

MULTIGRID INCOMPLETE FACTORIZATION METHODS IN KRYLOV SUBSPACES

V. P. Il'in*

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The paper studies multigrid methods for solving systems of linear algebraic equations resulting from the seven-point discretization of the three-dimensional Dirichlet problem for an elliptic differential equation of the second order in a parallelepipedal domain on a regular grid. The algorithms suggested are presented as special iteration processes of incomplete factorization in Krylov subspaces with a hierarchical recursive vector structure that corresponds to a sequence of embedded grids and gives rise to a block tridiagonal recursive representation of the coefficient matrix of the original linear algebraic system. The convergence of iterations is enhanced by using the principle of compensation of the row sums and also the symmetric successive block overrelaxation. An arbitrary m -grid method is defined recursively, based on the two-grid method. For simplicity, the algorithms are considered for linear systems with Stieltjes coefficient matrices. Issues related to generalization of the algorithms to larger classes of problems and, in particular, those with unsymmetric matrices are discussed. Bibliography: 22 titles.

1. INTRODUCTION

Multigrid methods for solving systems of linear algebraic equations (SLAEs) arising from approximation of multidimensional boundary-value problems are of special importance in computational algebra because they result in asymptotically optimal algorithms, for which the amount of computer resources is proportional to the number of unknowns. In the pioneering works by Fedorenko [1] and Bakhvalov [2], these approaches were based on spectral principles with separate suppression of error in low- and high-frequency components. In a large number of subsequent publications, they were developed in geometric terms (in particular, the so-called cascade method was considered [3–5]), in algebraic terms (Algebraic Multi Grid – AMG), and in combinatorial terms. The latter approach is based on transformations of grid graphs (e.g., with the formation of spanning trees, see [6–20] and the references therein). The traditional approaches are based on iterative processes using smoothing, reduction (or restriction), coarse grid correction, and prolongation operators. Various methodological results were also accompanied by software development and numerous practical applications, including parallelization of algorithms. In this paper, we investigate iterative multigrid methods as a special class of preconditioned Krylov type algorithms applied to linear systems with hierarchically or recursively ordered grid nodes.

The paper is organized as follows. In Sec. 2, we describe a general scheme for constructing algebraic multigrid methods based on a recursive ordering of vector components. Section 3 presents preconditioned iterative methods in Krylov subspaces in application to the AMG in question. Section 4 considers multigrid incomplete factorization methods for solving seven-point SLAEs resulting from approximation of three-dimensional boundary-value problems on a parallelepipedal grid. In the final section, possible generalizations of the algorithms proposed to a wider class of problems are discussed.

2. GENERAL SCHEME OF MULTIGRID APPROACHES

Consider a linear algebraic system

$$Au=f, \quad A=\{a_{t,s}\} \in \mathcal{R}^{N,N}, \quad u=\{u_t\}, \quad f=\{f_t\} \in \mathcal{R}^N, \quad (1)$$

*Institute of Computational Mathematics and Mathematical Geophysics SB RAS, e-mail: il'in@sscc.ru.

with a symmetric positive definite (s.p.d.) matrix resulting from approximation of a three-dimensional boundary-value problem for a second-order elliptic differential equation using a finite difference, a finite volume, or a finite element method, see [21]. For simplicity, the parallelepiped-shaped computational domain Ω will be considered, and its discretization will be carried out using a parallelepipedal grid consisting of m embedded grids of the same topological structure:

$$\Omega^h = \Omega_1^h \supset \Omega_2^h \supset \dots \supset \Omega_m^h.$$

For simplicity, it is assumed that the boundary Γ of the domain Ω passes along the faces of the coarsest grid Ω_m^h , and the finer grid of the l th level Ω_l^h is obtained by drawing new coordinate planes bisecting all grid intervals of the coarser grid Ω_{l+1}^h , $l = 1, 2, \dots, m - 1$. A possible generalization of the approaches considered to other types of domains and grids will be described below.

