

Comparative analysis of PCG solvers for voxel FEM systems

S. Margenov and Y. Vutov

Institute for Parallel Processing, Bulgarian Academy of Sciences
Acad. G. Bonchev, bl. 25A, 1113 Sofia, Bulgaria
margenov@parallel.bas.bg and *yavor@parallel.bas.bg*

Abstract. The presented comparative analysis concerns two iterative solvers for large-scale linear systems related to μ FEM simulation of human bones. The 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 elliptic problem. It is well known that the preconditioned conjugate gradient method is the best tool for efficient solution of large-scale symmetric systems with sparse positive definite matrices. Here, the performance of two preconditioners is studied, namely the modified incomplete Cholesky factorization MIC(0) and the algebraic multigrid. The comparative analysis is mostly based on the computing times to run the sequential codes. The number of iterations for both preconditioners are also discussed. Numerical tests of a novel parallel MIC(0) code are given at the end. The obtained parallel speed-ups and efficiencies well illustrate the scope of efficient applications for real-life large-scale problems.

Key words: FEM, PCG, MIC(0), AMG, parallel algorithms

1 Introduction

The recent computational science entails interdisciplinary research, tackling complex scientific and engineering problems under the unifying concept of computation. The explosive growth of computer performance and progress in numerical methods and interfaces extends the power of scientific computation to an ever larger set of problems, while suggesting new ideas for experimental research. The present study is motivated by the development and tuning of robust iterative solution methods, algorithms and software tools for μ FE (micro finite element) simulation of human bones. The problem includes a voxel representation of the bone structure based on micro computer tomography (CT) images. We consider an isotropic 3D elliptic partial differential equation. This scalar problem is an inherent brick in the development of efficient solvers for the related coupled problems involved in the nonlinear elasticity and porous elasticity μ FE simulation of bone structures.

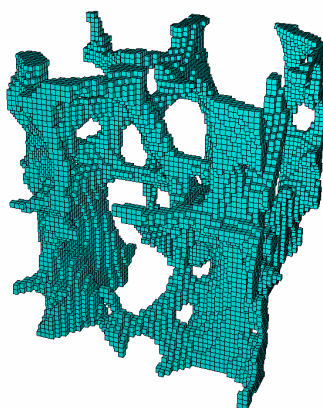


Fig. 1. Micro mesh detail of the solid phase of a human trabecular bone.

The computational domain is a complicated heterogeneous composition of solid and fluid phases. The figure below presents the solid phase of a micro mesh detail of 2.5 mm cubic portion of a bone specimen with 44 μ m voxels [1].

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 [5]. Here, the performance of the following two PCG codes is studied: a) the modified incomplete factorization, MIC(0), and b) the algebraic multigrid, AMG. The first code is developed in IPP-BAS, Sofia, while the AMG code is the BoomerAMG module of the software system Hypra 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.

The paper is organized as follows. In Section 2 we describe the Finite Element Method (FEM) setting of the problem. A short information about MIC(0) and BoomerAMG preconditioners is given in Section 3 ending with comparative numerical tests for the related sequential codes. Section 4 is devoted to the recently proposed parallel MIC(0) algorithm for 3D Rannacher-Turek FEM systems. The included parallel numerical tests are performed on an IBM SP Cluster.

2 Non-conforming FEM formulation of the problem

Consider the elliptic boundary value problem

$$\begin{aligned} Lu \equiv -\nabla \cdot (a(x)\nabla u(x)) &= f(x) && \text{in } \Omega, \\ u &= 0 && \text{on } \Gamma_D, \\ (a(x)\nabla u(x)) \cdot n &= 0 && \text{on } \Gamma_N, \end{aligned} \quad (1)$$

where Ω is a parallelogram domain in \mathbb{R}^3 which can be decomposed into $n_1 \times n_2 \times n_3$ cubes. Each of these cubes corresponds to a voxel from the CT image of the bone specimen. The problem is isotropic. The coefficient $a(x)$ is assumed to be piece-wise constant with jumps aligned with the voxel mesh, i.e.,

$$a(x) = \begin{cases} 1 & \text{for } x \in \Omega_s \\ \zeta & \text{for } x \in \Omega \setminus \Omega_s \end{cases},$$

where Ω_s stands for the solid phase of the bone volume, $\Omega \setminus \Omega_s$ corresponds to the fluid phase, and ζ is a constant parameter in $(0, 1]$.

