PRECONDITIONING BY APPROXIMATE SCHUR COMPLEMENTS ON HIERARCHICAL GRIDS

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Abstract. We present an algebraic multilevel preconditioning for M-matrices arising from finite-difference discretization of three-dimensional elliptic operators.

For the Poisson model problem with Dirichlet boundary conditions we show that the condition number of the preconditioned system is bounded by $O(h^{-\frac{16}{25}})$, which is better than the bound $O(h^{-1})$ for the standard modified incomplete LU factorization (MILU).

Our strategy for dropping fill-in terms during the incomplete factorization process is based on a special ordering of the gridpoints. The Schur complements that result from blockwise elimination of the unknowns refer to a sequence of hierarchical grids and we approximate the corresponding operators by simpler ones until we reach a final coarsest grid. For the remaining unknowns we use complete Gaussian elimination. This procedure results in a preconditioner that is well suited for parallel architectures.

Key Words. Algebraic Multigrid Methods, Approximate Schur Complement Preconditioners

1. Introduction. Iterative methods for solving large, sparse systems of linear equations need efficient preconditioning. For matrices arising from discretization of elliptic boundary value problems, incomplete LU (or Cholesky) factorization produces preconditioners frequently used in practice. Multilevel methods, on the other hand, solve many problems of that kind with less computational work. This paper combines both ideas; it discusses a preconditioner based on incomplete factorization and a multilevel ordering of the unknowns. It improves bounds on the condition number in the three-dimensional case.

For elliptic model problems, the condition number of systems preconditioned by conventional incomplete factorizations grows as $O(h^{-2})$ or $O(h^{-1})$, see e.g. [7], [8] and [5]. A specific ordering of the unknowns, introduced by Brand [4], improved the asymptotic bound to $O(h^{-\frac{1}{2}})$ in the two-dimensional case. Refining the estimates, Ciarlet [6] bounded the relative condition number by $O(h^{-\frac{1}{3}})$. Their preconditioners, while strictly within the framework of incomplete factorization, can be compared to a V-cycle in an algebraic multigrid method. Axelsson and Eijkhout investigated in their work [1] also W-cycles realized by employment of second order matrix polynomials. They showed that an alternating use of first and higher degree polynomials on different levels leads to a spectrally equivalent preconditioner of optimal order of computational complexity.

In this paper we discuss three-dimensional problems. For the analysis of our method we consider the Poisson equation on the unit cube with Dirichlet boundary conditions:

$$-\Delta u = f \quad \text{on} \quad \Omega = (0,1)\times(0,1)\times(0,1) \tag{1}$$

$$u = 0 \quad \text{on} \quad \Gamma = \partial\Omega \tag{2}$$

A second order difference approximation of (1)–(2) (7–point formula) on a uniform $N\times N\times N$–grid

$$G^h := \{(ih, jh, kh) \mid 1 \le i,j,k \le N\}$$

with meshsize $h = \frac{1}{N+1}$ leads us to a system of linear equations:

$$A \cdot \mathbf{u} = \mathbf{b} \tag{3}$$

It is convenient to represent the solution vector $\mathbf{u}$ by a triply indexed array

$$\mathbf{u} = (u_{ijk}) = u(ih, jh, kh) \quad (1 \le i, j, k \le N).$$

Numerical tests for more general problems will be given in the last section.

As for basic iterative schemes we consider a splitting

$$A = \tilde{A} - R, \tag{4}$$

where $\tilde{A}$ is a close approximation of A, which can easily be inverted. We will construct the preconditioner $\tilde{A} = L \cdot U$ by modified incomplete factorization so that the lower and upper triangular factors L and U are also sparse matrices, that is, the number of nonzero entries is proportional to the number of equations.

2. Ordering of the gridpoints. In this section we will illustrate an ordering strategy for the gridpoints of an $L \times M \times N$–grid G^0, i.e., the cartesian product graph of three paths of length $L-1$, $M-1$ and $N-1$. Of course this algorithm induces an ordering for any subgrid of G^0.

We start with the formal definition of a nested sequence of grids G^p with increasing meshsize $2^p h$ $(p = 0, 1, 2, 3, \ldots)$:

$$\begin{aligned} G^0 &:= G^h \\ G^p &:= \{(ih, jh, kh) \in G^0 \mid i, j, k \equiv 1 (mod\ 2^p)\} \quad \text{for } p \ge 1 \end{aligned}$$

In this definition the point (h, h, h) is element of all grids G^p $(p \ge 0)$. Next we associate with each grid G^p $(p \ge 1)$ four sets of indices:

$$\begin{aligned} B^p &:= \{(i,j,k) \mid (ih, jh, kh) \in G^p : 1 \le i, j, k \le N\} \\ R^p_{(1)} &:= \{(i,j,k) \mid \exists (i_p, j_p, k_p) \in B^p : d((i,j,k),(i_p,j_p,k_p)) = 2^{p-1}\} \\ R^p_{(2)} &:= \{(i,j,k) \mid \exists (i_p, j_p, k_p) \in B^p : d((i,j,k),(i_p,j_p,k_p)) = 2^{p-1}\sqrt{2}\} \\ R^p_{(3)} &:= \{(i,j,k) \mid \exists (i_p, j_p, k_p) \in B^p : d((i,j,k),(i_p,j_p,k_p)) = 2^{p-1}\sqrt{3}\} \end{aligned}$$

Here $d(.,.)$ symbolizes the Euclidian norm. Thus $R^p_{(1)}$ consists of those triples that have shortest distance 2^{p-1} to a triple in B^p. For $R^p_{(2)}$ and $R^p_{(3)}$ these characteristic distances are $2^{p-1}\sqrt{2}$ and $2^{p-1}\sqrt{3}$ respectively.