The common up-to-date approach to constructing multigrid algorithms is based on iterative processes in Krylov subspaces with preconditioning matrices corresponding to recursive data structures. We will investigate node-type SLAEs. In this case, every node of each of the grids corresponds to a single component of a given and an unknown vectors, and they are numbered in accordance with a recursive multilevel ordering of the nodes of the embedded grids. The set of nodes and vector components of the original SLAE on the finest (initial) grid is represented in the following two-level form:

$$\begin{aligned} \Omega^h &= \Omega_1^h = \widehat{\Omega}_1^h \cup \check{\Omega}_1^h, & \check{\Omega}_1^h &= \Omega_2^h, \\ u &= u^{(1)} = \left((\widehat{u}^{(1)})^\top, (\check{u}^{(1)})^\top \right)^\top, & \check{u}^{(1)} &= u^{(2)}. \end{aligned} \quad (2)$$

The second-level subsets and subvectors can be decomposed in a similar way. As a result, we obtain the following multilevel representations for m grids:

$$\begin{aligned} \Omega^h &= \Omega_1^h = \widehat{\Omega}_1^h \cup \widehat{\Omega}_2^h \dots \cup \widehat{\Omega}_{m-1}^h \cup \Omega_m^h, \\ u &= u^{(1)} = \left((\widehat{u}^{(1)})^\top, (\widehat{u}^{(2)})^\top, \dots, (\widehat{u}^{(m-1)})^\top, (u^{(m)})^\top \right)^\top, \end{aligned}$$

where every set of the l th level is split into two subsets, one of which belongs to the next level and is also split into two parts:

$$\Omega_l^h = \widehat{\Omega}_l^h \cup \check{\Omega}_l^h, \quad \check{\Omega}_l^h = \Omega_{l+1}^h, \quad u^{(l)} = \left((\widehat{u}^{(l)})^\top, (\check{u}^{(l)})^\top \right)^\top, \quad \check{u}^{(l)} = u^{(l+1)}.$$

The right-hand-side vector f is written in a similar hierarchical form as $f = f^{(1)} = (\widehat{f}^{(1)}, \check{f}^{(1)})$, $\check{f}^{(1)} = f^{(2)}$. In the case of the two-level node ordering (2) and the corresponding splitting into subvectors, the original linear system takes the following block form:

$$Au = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} \begin{bmatrix} \widehat{u}^{(1)} \\ u^{(2)} \end{bmatrix} = \begin{bmatrix} \widehat{f}^{(1)} \\ f^{(2)} \end{bmatrix} = f. \quad (3)$$

The simplest method (in the general case, the major component of the multigrid method) is the two-grid variant. The essence of this variant is as follows. Upon some transformations, the subvector $(u^{(2)})^0$ is computed by solving system (3) by a direct method. Actually, an initial approximation of this subvector is found by approximately eliminating the subvector $\widehat{u}^{(1)}$. This initial approximation is refined in the course of subsequent iterations.

Given an initial vector u^0 and a subvector $(u^{(2)})^0 \in \mathbb{R}_{i,s}^{N_2}$, the first iterative guess for Eq. (3) can schematically be represented as $u = u^0 + P(u^{(2)})^0$, where $P \in \mathbb{R}^{N, N_2}$ is a prolongation operator. The operator can be constructed, for example, using interpolation from the coarse

grid to the fine one. Upon substituting this expression into SLAE (3) preliminary multiplied on the left by the restriction operator $R=P^\top$, we obtain the equation

$$A_c(u^{(2)})^0=R(f - Au^0)=Rr^0, \quad A_c=RAP, \quad (4)$$

where $A_c \in \mathbb{R}^{N_2, N_2}$ is a low-rank approximation of the matrix A associated with the coarse grid. The prolongation operator P is considered to be a matrix of full rank. Then we have

$$u=u^0 + B_2^{-1}r^0, \quad B_2^{-1}=PA_c^{-1}R=B_2^{-T}=(B_2^{-1})^T. \quad (5)$$

Here, the symmetric matrix $B_2 \in \mathbb{R}^{N, N}$ can be treated as a preconditioner for A . The inversion of B_2 actually requires solving the algebraic system (4) on the coarse grid, and the vector relation (5) provides a foundation for constructing two-grid iterative methods. In this case, from the methodological point of view, there is the following alternative: SLAE (4) can be solved either by a direct or by an iterative method. The second option leads to a two-level process, but, in this paper, we only consider the first option, which allows us to use embedded grids in a uniform way (provided that the structure of the matrix A_c is similar to that of the matrix A).

The above form of the two-grid method is as yet incomplete, and at every iteration it must be supplemented with a pre-smoothing and a post-smoothing operations. In matrix terms, this is done by replacing the preconditioner B_2^{-1} in (5) with the preconditioning matrix

$$\overline{B}_2^{-1}=S_2PA_c^{-1}RS_1, \quad S_1=S_2^\top.$$

Here, the operators S_1 and S_2 , whose specific form will be discussed below, must ensure that the matrix \overline{B}_2 is symmetric.