The weak formulation of the problem (1) reads as follows: given $f \in L^2(\Omega)$ find $u \in \mathcal{V} \equiv H_D^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma_D\}$, satisfying

$$\mathcal{A}(u, v) = (f, v) \quad \forall v \in H_D^1(\Omega), \quad \text{where} \quad \mathcal{A}_h(u, v) = \int_{\Omega} a(x)\nabla u(x) \cdot \nabla v(x) dx. \quad (2)$$

The variational problem (2) is then discretized using the finite element method, i.e., the continuous space \mathcal{V} is replaced by a finite dimensional subspace \mathcal{V}_h . Then the finite element formulation is: find $u_h \in \mathcal{V}_h$, satisfying

$$\mathcal{A}(u_h, v_h) = (f, v_h) \quad \forall v_h \in \mathcal{V}_h, \quad \text{where} \quad \mathcal{A}_h(u_h, v_h) = \sum_{e \in \mathcal{T}_h} \int_e a(e)\nabla u_h \cdot \nabla v_h dx. \quad (3)$$

The resulting discrete problem to be solved is then a linear system of equations

$$A\mathbf{u}_h = \mathbf{f}_h, \quad (4)$$

where \mathbf{u}_h stands for the vector of unknown degrees of freedom, A and \mathbf{f}_h being the corresponding global stiffness matrix and global right hand side, and h being the discretization (mesh size) parameter for the underlying partition \mathcal{T}_h of Ω . The aim of this paper is to investigate high performance preconditioners for solving the system (4).

Non-conforming finite elements based on *rotated* multilinear shape functions were introduced by Rannacher and Turek [15] as a class of simple elements for the Stokes problem. More generally, the recent activities in the development of efficient solution methods for non-conforming finite element systems are inspired by their attractive properties as a stable discretization tool for ill-conditioned problems. Some more details about non-conforming finite elements can be found, e.g., in [4,6,8]. The cube $[-1, 1]^3$ is used as a reference element \hat{e} to define the isoparametric rotated trilinear element $e \in \mathcal{T}_h$. Let $\Psi_e : \hat{e} \rightarrow e$ be

the corresponding trilinear one-to-one transformation, and let the nodal basis functions be determined by the relation

$$\{\phi_i\}_{i=1}^6 = \{\hat{\phi}_i \circ \Psi_e^{-1}\}_{i=1}^6, \quad \{\hat{\phi}_i\} \in \text{span}\{1, x, y, z, y^2 - x^2, x^2 - z^2\},$$

where $(x_1, x_2, x_3) \equiv (x, y, z)$, ' \circ ' denotes the composition of functions. For the variant MP (mid point), $\{\hat{\phi}_i\}_{i=1}^6$ are found by the point-wise interpolation condition

$$\hat{\phi}_i(b_e^j) = \delta_{ij},$$

where b_e^j , $j=1,6$ are the centers of gravity of the walls of the cube \hat{e} . Then,

$$\begin{aligned} \hat{\phi}_1(x, y, z) &= (1 - 3x + 2x^2 - y^2 - z^2) / 6, \\ \hat{\phi}_2(x, y, z) &= (1 + 3x + 2x^2 - y^2 - z^2) / 6, \\ \hat{\phi}_3(x, y, z) &= (1 - x^2 - 3y + 2y^2 - z^2) / 6, \\ \hat{\phi}_4(x, y, z) &= (1 - x^2 + 3y + 2y^2 - z^2) / 6, \\ \hat{\phi}_5(x, y, z) &= (1 - x^2 - y^2 - 3z + 2z^2) / 6, \\ \hat{\phi}_6(x, y, z) &= (1 - x^2 - y^2 + 3z + 2z^2) / 6. \end{aligned}$$