Remark. The sets $R^p_{(r)}, B^p$ are disjoint $(p = 1, 2, 3, \ldots;\ r = 1, 2, 3)$ and

$$\bigcup_{1 \le p \le s} \left(R^p_{(1)} \cup R^p_{(2)} \cup R^p_{(3)} \right) \cup B^s = \{(i,j,k) \mid 1 \le i, j, k \le N\}$$

Now an s-step ordering assigns the numbers $1, 2, 3, \ldots, N^3$ to the gridpoints of G^0 according to the following nested loop:

```
for p = 1 to s do
  for r = 1 to 3 do
    for all points in R^p_(r)
    assign next number
  end for
end for
```

for all points in B^s
assign next number

Thereby our convention, which is of course not necessary, is to perform a natural ordering of the sets $R^p_{(r)}$ and B^s, that is, a numbering first in the direction from east to west (i) then from south to nord (j) and, finally, from down to up (k) beginning in the down-south-east corner. Table 1 shows a two-step ordering.

TABLE 1
A two-step ordering of a $5{\times}5{\times}5$*–cube*

k=1

120	11	102	12	121
8	81	9	82	10
100	6	115	7	101
3	79	4	80	5
118	1	99	2	119

k=2

19	71	20	72	21
58	93	59	94	60
16	69	17	70	18
55	91	56	92	57
13	67	14	68	15

k=3

105	32	114	33	106
29	85	30	86	31
111	27	117	28	112
24	83	25	84	26
103	22	113	23	104

k=4

40	77	41	78	42
64	97	65	98	66
37	75	38	76	39
61	95	62	96	63
34	73	35	74	36

k=5

124	53	110	54	125
50	89	51	90	52
108	48	116	49	109
45	87	46	88	47
122	43	107	44	123

3. Approximation of the Schur complements.

Before we begin to construct our modified incomplete Schur complement factorization (MISCLU) of the matrix A let us make clear the notation. Strictly speaking, we deal with equivalence classes of matrices, where members of the same equivalence class differ only by a permutation of corresponding rows and columns. For example, we denote by A its equivalence class and also the stencil that generated A, i.e.,

$$A : u_{ijk} \to 6u_{ijk} - u_{(i+1)jk} - u_{(i-1)jk} - u_{i(j+1)k} - u_{i(j-1)k} - u_{ij(k+1)} - u_{ij(k-1)}$$

Additionally the common stencil arithmetic will be used.

So let us now consider a one-step ordering of the matrix A in (3):

$$A = \begin{pmatrix} 6I & -F \\ -F^T & 6I \end{pmatrix}$$

Elimination of the unknowns with indices in $R^1_{(1)}$ yields the decomposition

$$A = \begin{pmatrix} I & \\ -\frac{1}{6}F^T & I \end{pmatrix} \cdot \begin{pmatrix} 6I & -F \\ & B_1 \end{pmatrix}$$

with the Schur complement $B_1 = 6I - \frac{1}{6}F^T F$. To give a formal description of the following elimination steps we define some stencils:

$$
\begin{aligned}
J_x : \mathbf{u} &\rightarrow J_x(\mathbf{u}) \\
u_{ijk} &\rightarrow u_{(i+1)jk} + u_{(i-1)jk}
\end{aligned}
$$

$$
\begin{aligned}
K_{x^2+y^2+z^2} &= J_x^2 + J_y^2 + J_z^2 - 6I \\
K_{x^2+y^2} &= J_x^2 + J_y^2 - 4I \\
M_{xy} &= J_x J_y \\
M_{xyz} &= J_x J_y J_z \\
M_{x^2y^2} &= \left(J_x^2 - 2I\right)\left(J_y^2 - 2I\right) \\
M_{x^2y^2z^2} &= \left(J_x^2 - 2I\right)\left(J_y^2 - 2I\right)\left(J_z^2 - 2I\right)
\end{aligned}
$$

$$
J_y, J_z, K_{y^2+z^2}, K_{x^2+z^2}, M_{yz}, M_{xz}, M_{y^2z^2}, M_{x^2z^2} \quad \text{analog.}
$$