When using an m -grid algorithm, the subvectors $u^{(l)}$, $l=2, \dots, m-1$, are successively split, and the resulting SLAE to be solved can be represented in the following form:

$$Au=Au^{(1)}=\begin{bmatrix} A_{1,1} & A_{1,2} & 0 & & & \\ A_{2,1} & A_{2,2} & A_{2,3} & & & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & A_{m-1,m-1} & A_{m-1,m} & \\ 0 & \dots & 0 & A_{m,m-1} & A_{m,m} & \end{bmatrix} \begin{bmatrix} \widehat{u}^{(1)} \\ \widehat{u}^{(2)} \\ \vdots \\ \widehat{u}^{(m-1)} \\ u^{(m)} \end{bmatrix} = \begin{bmatrix} \widehat{f}^{(1)} \\ \widehat{f}^{(2)} \\ \vdots \\ \widehat{f}^{(m-1)} \\ f^{(m)} \end{bmatrix}. \quad (6)$$

It is important to observe that this system has a block tridiagonal coefficient matrix (this is a necessary requirement imposed on the grids constructed and the corresponding matrix blocks). Formally, system (6) only differs from (1) or (3) in the ordering of unknowns. Representing SLAE (6) in the two-by-two block form as

$$Au=\begin{bmatrix} \overline{A}_{1,1} & \overline{A}_{1,m-1} \\ \overline{A}_{m-1,1} & \overline{A}_{m,m} \end{bmatrix} \begin{bmatrix} \overline{u}^{(1)} \\ u^{(m)} \end{bmatrix} =f, \quad \overline{A}_{m-1,1}=\overline{A}_{1,m-1}^\top,$$

we can apply to it the principles of constructing multigrid preconditioned iterative algorithms, as it was done in Eqs. (4), (5) for the two-grid variant.

3. PRECONDITIONED CONJUGATE DIRECTION METHODS

In the problem statement with a recursive ordering of unknowns, the problem of constructing an iterative process reduces to finding a preconditioning matrix for the SLAE (6) and to applying a conjugate direction method in Krylov subspaces.

First consider a two-sided preconditioning based on a matrix that allows for an efficient Cholesky factorization,

$$B=L_BU_B, \quad B^{-1}=U_B^{-1}L_B^{-1}, \quad U_B=L_B^\top. \quad (7)$$

The preconditioned SLAE resulting from (1) is written as

$$\overline{A}\overline{u}=\overline{f}, \quad \overline{A}=L_B^{-1}AU_B^{-1}, \quad \overline{u}=U_Bu, \quad \overline{f}=L_B^{-1}f. \quad (8)$$

Krylov type iterative methods for solving the symmetric system (8) are then represented in the form

$$\begin{aligned} \overline{r}^0 &= \overline{f} - \overline{A}\overline{u}^0, \quad \overline{p}^0 = \overline{r}^0, \quad n = 0, 1, \dots: \quad \overline{u}^{n+1} = \overline{u}^n + \alpha_n \overline{p}^n = \overline{u}^0 + \alpha_0 \overline{p}^0 + \dots + \alpha_n \overline{p}^n, \quad (9) \\ \overline{r}^{n+1} &= \overline{f} - \overline{A}\overline{u}^{n+1} = \overline{r}^n - \alpha_n \overline{A}\overline{p}^n = \overline{r}^0 - \alpha_0 \overline{A}\overline{p}^0 - \dots - \alpha_n \overline{A}\overline{p}^n, \end{aligned}$$

where u^0 is an arbitrary initial guess, and \overline{p}^n are the direction vectors satisfying the following orthogonality conditions:

$$\left(\overline{A}^\gamma \overline{p}^n, \overline{p}^k \right) = \left(\overline{p}^n, \overline{p}^k \right)_\gamma = \rho_n^{(\gamma)} \delta_{k,n}, \quad \rho_n^{(\gamma)} = \left(\overline{p}^n, \overline{p}^n \right)_\gamma. \quad (10)$$