Alternatively, for the variant *MV*, the integral mean-value interpolation operator is applied in the form

$$|\Gamma_e^j|^{-1} \int_{\Gamma_e^j} \hat{\phi}_i d\Gamma_e^j = \delta_{ij},$$

Γ_e^j , $j=1,6$ are the walls of the cube, and then

$$\begin{aligned} \hat{\phi}_1(x, y, z) &= (2 - 6x + 6x^2 - 3y^2 - 3z^2) / 12, \\ \hat{\phi}_2(x, y, z) &= (2 + 6x + 6x^2 - 3y^2 - 3z^2) / 12, \\ \hat{\phi}_3(x, y, z) &= (2 - 3x^2 - 6y + 6y^2 - 3z^2) / 12, \\ \hat{\phi}_4(x, y, z) &= (2 - 3x^2 + 6y + 6y^2 - 3z^2) / 12, \\ \hat{\phi}_5(x, y, z) &= (2 - 3x^2 - 3y^2 - 6z + 6z^2) / 12, \\ \hat{\phi}_6(x, y, z) &= (2 - 3x^2 - 3y^2 + 6z + 6z^2) / 12. \end{aligned}$$

Both variants *MP* and *MV* have similar properties with respect to the solution methods for the related FEM systems. In what follows we present numerical tests for the case *MV* which is motivated by some approximation advantages of this variant as reported in the literature, see e.g. [15].

3 PCG algorithms

The PCG is known to be the best algorithm for solution of large sparse systems of linear equations with a positive definite matrix. Crucial for its performance is the preconditioning technique used. Here we focus on two preconditioners: the modified incomplete Cholesky factorization MIC(0) and the algebraic multigrid method in the variant BoomerAMG, developed at Lawrence Livermore National Laboratory (LLNL).

3.1 MIC(0) preconditioning

In this section we briefly recall some known facts about the modified incomplete factorization [9], see also [10,11]. Our presentation at this point follows those from [7]. Let us rewrite the real $N \times N$ matrix $A = (a_{ij})$ in the form

$$A = D - L - L^T$$

where D is the diagonal and $(-L)$ is the strictly lower triangular part of A . Then we consider the approximate factorization of A which has the following form:

$$C_{MIC(0)} = (X - L)X^{-1}(X - L)^T$$

where $X = \text{diag}(x_1, \dots, x_N)$ is a diagonal matrix determined by the condition of equal rowsums. We are interested in the case when $X > 0$ and thus $C_{MIC(0)}$ is positive definite for the purpose of preconditioning. If this holds, we speak about *stable* MIC(0) factorization. Concerning the stability of MIC(0) factorization, we have the following theorem.

Theorem 1. Let $A = (a_{ij})$ be a symmetric real $N \times N$ matrix and let $A = D - L - L^T$ be the splitting of A . Let us assume that

$$\begin{aligned} L &\geq 0, \\ A\mathbf{e} &\geq 0, \\ A\mathbf{e} + L^T\mathbf{e} &> 0, \quad \mathbf{e} = (1, \dots, 1)^T \in \mathbb{R}^N, \end{aligned}$$

i.e. that A is a weakly diagonally dominant matrix with nonpositive offdiagonal entries and that $A + L^T = D - L$ is strictly diagonally dominant. Then the relation

$$x_i = a_{ii} - \sum_{k=1}^{i-1} \frac{a_{ik}}{x_k} \sum_{j=k+1}^N a_{kj} > 0$$

holds and the diagonal matrix $X = \text{diag}(x_1, \dots, x_N)$ defines stable MIC(0) factorization of A .

Remark 1. The presented numerical tests are performed using the perturbed version of MIC(0) algorithm, where the incomplete factorization is applied to the matrix $\tilde{A} = A + \tilde{D}$. The diagonal perturbation $\tilde{D} = \tilde{D}(\xi) = \text{diag}(\tilde{d}_1, \dots, \tilde{d}_N)$ 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 parameter, and $w_i = \sum_{j>i} -a_{ij}$.