In points where some arm of a stencil reaches (or crosses) the boundary the operator has to be modified according to the specific boundary condition. Then B_1 has the form

$$
\begin{pmatrix}
\frac{16}{3}I - \frac{1}{6}K_{y^2+z^2} & -\frac{1}{6}M_{xy} & -\frac{1}{6}M_{xz} & -J_x & -\frac{1}{3}M_{yz} \\
-\frac{1}{6}M_{xy}^T & \frac{16}{3}I - \frac{1}{6}K_{x^2+z^2} & -\frac{1}{6}M_{yz} & -J_y & -\frac{1}{3}M_{xz} \\
-\frac{1}{6}M_{xz}^T & -\frac{1}{6}M_{yz}^T & \frac{16}{3}I - \frac{1}{6}K_{x^2+y^2} & -J_z & -\frac{1}{3}M_{xy} \\
-J_x^T & -J_y^T & -J_z^T & 6I & 0 \\
-\frac{1}{3}M_{yz}^T & -\frac{1}{3}M_{xz}^T & -\frac{1}{3}M_{xy}^T & 0 & 5I - \frac{1}{6}K_{x^2+y^2+z^2}
\end{pmatrix}.
$$

We replace B_1 by $\tilde{B}_1$:

$$
\begin{aligned}
\tilde{B}_1 &:= \begin{pmatrix}
\frac{10}{3}I & 0 & 0 & -J_x & -\frac{1}{3}M_{yz} \\
0 & \frac{10}{3}I & 0 & -J_y & -\frac{1}{3}M_{xz} \\
0 & 0 & \frac{10}{3}I & -J_z & -\frac{1}{3}M_{xy} \\
-J_x^T & -J_y^T & -J_z^T & 6I & 0 \\
-\frac{1}{3}M_{yz}^T & -\frac{1}{3}M_{xz}^T & -\frac{1}{3}M_{xy}^T & 0 & 5I - \frac{1}{6}K_{x^2+y^2+z^2}
\end{pmatrix} \\
&=: \begin{pmatrix}
\frac{10}{3}I & -D_2 \\
-D_2^T & C_2
\end{pmatrix}
\end{aligned}
$$

After elimination of the block of unknowns belonging to $R^1_{(2)}$ we have

$$
\tilde{B}_1 = \begin{pmatrix}
I & \\
-\frac{3}{10}D_2^T & I
\end{pmatrix} \cdot \begin{pmatrix}
\frac{10}{3}I & -D_2 \\
 & B_2
\end{pmatrix},
$$

with

$$
\begin{aligned}
B_2 &= \begin{pmatrix} \frac{21}{5}I - \frac{3}{10}K_{x^2+y^2+z^2} & -\frac{3}{10}M_{xyz} \\ -\frac{3}{10}M_{xyz}^T & \frac{23}{5}I - \frac{3}{10}K_{x^2+y^2+z^2} - \frac{1}{30}(M_{x^2y^2} + M_{x^2z^2} + M_{y^2z^2} \end{pmatrix} \\
&=: \begin{pmatrix} \frac{21}{5}I - \frac{3}{10}K_{x^2+y^2+z^2} & -D_3 \\ -D_3^T & C_3 \end{pmatrix}.
\end{aligned}
$$

The approximation for B_2 is $\tilde{B}_2$:

$$
\tilde{B}_2 := \begin{pmatrix} \frac{12}{5}I & -D_3 \\ -D_3^T & C_3 \end{pmatrix}
$$

A factorization of $\tilde{B}_2$ with respect to the blocks $R^1_{(3)}$ and B^1 gives

$$
\tilde{B}_2 = \begin{pmatrix} I & \\ -\frac{1}{8}M_{xyz}^T & I \end{pmatrix} \cdot \begin{pmatrix} \frac{12}{5}I & -\frac{3}{10}M_{xyz} \\ & B_3 \end{pmatrix},
$$

with

$$
B_3 = \frac{43}{10}I - \frac{9}{20}K_{x^2+y^2+z^2} - \frac{13}{120}(M_{x^2y^2} + M_{x^2z^2} + M_{y^2z^2}) - \frac{3}{80}M_{x^2y^2z^2}.
$$

If we replace B_3 by $B_3^* := \frac{27}{10}I - \frac{9}{20}K_{x^2+y^2+z^2}$ then the error matrix R of (4) has the representation

$$
R = \begin{pmatrix}
2I - \frac{1}{6}K_{y^2+z^2} & -\frac{1}{6}M_{xy} & -\frac{1}{6}M_{xz} & 0 & 0 \\
-\frac{1}{6}M_{xy}^T & 2I - \frac{1}{6}K_{x^2+z^2} & -\frac{1}{6}M_{yz} & 0 & 0 \\
-\frac{1}{6}M_{xz}^T & -\frac{1}{6}M_{yz}^T & 2I - \frac{1}{6}K_{x^2+y^2} & 0 & 0 \\
0 & 0 & 0 & \frac{9}{5}I - \frac{3}{10}K_{x^2+y^2+z^2} & 0 \\
0 & 0 & 0 & 0 & R^*
\end{pmatrix},
$$

where

$$
R^* = \frac{8}{5}I - \frac{13}{120}(M_{x^2y^2} + M_{x^2z^2} + M_{y^2z^2}) - \frac{3}{80}M_{x^2y^2z^2}.
$$

The remaining unknowns refer to the grid G^1 with meshsize $2h$, and the indices of the gridpoints are given by B^1. If we apply an s-step ordering ($s > 1$) to the matrix A in (3) we are able to continue this incomplete decomposition recursively until we reach a final coarsest grid G^s. There we perform a complete Cholesky factorization. It should be mentioned here that it is not necessary to replace 27–point stencils by 7–point stencils in all nodes of G^p ($p = 1, 2, \ldots, s-1$). We did so by the approximation B_3^* of B_3 on G^1. This will enable us to derive a first upper bound for the relative condition number of an s-step MISCLU preconditioner.