Here, $\delta_{k,n}$ is the Kronecker symbol, and the values $\gamma = 0, 1, 2$ correspond to the minimal error, conjugate gradient, and conjugate residual algorithms, respectively. This family of iterative processes, with the chosen hierarchical ordering of grid nodes and the corresponding structures of the coefficient and preconditioning matrices, will be referred to as the multigrid conjugate direction methods. Relations (9), (10) provide for minimization of the functionals $\left(\overline{r}^{n+1}, \overline{r}^{n+1} \right)_{\gamma-2}$ in the Krylov subspaces

$$\mathcal{K}_{n+1}(\overline{r}^0, \overline{A}) = \text{Span} \{ \overline{r}^0, \overline{A}\overline{r}^0, \dots, \overline{A}^n \overline{r}^0 \}, \quad (11)$$

and the following relations are valid:

$$\Phi_\gamma(\overline{r}^{n+1}) = \left(\overline{r}^{n+1}, \overline{r}^{n+1} \right)_{\gamma-2} = \Phi_\gamma(\overline{r}^0) - \sum_{k=0}^n (\sigma_k^{(\gamma)})^2 / \rho_k^{(\gamma)}, \quad \sigma_k^{(\gamma)} = \left(\overline{r}^0, \overline{p}^k \right)_{\gamma-1}.$$

For $\gamma = 1, 2$, these optimization properties are achieved by computing the iterative parameters and direction vectors via the following formulas:

$$\begin{aligned} \alpha_n^{(\gamma)} &= \sigma_n^{(\gamma)} / \rho_n^{(\gamma)}, \quad \overline{p}^0 = \overline{r}^0, \quad \overline{p}^{n+1} = \overline{r}^{n+1} + \beta_n^{(\gamma)} \overline{p}^n, \\ \beta_n^{(\gamma)} &= - \left(\overline{r}^{n+1}, \overline{p}^n \right)_\gamma / \rho_n^{(\gamma)} = \sigma_{n+1}^{(\gamma)} / \sigma_n^{(\gamma)}. \end{aligned} \quad (12)$$

For $\gamma = 0$, the above formulas are not applicable because they involve the inverse matrix \overline{A}^{-1} . An alternative approach to finding the direction vectors is to apply the Lanczos orthogonalization process. The coefficients $\alpha_n^{(0)}$ can be found from the representations of the error vectors $v^n = \overline{u} - u^n$ and the residual vectors $\overline{r}^n = \overline{A}v^n$ resulting from the following representation of the exact solution $\overline{u} = U_B u$:

$$\begin{aligned} \overline{u} &= \overline{u}^0 + \alpha_0^{(0)} \overline{p}^0 + \dots + \alpha_n^{(0)} \overline{p}^n + \dots, \\ v^n &= \alpha_n^{(0)} \overline{p}^n + \alpha_{n+1}^{(0)} \overline{p}^{n+1} + \dots, \\ \overline{r}^n &= \alpha_n^{(0)} \overline{A}\overline{p}^n + \alpha_{n+1}^{(0)} \overline{A}\overline{p}^{n+1} + \dots. \end{aligned}$$

Thus, we obtain

$$\alpha_n^{(0)} = (v^n, \overline{p}^n) / \rho_n^{(0)} = - \alpha_{n-1}^{(0)} (v^n, \overline{A}\overline{p}^{n-1}) / \rho_n^{(0)} = - \alpha_{n-1}^{(0)} (r^n, \overline{p}^{n-1}) / \rho_n^{(0)}.$$

It should be kept in mind that since $\sigma_0^{(0)} = (\overline{r}^0, \overline{A}^{-1} \overline{p}^0)$, the initial direction vector cannot be arbitrary and must be determined as follows:

$$\overline{p}^0 = \overline{A}\overline{r}^0, \quad \sigma_0^{(0)} = (\overline{r}^0, \overline{r}^0).$$

Now the Lanczos process for computing p^n is as follows:

$$\begin{aligned}\bar{p}^0 &= \bar{A}r^0, & \bar{p}^1 &= \bar{A}\bar{p}^0 - \bar{\alpha}_0 p^0, \\ n = 1, 2, \dots &: & \bar{p}^{n+1} &= \bar{A}\bar{p}^n - \bar{\alpha}_n \bar{p}^n - \bar{\beta}_n \bar{p}^{n-1}, \\ \bar{\alpha}_n &= (\bar{A}\bar{p}^n, \bar{p}^n) / \rho_n^{(0)}, & \bar{\beta}_n &= (\bar{A}\bar{p}^n, \bar{p}^{n-1}) / \rho_{n-1}^{(0)}, & \rho_n^{(0)} &= (\bar{p}^n, \bar{p}^n).\end{aligned}\tag{13}$$

Note that if at every iteration the computations in (13) and (9) are carried out simultaneously, then there is no need in storing all the direction vectors \bar{p}^n . The commonly used simplest stopping criterion is the condition $\|r^n\| \leq \varepsilon \|f\|$, with a given $\varepsilon \ll 1$ (for more subtle approaches and error estimates, see the survey [20]). Note that for $\gamma = 0$, the direction vectors can also be computed by formulas (12), except for using $\sigma_n^{(0)}$.

