In the presented tests, the computational domain is a composition of solid and fluid phases. The CT image is extracted from the dataset [8]. The voxel size is $37\mu$m. Each voxel corresponds to a macroelement from the RSI FEM discretization. The bone specimen is placed between two plates (see Figure 2). The thickness of the plates is 1 voxel. The position of the bottom plate is fixed (homogeneous Dirichlet boundary conditions), and a force of $||g|| = 1$ is uniformly distributed on the top one. This setting simulates a vertically loaded bone specimen.

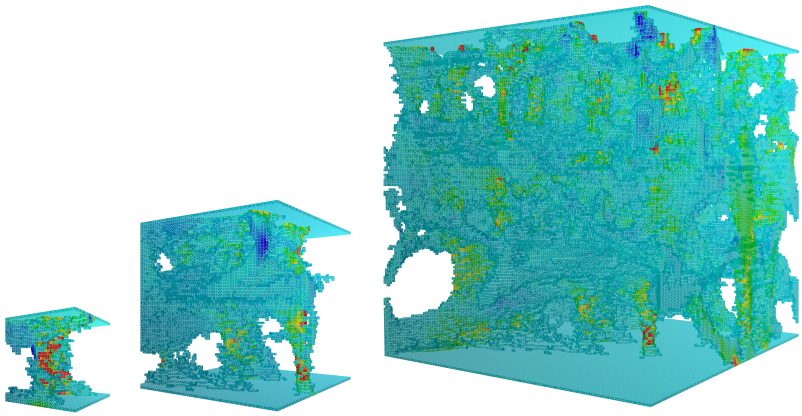

Figure 2: Vertical stresses: $n = 64$ - left, $n = 128$ - middle, $n = 256$ - right; red indicates areas with maximal stress, blue - with minimal.

The considered test problems are given by the following parameters: $E_p = 10$, $E_s = 1$, $E_f = \zeta \in \{0.1, 0.01, 0.001\}$, $\nu = 0.3$. Here, $E_p$ is the elasticity modulus of the two plates, $E_s$ stands for a scaled elasticity modulus of the solid phase, while $E_f$ introduces varying coefficient jumps between solid and fluid phases.

The results presented in Table 2 are obtained on the platform C2. For the case of the biggest coefficient jumps ($\zeta$=0.001) and the biggest problem (N=151 584 768), outer PCG iteration with AMG preconditioner fails to converge within the specified time limit of 7200 seconds. This test was repeated with an increased number of inner

iterations. The corresponding values in the table are obtained with $It_{in} = 6$. On Figure 2 with different colors are shown vertical stresses.

Table 2: Parallel Tests II

| | | $\zeta = 0.1$ | | | | $\zeta = 0.01$ | | | | $\zeta = 0.001$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | MIC(0) | | AMG | | MIC(0) | | AMG | | MIC(0) | | AMG | |
| $n$ | $p$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ | $T[s]$ | $It$ |
| 64 | 1 | 239.3 | 330 | 374.9 | 27 | 348.3 | 505 | 757.9 | 57 | 588.6 | 823 | 1040.5 | 78 |
| 128 | 8 | 833.2 | 708 | 681.0 | 25 | 975.5 | 830 | 1501.3 | 60 | 2166.7 | 1850 | 2908.9 | 107 |
| 256 | 64 | 2393.8 | 1237 | 945.4 | 25 | 3495.7 | 1831 | 2114.4 | 57 | 6025.8 | 3150 | 5520.1 | 114 |

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