A proof for the existence of this type of modified incomplete factorizations can be found in [4]. It makes use of the assumption that A is a weakly diagonally dominant M-matrix. (A matrix $A = (a_{ij})$ is a M-matrix, if it is nonsingular, $A^{-1} \geq 0$ and $a_{ij} \leq 0$ for $i \neq j$.)

4. Spectral analysis.

4.1. Eigenvector bases for A and R. An important criterion for the convergence rate of iterative methods that are based on the splitting (4) is the condition number κ of $\tilde{A}^{-1}A$. Because the matrix A from (3) is symmetric positive definite the error matrix R of the MISCLU factorization described in Section 3 is symmetric positive semidefinite. Consequently we have

$$\kappa(\tilde{A}^{-1}A) \leq \rho(\tilde{A}^{-1}A) = \frac{1}{\rho(I - A^{-1}R)} = \frac{1}{1-\rho(A^{-1}R)}. \tag{5}$$

Therefore we are interested in a close upper bound for the largest eigenvalue λ_{max} of $A^{-1}R$.

An orthogonal set of eigenvectors for the discrete Dirichlet operator A consists of the N^3 vectors $\Phi^{(lmn)}$ $(1 \leq l,m,n \leq N)$ with components $\Phi^{(lmn)}_{ijk}$:

$$\Phi^{(lmn)}_{ijk} = \sin(\frac{i\pi l}{N+1})\sin(\frac{j\pi m}{N+1})\sin(\frac{k\pi n}{N+1}),\ 1 \leq i,j,k \leq N.$$

The underlying grid contains eight disjoint subgrids with double meshsize. Correspondingly we partition each vector $\Phi^{(lmn)}$ in

$$\Phi^{(lmn)} = (x_1^{(lmn)}, x_2^{(lmn)}, \ldots, x_8^{(lmn)})^T,$$

where $x_1^{(lmn)}, x_2^{(lmn)}, \ldots, x_8^{(lmn)}$ are the projections of $\Phi^{(lmn)}$ onto the eight coarse grids, respectively. We specify in Table 2 each grid by the index triple of one representative gridpoint.

TABLE 2
Correspondence between vectors and coarse subgrids

coarse subgrid	representative index triple
x_1	$(2,1,1)$
x_2	$(1,2,1)$
x_3	$(1,1,2)$
x_4	$(1,2,2)$
x_5	$(2,1,2)$
x_6	$(2,2,1)$
x_7	$(2,2,2)$
x_8	$(1,1,1)$

Now we are able to construct an eigenvector basis Ψ for R.

$$\begin{aligned}
\Psi_1^{(lmn)} &= (x_1^{(lmn)},0,0,0,0,0,0,0)^T \\
\Psi_2^{(lmn)} &= (0,x_2^{(lmn)},0,0,0,0,0,0)^T \\
&\vdots \\
\Psi_7^{(lmn)} &= (0,0,0,0,0,0,x_7^{(lmn)},0)^T \\
\Psi_8^{(lmn)} &= (0,0,0,0,0,0,0,x_8^{(lmn)})^T
\end{aligned}$$

For $1 \leq l,m,n \leq \frac{N}{2}$ let $l' = N - l + 1,\ m' = N - m + 1,\ n' = N - n + 1$. Then every vector $\Psi_t^{(lmn)}$ $(1 \leq t \leq 8)$ is a linear combination of the eight vectors $\Phi^{(lmn)}, \Phi^{(l'mn)}, \ldots, \Phi^{(l'm'n')}$. (This can easily be seen if one uses the identity $\sin(\frac{i\pi l}{N+1}) = (-1)^{i+1}\sin(\frac{i\pi l'}{N+1})$.) The bases Φ and Ψ are related through the orthogonal transformation

$$
\begin{pmatrix} \Psi_1^{(lmn)} \\ \Psi_2^{(lmn)} \\ \Psi_3^{(lmn)} \\ \Psi_4^{(lmn)} \\ \Psi_5^{(lmn)} \\ \Psi_6^{(lmn)} \\ \Psi_7^{(lmn)} \\ \Psi_8^{(lmn)} \end{pmatrix} = S \cdot \begin{pmatrix} \Phi^{(lmn')} \\ \Phi^{(lm'n)} \\ \Phi^{(l'mn)} \\ \Phi^{(l'm'n)} \\ \Phi^{(l'mn')} \\ \Phi^{(lm'n')} \\ \Phi^{(l'm'n')} \\ \Phi^{(lmn)} \end{pmatrix}, \tag{6}
$$

where

$$
S = \frac{1}{8} \cdot \begin{pmatrix} 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.
$$