Consider a special cost-effective variant of the two-sided preconditioning where the coefficient matrix is split as $A = D + L + U$, where D, L , and U are the diagonal, lower triangular, and upper triangular parts of A , respectively, and the preconditioning matrix is constructed using the following incomplete factorization method:

$$\begin{aligned}B &= (G + L)G^{-1}(G + U) = G + L + U + LG^{-1}U, \\ G &= D - \overline{LG^{-1}U} - \theta S & Se &= (LG^{-1}U - \overline{LG^{-1}U})e,\end{aligned}\tag{14}$$

where the overline means an approximation of a matrix; S is a diagonal matrix; e is a trial (frequently, the unit) vector, and $\theta \in [0, 1]$ is a compensation parameter, see [22].

In what follows, we will use banded approximations (by $\overline{C} = (C)_s$ the band part of the matrix C with bandwidth s is denoted). If the matrix factors are defined by the relations

$$L_B = (G + L)U_G^{-1}, \quad U_B = L_G^{-1}(G + U), \quad G = L_G U_G, \quad U_G = L_G^\top,\tag{15}$$

then the preconditioned matrix can be represented as follows:

$$\begin{aligned}\bar{A} &= (I + \bar{L})^{-1} + (I + \bar{U})^{-1} + (I + \bar{L})^{-1}(\bar{D} - 2I)(I + \bar{U})^{-1}, \\ \bar{D} &= L_G^{-1} D U_G^{-1}, & \bar{L} &= L_G^{-1} L U_G^{-1}, & \bar{U} &= L_G^{-1} U U_G^{-1}, \\ \bar{A}v &= (I + \bar{L})^{-1}[v + (\bar{D} - 2I)v] + w, & w &= (I + \bar{U})^{-1}v.\end{aligned}\tag{16}$$

If we apply this approach to a banded (for example, a diagonal or a tridiagonal) matrix G , then the operations of multiplying a vector by the original matrix A and by the preconditioned matrix \bar{A} have approximately the same complexity.

In some cases, factorization of the preconditioning matrix is impractical. Then a one-sided preconditioning of the SLAE is used. For $\gamma = 1, 2$, from the above relations we obtain the following formulas in terms of the matrices A and B (the superscripts γ are omitted for brevity):

- for the conjugate gradient methods,

$$\begin{aligned}r^0 &= f - Au^0, & p^0 &= B^{-1}r^0, & \alpha_n &= \sigma_n / \rho_n, \\ u^{n+1} &= u^n + \alpha_n p^n, & r^{n+1} &= r^n - \alpha_n A p^n, & p^{n+1} &= B^{-1}r^{n+1} + \beta_n p^n, \\ \sigma_n &= (r^n, p^n) = (B^{-1}r^n, r^n), & \rho_n &= (A p^n, p^n), & \beta_n &= \sigma_{n+1} / \sigma_n;\end{aligned}\tag{17}$$

- for the conjugate residual methods,

$$\begin{aligned}r^0 &= f - Au^0, & \hat{r}^0 &= \hat{p}^0 = B^{-1}r^0, & \alpha_n &= \sigma_n / \rho_n, \\ u^{n+1} &= u^n + \alpha_n \hat{p}^n, & \hat{r}^{n+1} &= \hat{r}^n - \alpha_n B^{-1}A \hat{p}^n, & \hat{p}^{n+1} &= \hat{r}^{n+1} + \beta_n \hat{p}^n, \\ \sigma_n &= (B^{-1}\hat{r}^n, A \hat{p}^n) = (A \hat{r}^n, \hat{r}^n), & \rho_n &= (B^{-1}A \hat{p}^n, A \hat{p}^n), & \beta_n &= \sigma_{n+1} / \sigma_n.\end{aligned}\tag{18}$$

Note that in both methods, at every iteration one multiplication by A and one multiplication by B^{-1} are required, and in formulas (18) the vector \hat{r}^n is the preconditioned residual, i.e., in

the exact arithmetic, $\hat{r}^n = B^{-1}r^n = B^{-1}(f - Au^n)$, and at every iteration the value $(B^{-1}r^n, r^n)$ is minimized.

