Parallel PCG Algorithms for Voxel Elasticity Problems

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Two parallel iterative solvers for large-scale linear systems related to μFEM simulation are presented. The problems solved represent the strongly heterogeneous structure of real bone specimens or a geocomposite material. The voxel data are obtained by a high resolution computer tomography.
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

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

$\forall \mathbf{v} \in [H^1_0(\Omega)]^3 = \{\mathbf{v} = [H^1(\Omega)]^3 : \mathbf{v}_{\Gamma_D} = 0\}$, with the positive constants λ and μ 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 $\operatorname{div}\mathbf{u}$. 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]. The discretization of (1) using nonconforming rotated trilinear elements of Rannacher-Turek [4] leads to the coupled system of linear equations

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

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 algorithm to solve the system (2). Crucial for its performance is the preconditioning technique used. Here we focus on two preconditioners based on the isotropic variant of the displacement decomposition (DD)[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

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

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 of the studied preconditioners is obtained by parallel MIC(0) factorization of the blocks in (3). As an alternative, inner PCG iterations with BoomerAMG preconditioner for A are used to approximate the DD block-diagonal matrix (3). BoomerAMG is a parallel algebraic multigrid implementation from the package Hypre, developed in LLNL, Livermore. For a description of the algorithms used and their settings, see [3] and the references therein.
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 for a model problem representing vertically loaded brick. The computer platforms C1, C2 and C3 are described in [3].

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

In a good agreement with the theory, the number of iterations for MIC(0) increases as $O(\sqrt{n})$, while the AMG iterations stay about the same. For the smallest problem (N=2 396 160) MIC(0) clearly outperforms the AMG code. For the medium size (N= 19 021 824) the times are rather similar. However, for the largest problem (N=151 584 768) the advantage of AMG is well expressed.
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 [1]. The voxel size is 37μm. Each voxel corresponds to a macroelement from the RSI FEM discretization. The bone specimen is placed between two plates (see Fig. 1). 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.

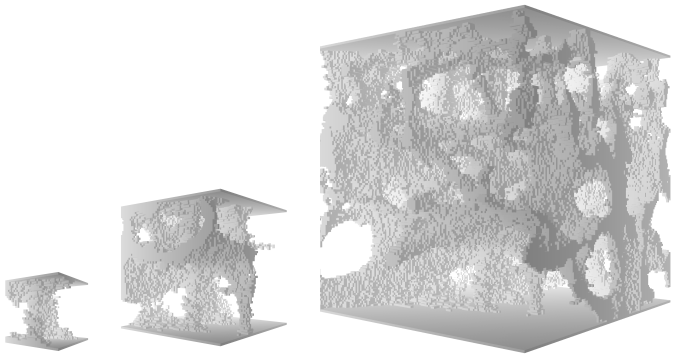

Figure 1: Structure of the solid phase: $32 \times 32 \times 32$ - left, $64 \times 64 \times 64$ - middle, and $128 \times 128 \times 128$ - right.

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.

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

The considered algorithms were successfully applied to another test problem. The voxel data represents a coal-polyurethane geocomposite (see Fig. 2 left). The domain is cubic – 75x75x75mm, but the scan is non-uniform in all directions – 35x110x110 voxels. The mechanical properties used were: Coal – $\nu = 0.25$, $E = 4000$MPa; Polyurethane – $\nu \in [0.1, 0.25]$, $E \in [200, 2100]$MPa. The setting used was the same – vertically loaded specimen. On the right on Fig. 2 are shown vertical displacements.

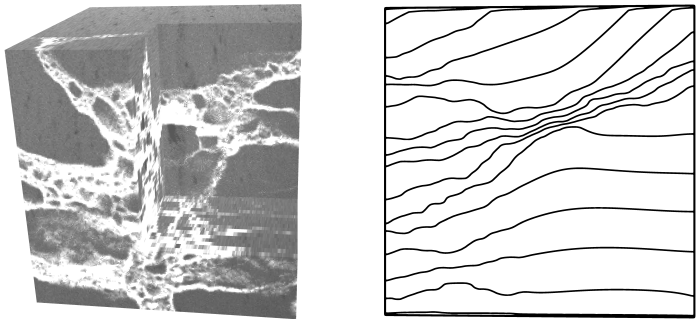

Figure 2: Left: coal-polyurethane geocomposite brick; right: vertical displacements.

The general conclusion is that the studied codes provide a stable toolkit for computer simulation of the bone microstructure. Both approaches have their advantages depending on the size of the FEM systems and the level of heterogeneity of the bone specimens. The achieved parallel scalability well corresponds to the connectivity of the considered problems.

References

[1] Gisela Beller, Markus Burkhart, Dieter Felsenberg, Wolfgang Gowin, Hans-Christian Hege, Bruno Koller, Steffen Prohaska, Peter I. Saparin and Jesper S. Thomsen: Vertebral Body Data Set ESA29-99-L3, http://bone3d.zib.de/data/2005/ESA29-99-L3/

[2] D. Malkus, T. Hughes. Mixed finite element methods. Reduced and selective integration techniques: an uniform concepts. *Comp. Meth. Appl. Mech. Eng.,*15: 63-81, 1978.

[3] Svetozar Margenov, Yavor Vutov, Parallel PCG Algorithms for Voxel FEM Elasticity Systems, Proceedings of the International Multiconference on Computer Science and Information Technology, 2007, pp. 517-526

[4] R. Rannacher, S. Turek: *Simple nonconforming quadrilateral Stokes Element*, Numer. Methods Partial Differential Equations 8(2), 1992, 97-112.

[5] R. Blaheta: *Displacement Decomposition - incomplete factorization preconditioning techniques for linear elasticity problems*, Numer. Lin. Alg. Appl., **1** (1994), 107–126