For the subspace spanned by the eigenvectors

$$\Phi^{(lmn')}, \Phi^{(lm'n)}, \Phi^{(l'mn)}, \Phi^{(l'm'n)}, \Phi^{(l'mn')}, \Phi^{(lm'n')}, \Phi^{(l'm'n')}, \Phi^{(lmn)},$$

or alternatively via the transformation (6), by the eigenvectors

$$\Psi_1^{(lmn)}, \Psi_2^{(lmn)}, \Psi_3^{(lmn)}, \Psi_4^{(lmn)}, \Psi_5^{(lmn)}, \Psi_6^{(lmn)}, \Psi_7^{(lmn)}, \Psi_8^{(lmn)},$$

the corresponding diagonalized parts of A and R are given by

$$
\begin{aligned}
A^{(lmn)} &= diag[6 - 2(u + v - w), 6 - 2(u - v + w), 6 - 2(-u + v + w) \\
&, \quad 6 - 2(-u - v + w), 6 - 2(-u + v - w), 6 - 2(u - v - w) \\
&, \quad 6 - 2(-u - v - w), 6 - 2(u + v + w)] \\
R^{(lmn)} &= diag[0, 0, 0 \\
&, \quad \frac{8}{3} - \frac{2}{3}(uv + uw + v^2 + w^2), \frac{8}{3} - \frac{2}{3}(uv + vw + u^2 + w^2) \\
&, \quad \frac{8}{3} - \frac{2}{3}(uw + vw + u^2 + v^2), \frac{18}{5} - \frac{6}{5}(u^2 + v^2 + w^2) \\
&, \quad \frac{9}{15} - \frac{1}{15}(36u^2v^2w^2 + 8(u^2v^2 + u^2w^2 + v^2w^2) - 17(u^2 + v^2 + w^2))].
\end{aligned}
$$

Here we used the substitution $u = \cos(\frac{l\pi}{N+1}),\ v = \cos(\frac{m\pi}{N+1})$ and $w = \cos(\frac{n\pi}{N+1})$.

Remark. For the eigenvectors $\Phi^{(lmn)}$ $(1 \le l, m, n \le \frac{N}{2})$ the corresponding eigenvalues of the operators J_x, J_y and J_z are given by $2u$, $2v$ and $2w$ respectively. The eigenvalues for the other modes are the same except for the sign. Taking into account the construction of Ψ, we are able to calculate the eigenvalues of the more complicated operators involved in R in a simple way. For example the eigenvalues of

$$2I - \frac{1}{6}K_{y^2+z^2} - \frac{1}{6}M_{xy} - \frac{1}{6}M_{xz}$$

have the form:

$$2 - \frac{1}{6}\left(4v^2 + 4w^2 - 4\right) - \frac{1}{6}\left(2u2v\right) - \frac{1}{6}\left(2u2w\right) = \frac{8}{3} - \frac{2}{3}\left(uv + uw + v^2 + w^2\right)$$

4.2. Bounding the condition number. The special form of Φ and Ψ allows us to restrict our spectral analysis to the 8×8–matrices

$$S\ (A^{(lmn)})^{-1} S^{-1} R^{(lmn)}. \tag{7}$$

We were not able to find simple analytic expressions for the eigenvalues of (7). Nevertheless we established the sharp upper bound $\lambda_{max} \le \frac{31}{40}$ by using Gershgorin's theorem (with row sums). Therefore we get from inequality (5)

$$\kappa(\tilde{A}^{-1}A) \le \frac{40}{9} \tag{8}$$

The error matrix R from Section 3 was determined by a one-step MISCLU decomposition, thus assuming that the factorization of the approximated Schur complement B_3^* is done by complete Gaussian elimination. As already mentioned in the introduction the factors L and U of $\tilde{A}$ should be sparse. For the model problem on an $N\times M\times L$ cube we have the following lemma.

LEMMA 4.1. *Let A be the difference matrix with 7–point stencil that results from discretization of the model problem on an $N\times M\times L$–grid. (Without loss of generality we assume that $L \le M \le N$.) Then for $s := [\frac{1}{5}(\mathrm{ld}L + \mathrm{ld}M)]$ the number of nonzero entries in the lower and upper triangular factors L and U arising from an s-step MISCLU factorization is proportional to LMN.*

Proof. The grid corresponding to the completely factorized Schur complement B_{3s} is G^s. It contains $O\left(\frac{LMN}{2^{3s}}\right)$ gridpoints. Because of the 27–point coupling on this coarsest grid the bandwidth of B_{3s} is $O\left(\frac{LM}{2^{2s}}\right)$. Complete elimination at this level will cause $O\left(\frac{L^2M^2N}{2^{5s}}\right)$ fill-in terms in L and U. So the desired result is obtained if $\frac{L^2M^2N}{2^{5s}} = LMN$ or, equivalently, $s = [\frac{1}{5}(\mathrm{ld}L + \mathrm{ld}M)]$. $\square$

The next lemma is essential for our conditioning analysis.