3.2 BoomerAMG

BoomerAMG contains sequential and parallel implementations of algebraic multigrid methods [16]. It can be used both as a solver or as a preconditioner. Various different parallel coarsening techniques and relaxation schemes are available. See [12,18] for a detailed description of the coarsening algorithms, the interpolation and numerical results. The following coarsening techniques are available:

- the Cleary-Luby-Jones-Plassman (CLJP) coarsening,
- various variants of the classical Ruge-Stüben (RS) coarsening algorithm, and
- the Falgout coarsening which is a combination of CLJP and the classical RS coarsening algorithm.

The following relaxation techniques are available:

- Jacobi relaxation,
- hybrid Gauss-Seidel / Jacobi relaxation scheme,
- symmetric hybrid Gauss-Seidel / Jacobi relaxation scheme, and
- Gauss-Seidel relaxation.

3.3 Sequential numerical tests

The tests included in this section are performed on a computer with Athlon64 processor running on 2.0GHz with 4GB of RAM. The structure of the solid phase for the domains $(32 \times 32 \times 32)$ and $(64 \times 64 \times 64)$ is extracted from a real CT image of a human bone. Then, a mirror reflection technique is applied to get the larger problems (see Fig. 2). Both, MIC(0) and BoomerAMG are used as preconditioners with a relative stopping criteria in the form

$$(C^{-1}r^{N_{it}}, r^{N_{it}})/(C^{-1}r^0, r^0) < 10^{-6},$$

where r^i is the current residual and C stands for the used preconditioner. The size of the discrete problem N and the coefficient jump ζ are varied, where $N = (n_1 + 1)n_2n_3 + n_1(n_2 + 1)n_3 + n_1n_2(n_3 + 1)$, n_i is the number of mesh intervals along x_i direction, $i \in \{1, 2, 3\}$.

The numerical tests for the preconditioners MIC(0) and BoomerAMG are presented in Table 1 and Table 2 respectively. They include the obtained numbers of iterations N_{it} and the related total execution times t measured in seconds. The default settings of BoomerAMG were used: The Falgout coarsening consists of the classical Ruge-Stueben coarsening, followed by CLJP using the interior coarse points generated by Ruge-Stueben coarsening as its first independent set. A V(1, 1)-cycle was performed with hybrid Gauss-Seidel smoothing. The related AMG strength threshold was 0.25.

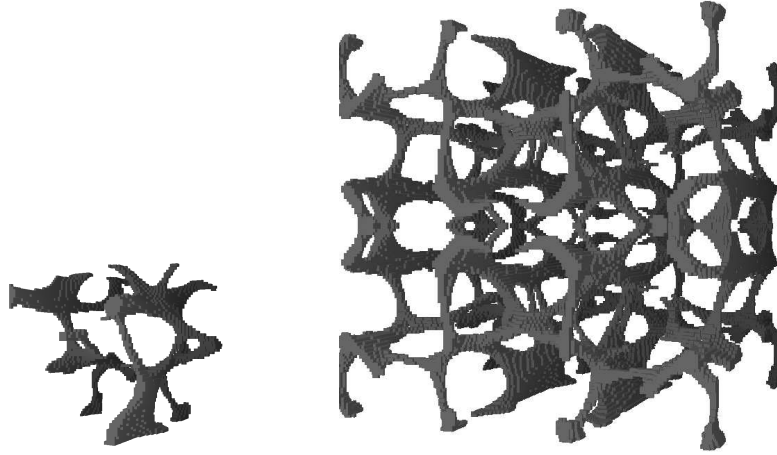


Fig. 2. Structure of the solid phase: $64 \times 64 \times 64$ - left, and $128 \times 128 \times 128$ - right.