LEMMA 4.2. *Let A, B and C be SPD matrices. Then*

$$\rho(AB) \le \rho(AC)\rho(C^{-1}B)$$

Proof.

$$\begin{aligned}\rho(AB) &= \sup_x \frac{(Cx,x)(Bx,x)}{(A^{-1}x,x)(Cx,x)}\\ &\leq \sup_x \frac{(Cx,x)}{(A^{-1}x,x)} \sup_x \frac{(Bx,x)}{(Cx,x)}\\ &= \rho(AC)\rho(C^{-1}B) \qquad \square\end{aligned}$$

We come to a first result. In the model problem (3) and for $s := [\frac{2}{5}\mathrm{ld}N]$ the relative condition number of the s-step MISCLU preconditioner $\tilde{A}_s$ can be estimated by

$$(9) \quad \rho(\tilde{A}_s^{-1}A) \leq \rho(\tilde{A}_s^{-1}\tilde{A}_{s-1}^{-1})\rho(\tilde{A}_{s-1}^{-1}\tilde{A}_{s-2}^{-1})\ldots\rho(\tilde{A}_1^{-1}A) \leq \left(\frac{40}{9}\right)^{\frac{2}{5}\mathrm{ld}N} \approx N^{0.861}.$$

This improves the asymptotic bound for the standard MILU factorization. An evaluation of the maximal eigenvalue on the first two steps of approximation indicates already that the factor $\frac{40}{9}$ in (9) is rather pessimistic. Table 3 shows the increase of the relative condition number $\kappa(\tilde{A}_s^{-1}A)$ from $s = 1$ to $s = 2$.

TABLE 3

Condition number $\dfrac{1}{1-\lambda_{max}}$

N	$s=1$	$s=2$
12	2.65	
16	2.74	
20	2.78	6.04
24	2.80	6.48
28		6.79
32		6.97

4.3. A better asymptotic bound. To get a closer estimate we start with the 27–point operator T_p on the grid G^p $(p = 1, 2, \ldots, s-1)$. We can express T_p in terms of our stencils from Section 3.

$$\begin{aligned}T_p &= (6a_p + 12b_p + 8c_p)I - a_p K_{x^m+y^m+z^m}\\ &- b_p(M_{x^m y^m} + M_{x^m z^m} + M_{y^m z^m}) - c_p M_{x^m y^m z^m}\end{aligned}$$

with

$$\begin{aligned}m &= m(p) = 2^p,\ p = 1, 2, 3\ldots,\\ a_1 &= \frac{9}{20},\ b_1 = \frac{13}{120},\ c_1 = \frac{3}{80},\\ a_{p+1} &= \frac{9a_p{}^2 + 29a_pb_p + 10a_pc_p + 24b_p{}^2 + 12b_pc_p}{20a_p + 24b_p},\\ b_{p+1} &= \frac{13a_p{}^2 + 51a_pb_p + 30a_pc_p + 36b_p{}^2 + 36b_pc_p}{120a_p + 144b_p},\\ c_{p+1} &= \frac{3a_p{}^2 + 9a_pb_p + 10a_pc_p + 12b_pc_p}{80a_p + 96b_p}.\end{aligned}$$

For $m = 2$ the stencils $K_{x^m+y^m+z^m}$, $M_{x^m y^m}$, $M_{x^m z^m}$, $M_{y^m z^m}$ and $M_{x^m y^m z^m}$ have already been defined in Section 3. In the more general case $m \geq 2$ they couple neighbors at distance mh, $m\sqrt{2}h$ and $m\sqrt{3}h$.

To obtain again a 27–point stencil on G^{p+1} we perform three Schur complement approximations. There are several possibilities of dropping (and keeping) fill-in terms during the incomplete factorization process. Our strategy can be summarized in the following way:
For nodes referring to $R^p_{(1)}$, $R^p_{(2)}$ and $R^p_{(3)}$ only keep those connections that are listed in Table 4.

Table 4
Coupling directions of the simplified operators

$R^p_{(r)}$	subset	coupling directions
$R^p_{(1)}$	–	n, s, e, w, u, d
$R^p_{(2)}$	$j \equiv 0(mod\ 2^p) \wedge k \equiv 0(mod\ 2^p)$	e, w, nu, nd, su, sd
$R^p_{(2)}$	$i \equiv 0(mod\ 2^p) \wedge k \equiv 0(mod\ 2^p)$	n, s, eu, ed, wu, wd
$R^p_{(2)}$	$i \equiv 0(mod\ 2^p) \wedge j \equiv 0(mod\ 2^p)$	u, d, ne, nw, se, sw
$R^p_{(3)}$	–	neu, nwu, seu, swu, ned, nwd, sed, swd

For example the entry “neu” in the column “coupling directions” means that the corresponding operator couples each element with its neighbor in the direction north-east-up on the grid G^p.