Table 1. MIC(0)

$n_1 \times n_2 \times n_3$	N	$\zeta = 1$		$\zeta = 0.1$		$\zeta = 0.01$		$\zeta = 0.001$	
		N_{it}	t	N_{it}	t	N_{it}	t	N_{it}	t
$32 \times 32 \times 32$	101 376	27	0.86	46	1.55	121	3.22	187	5.11
$32 \times 32 \times 64$	798 720	26	1.58	36	2.27	115	6.08	296	15.3
$32 \times 64 \times 64$		26	3.04	41	5.51	117	13.1	379	47.8
$64 \times 64 \times 64$		35	7.84	56	14.5	166	41.3	417	103
$64 \times 64 \times 128$		33	14.6	52	28.1	141	69.3	453	220
$64 \times 128 \times 128$	6 340 608	33	27.7	53	54.2	142	134	467	440
$128 \times 128 \times 128$		47	76.8	72	122	197	337	575	981

The first observation is that $N_{it} = O(\sqrt{n_1})$ in the case of MIC(0). This is in a full agreement with the existing theoretical estimates, and with the much richer computational practice. For the largest problem $128 \times 128 \times 128$, N_{it} increases more than 12 times when ζ decreases from 1 to 0.001. The iteration counts are much better for BoomerAMG. What we see from the tests is that the multigrid iterations are almost optimal with respect to the problem size N , slightly increasing with the coefficient jumps. Let us remind that the AMG theory does not support the case of so strongly heterogeneous media.

It is important to note that structure of the algorithm and the memory consumption of the MIC(0) code does not depend on the coefficients. This is not the case with BoomerAMG, which uses about 4 times more memory than the MIC(0) for the Laplace equation ($\zeta = 1$) and about 10 times more when the coefficient jump increases. The shortage of the available RAM was the reason to skip the last two largest tests for BoomerAMG in the cases $\zeta \in \{0.1, 0.01, 0.001\}$.

Table 2. BoomerAMG

$n_1 \times n_2 \times n_3$	N	$\zeta = 1$		$\zeta = 0.1$		$\zeta = 0.01$		$\zeta = 0.001$	
		N_{it}	t	N_{it}	t	N_{it}	t	N_{it}	t
$32 \times 32 \times 32$	101 376	7	3.65	8	5.42	9	5.79	11	6.18
$32 \times 32 \times 64$	798 720	7	6.83	8	9.55	8	10.0	10	10.0
$32 \times 64 \times 64$		7	13.4	8	27.3	10	29.2	11	30.5
$64 \times 64 \times 64$		8	28.5	9	58.9	12	57.1	13	52.7
$64 \times 64 \times 128$		8	58.1	9	145	11	153	15	181
$64 \times 128 \times 128$	6 340 608	8	123						
$128 \times 128 \times 128$		8	252						

The final goal of this analysis is to compare the total computing times. The presented tests show that MIC(0) performs better in all cases excluding the strongest coefficient jump of $\zeta = 0.001$. Here is the place to note that the time to construct the preconditioner (for the recursive approximate factorization) is relatively big for the BoomerAMG implementation of the general purpose algebraic multigrid algorithms. The better times for BoomerAMG are indicated in Table 2 by gray background. The important conclusion is that MIC(0) provides an alternative choice for efficient solution of voxel FEM elliptic systems in cases of small to moderate coefficient jump. For stronger jumps and larger problems (if fit to the available RAM), the BoomerAMG will outperform the tested MIC(0) code.

4 Parallel MIC(0)

As was already mentioned, BoomerAMG has also a parallel implementation. What is not so popular is the parallel algorithm for MIC(0) preconditioning of Rannacher-Turek FEM systems. The last section of this article is concerned with the recently developed parallel MIC(0) for 3D Rannacher-Turek problems. A separate article will be devoted to the comparative analysis of the parallel performance of MIC(0) and BoomerAMG.

4.1 The parallel algorithm

The idea of the algorithm is to apply the MIC(0) factorization on an auxiliary matrix B . The matrix B has a special block structure, which allows a scalable parallel implementation.

Following the standard FEM assembling procedure we write A in the form $A = \sum_{e \in \omega_h} L_e^T A_e L_e$, where A_e is the element stiffness matrix, L_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 :

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

The local numbering follows the pairs of the opposite nodes of the reference element. The diagonal entries of B_e are modified to hold the rowsum criteria. Assembling the locally defined matrices B_e we get the global matrix $B = \sum_{e \in \omega_h} L_e^T B_e L_e$.

The sparsity structure of the matrices A and B is illustrated by Fig. 3. Lexicographic node numbering is used. The important property of the matrix B is that its diagonal blocks are diagonal matrices. This allows a well scalable parallel implementation, see [2,3,17], which is confirmed by the tests presented at the end of this section.

4.2 Convergence tests

The definition of B ensures the uniform spectral condition number estimate $\kappa(B^{-1}A) = O(1)$. Here we compare the convergence of the sequential MIC(0) and the parallel variant, i.e., MIC(0) applied to the auxiliary matrix B . Diagonal compensation is used for removing the positive offdiagonal entries to ensure a stable MIC(0) factorization of A in the sequential algorithm. The number of iterations for both methods are collected in Table 3

Table 3. Number of iterations for MIC(0) and Parallel MIC(0)

$n_1 \times n_2 \times n_3$	MIC(0)	Parallel MIC(0)
$32 \times 32 \times 32$	23	27
$64 \times 64 \times 64$	33	35
$128 \times 128 \times 128$	46	47

As we see, the convergence is very similar. What is important to note is that the computational complexity of one PCG iteration is cheaper for the second variant because B is considerably sparser than A .

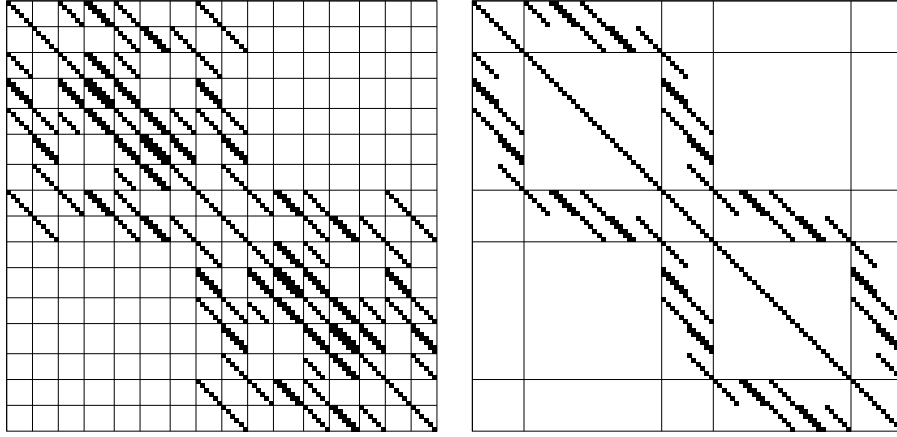


Fig. 3. Sparsity structure of the matrix A on the left and matrix B on the right, for the division of Ω into $2 \times 2 \times 6$ hexahedrons. Non-zero elements are drawn with small squares.

Remark 2. As seen from Tables 1-3, the sequential tests presented in Section 3.3 are performed using the modified (parallel) version of MIC(0).

4.3 Parallel tests

The parallel MIC(0) algorithm was programmed using the Message Passing Interface library (MPI). The presented tests are performed on “IBM SP Cluster 1600” made of 64 nodes p5-575 interconnected with a pair of connections to the Federation HPS (High Performance Switch). Each p5-575 node contains 8 SMP processors Power5 at 1.9GHz and 16GB of RAM. Based on the conclusions from the previous subsections we concentrate here on the parallel speedups and efficiencies which are presented in Table 4. The good scalability of the algorithm is well expressed for the larger of the test problems. Let us note

Table 4. Parallel speedups and efficiencies

$n_1 \times n_2 \times n_3$	n_p	Speedup	Efficiency
$32 \times 32 \times 32$	2	2.00	1.00
	4	3.05	0.76
	8	3.58	0.45
	16	7.09	0.44
$64 \times 64 \times 64$	2	1.95	0.97
	4	3.58	0.89
	8	6.42	0.80
	16	10.57	0.66
$128 \times 128 \times 128$	2	1.94	0.97
	4	3.56	0.89
	8	6.94	0.86
	16	13.14	0.82

that the speedups and efficiencies of the parallel MIC(0) algorithm are practically independent of the number of iterations.

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