To apply the same spectral analysis as before we considered the ratio of the weights a_p, b_p and c_p in T_p. A careful study of the normalized sequences

$$\tilde{a}_{p+1} = \frac{12\left(9\tilde{a}_p^2 + 29\tilde{a}_p\tilde{b}_p + 10\tilde{a}_p\tilde{c}_p + 24\tilde{b}_p^2 + 12\tilde{b}_p\tilde{c}_p\right)}{143\tilde{a}_p^2 + 477\tilde{a}_p\tilde{b}_p + 360\tilde{b}_p^2 + 210\tilde{a}_p\tilde{c}_p + 252\tilde{b}_p\tilde{c}_p} \tag{10}$$

$$\tilde{b}_{p+1} = \frac{2\left(13\tilde{a}_p^2 + 51\tilde{a}_p\tilde{b}_p + 30\tilde{a}_p\tilde{c}_p + 36\tilde{b}_p^2 + 36\tilde{b}_p\tilde{c}_p\right)}{143\tilde{a}_p^2 + 477\tilde{a}_p\tilde{b}_p + 360\tilde{b}_p^2 + 210\tilde{a}_p\tilde{c}_p + 252\tilde{b}_p\tilde{c}_p} \tag{11}$$

$$\tilde{c}_{p+1} = \frac{3\left(3\tilde{a}_p^2 + 9\tilde{a}_p\tilde{b}_p + 10\tilde{a}_p\tilde{c}_p + 12\tilde{b}_p\tilde{c}_p\right)}{143\tilde{a}_p^2 + 477\tilde{a}_p\tilde{b}_p + 360\tilde{b}_p^2 + 210\tilde{a}_p\tilde{c}_p + 252\tilde{b}_p\tilde{c}_p} \tag{12}$$

showed a very rapid convergence (i.e., we got a Lipschitz constant less than 0.56 for use with the fix-point theorem of Banach).

Now we need an upper bound for the largest eigenvalue of (13), the counterpart of (7).

$$S\ (B^p)^{-1} S^{-1} R^p \tag{13}$$

With respect to the eigenvector bases Φ and Ψ the diagonal matrices B^p and R^p are given by

$$
\begin{aligned}
B^p &= diag[6a_p + 12b_p + 8c_p \\
&- 2a_p(+u+v-w) - 4b_p(+uv-uw-vw) - 8c_p(-uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(+u-v+w) - 4b_p(-uv+uw-vw) - 8c_p(-uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(-u+v+w) - 4b_p(-uv-uw+vw) - 8c_p(-uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(-u-v+w) - 4b_p(+uv-uw-vw) - 8c_p(+uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(-u+v-w) - 4b_p(-uv+uw-vw) - 8c_p(+uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(+u-v-w) - 4b_p(-uv-uw+vw) - 8c_p(+uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(-u-v-w) - 4b_p(+uv+uw+vw) - 8c_p(-uvw) \\
&, \ 6a_p + 12b_p + 8c_p \\
&- 2a_p(+u+v+w) - 4b_p(+uv+uw+vw) - 8c_p(+uvw)] \\
R_2^{(lmn)} &= diag[12b_p + 8c_p - 4b_p(uv+uw+vw) - 8c_p(uvw) \\
&, \ 12b_p + 8c_p - 4b_p(uv+uw+vw) - 8c_p(uvw) \\
&, \ 12b_p + 8c_p - 4b_p(uv+uw+vw) - 8c_p(uvw) \\
&, \ \frac{8}{3}a_p + 8b_p + 8c_p - \frac{2}{3}a_p(uv+uw+v^2+w^2) \\
&- 4b_p(uv+uw) - 8c_p(uvw) \\
&, \ \frac{8}{3}a_p + 8b_p + 8c_p - \frac{2}{3}a_p(uv+vw+u^2+w^2) \\
&- 4b_p(uv+vw) - 8c_p(uvw) \\
&, \ \frac{8}{3}a_p + 8b_p + 8c_p - \frac{2}{3}a_p(uw+vw+u^2+v^2) \\
&- 4b_p(uw+vw) - 8c_p(uvw) \\
&, \ \frac{18{a_p}^2}{5a_p + 6b_p} + 12b_p \\
&- \frac{6{a_p}^2}{5a_p + 6b_p}(u^2+v^2+w^2) - 4b_p(uv+uw+vw), \ 0]
\end{aligned}
$$

We did not get analytic expressions for the eigenvalues of (13). A numerical analysis led us to the bound

$$
\frac{1}{1-\lambda_{max}} \le 2^{\frac{8}{5}}, \tag{14}
$$

which improves (9). Table 5 contains the normalized weights of the 27–point stencils T_p on the grids G^p and the relative condition number for a one step MISCLU approximation at these levels.

TABLE 5
Growth factor of the condition number for different levels

p	$\tilde{a}_p$	$\tilde{b}_p$	$\tilde{c}_p$	$1/(1-\lambda_{max})$
0	1.000000	0.000000	0.000000	2.7403
1	0.755245	0.181818	0.062937	2.9906
2	0.734791	0.203061	0.062148	3.0288
3	0.735295	0.203838	0.060866	3.0313
4	0.735566	0.203727	0.060707	3.0312
5	0.735596	0.203705	0.060699	3.0312
6	0.735597	0.203704	0.060700	3.0312
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

So we formulate our main result.

THEOREM 4.3. *For the model problem (3) on an $N \times N \times N$–cube, let $s := [\frac{2}{5}\mathrm{ld}N]$. Then the relative condition number of the s-step MISCLU preconditioner is bounded by $N^{\frac{16}{25}}$.*

Proof. This follows immediately by application of Lemma 4.2 (see (9)). □

5. Numerical results. To confirm the theoretical results of the previous section and to show the performance of our new preconditioning technique we give three test problems.

In each case we used the preconditioned conjugate gradient method to solve the system of difference equations. The right-hand side of (3) corresponds to the solution

$$u(x_j, y_j, z_j) = (1 - \cos(2\pi x_j))(1 - \cos(2\pi y_j))(1 - \cos(2\pi z_j))\exp(-2(x_j + y_j + z_j))$$

at a point (x_j, y_j, z_j). The starting vector has random elements in $[0, 1]$. The stopping criterion for the iteration was $\|r^k\|_2/\|r^0\|_2 \leq 10^{-6}$.

We compared the following three preconditioners.

MISCLU(2): Our method of (repeated) incomplete Schur complement decomposition using two approximation steps (i.e., complete Gaussian elimination for the unknowns of G^2).

MIC(2) and MIC(3): Second and third degree modified incomplete Cholesky factorization based on natural ordering. These methods take into account fill-in terms up to the order two and three, respectively. Entries in those positions where A has nonzero elements have order one. The terms of higher order form additional off-diagonal bands in L and U.

First test problem. (Dirichlet boundary conditions.) This is the model problem (1)–(2) discretized on an $N \times N \times N$–grid.

Second test problem. (Mixed boundary conditions.) As Problem 1 but on the up, north and east faces Neumann boundary conditions.

Third test problem. (Jumping coefficients.) The same domain and boundary conditions as in Problem 2 but instead of (1) we consider now the equation

$$-q\Delta u \;=\; f,$$

where

$$\begin{array}{lll} q = & 1 & \text{for} \quad (x,y,z) \in \Omega_1 := (0,\frac{1}{2})\times(0,\frac{1}{2})\times(0,\frac{1}{2}), \text{ and} \\ q = & 100 & \text{for} \quad (x,y,z) \in \Omega_2 := \Omega\backslash\Omega_1. \end{array}$$

We tested a sequence of uniform discretizations with increasing fineness going up from $8\times8\times8$ to $40\times40\times40$ gridpoints. The number of nonzero off-diagonal entries in the factors L and U is listed in Table 6.

TABLE 6
Number of nonzero offdiagonal entries in the triangular factors L and U

N	MISCLU(2)	MIC(2)	MIC(3)
8	2519	2520	4214
12	9287	9108	15730
16	23177	22320	39150
20	46787	44460	78698
24	83754	77832	138598
28	136204	124740	223074
32	210593	187488	336350
36	306605	268380	482650
40	436997	369720	666198

The resulting number of cg-iterations for the test problems 1, 2 and 3 is summarized in Tables 7, 8 and 9 respectively.

We see in all three examples that for sufficiently large problems our new preconditioner performs better than the standard MILU factorization.

TABLE 7
Number of cg-iterations for the first test problem

N	MISCLU(2)	MIC(2)	MIC(3)
8	10	8	7
12	12	11	9
16	14	13	11
20	15	15	13
24	16	17	14
28	16	19	16
32	17	21	17
36	17	22	19
40	17	24	20

TABLE 8
Number of cg-iterations for the second test problem

N	MISCLU(2)	MIC(2)	MIC(3)
8	11	10	9
12	14	13	11
16	15	16	14
20	16	18	16
24	16	21	18
28	17	23	20
32	17	25	22
36	17	28	24
40	17	30	26

TABLE 9
Number of cg-iterations for the third test problem

N	MISCLU(2)	MIC(2)	MIC(3)
8	12	10	9
12	14	13	11
16	17	17	14
20	16	20	16
24	18	22	19
28	16	25	21
32	19	28	23
36	17	31	26
40	19	34	28

6. Conclusions. We have shown for the three-dimensional model problem that a multilevel ordering improves the preconditioner constructed by incomplete factorization. The asymptotic bound on the condition number in the three-dimensional case is weaker than in two dimensions ($O(h^{-\frac{16}{25}})$ versus $O(h^{-\frac{1}{3}})$), but still better than the $O(h^{-2})$ or $O(h^{-1})$ bounds for conventional incomplete factorizations.

Numerical experiments suggest that our estimates hold not only for the simple model problem (1)–(2) but for Neumann boundary conditions or jumping coefficients as well.

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