Similarly, one can switch to one-sided preconditioning in the minimum error method, in which the coefficients are computed by the formulas

$$\alpha_n^{(0)} = -\alpha_{n-1}^{(0)}(B^{-1}r^n, p^{n-1}) / (B^{-1}p^n, p^n), \quad \alpha_0^{(0)} = -\alpha_0^{(0)}(B^{-1}r^0, r^0) / (B^{-1}p^0, p^0),$$

and the direction vectors are found by substituting $\bar{p}^n = L_B^{-1}p^n$ into the Lanczos orthogonalization formulas (13).

4. MULTIGRID INCOMPLETE FACTORIZATION METHODS

Now, from the abstract algebraic representation of the algorithms we pass to their specifications for seven-point SLAEs obtained using 3D parallelepipedal grids. Assume that the coefficient matrix A in SLAE (1) is a Stieltjes matrix, i.e., it is symmetric positive definite (s.p.d.), diagonally dominant (in general, not necessarily strictly but with at least one strictly diagonally dominant row), and has positive diagonal and nonpositive off-diagonal entries. Auxiliary matrices $A^{(l)}$ of the same type will be constructed for each of the grids Ω_i^h . The corresponding SLAEs will be written in the form

$$(A^{(l)}u^{(l)})_t = a_{t,t}^{(l)}u_t + \sum_{q=1}^6 a_{t,t+s_{t,q}}^{(l)}u_{t+s_{t,q}}^{(l)} = \bar{f}_t, \quad t = 1, \dots, N_l, \quad l = 1, 2, \dots, m, \quad (19)$$

where N_l is the order of the system, $q = 1, 2, \dots, 6$ are the numbers of diagonals (possibly curved) from the lower triangular or upper triangular part of the matrix $A^{(l)}$.

In order to simplify the notation in (19), in what follows we consider uniform grids of the form

$$\begin{aligned} \Omega_1^h: \quad & x_{i+1} = x_i + h, \quad y_{j+1} = y_j + h, \quad z_{k+1} = z_k + h; \quad i, j, k = 0, 1, 2, \dots, \\ \Omega_l^h: \quad & x_{i+2^{l'}} = x_i + 2^{l'}h^x, \quad y_{j+2^{l'}} = y_j + 2^{l'}h^y, \quad z_{k+2^{l'}} = z_k + 2^{l'}h^z, \\ & i, j, k = 0, 2^{l'}, 2 \cdot 2^{l'}, 3 \cdot 2^{l'}, \dots, \quad l' = l - 1, \dots, m - 1. \end{aligned}$$

In the case of nonuniform grids, only the coefficients of arithmetic expressions change, whereas the general computational scheme of the algorithms described below remains the same.

Consider a pair of neighboring systems from the family of algebraic systems (19),

$$A^{(l)}u^{(l)} = f^{(l)}, \quad A^{(l+1)}u^{(l+1)} = f^{(l+1)}, \quad l = 1, \dots, m - 1,$$

where l corresponds to the finer grid and $l + 1$ corresponds to the coarser one. We subdivide the nodes of Ω_i^h into four subsets of different types and number them in the following way:

$$\Omega_i^h = \Omega_i^1 \cup \Omega_i^2 \cup \Omega_i^3 \cup \Omega_i^4, \quad \Omega_i^4 = \Omega_{i+1}^h.$$

Here, the subsets consist of the centers of volumes and faces, the midpoints of edges, and the nodes of the embedded coarser grid Ω_{i+1}^h , respectively, which are denoted by the symbols \otimes, \circ, \times , and \bullet in Fig. 1). Denoting the associated subvectors (of dimensions $N_1^{(l)}, N_2^{(l)}, N_3^{(l)}, N_4^{(l)}$) in the l th SLAE by $\bar{u}_1^{(l)}, \bar{u}_2^{(l)}, \bar{u}_3^{(l)}, \bar{u}_4^{(l)}$ and $\bar{f}_1^{(l)}, \bar{f}_2^{(l)}, \bar{f}_3^{(l)}, \bar{f}_4^{(l)}$, we write it in the resulting block form as

$$A^{(l)}u^{(l)} = \begin{bmatrix} A_{1,1}^{(l)} & A_{1,2}^{(l)} & 0 & 0 \\ A_{2,1}^{(l)} & A_{2,2}^{(l)} & A_{2,3}^{(l)} & 0 \\ 0 & A_{3,2}^{(l)} & A_{3,3}^{(l)} & A_{3,4}^{(l)} \\ 0 & 0 & A_{4,3}^{(l)} & A_{4,4}^{(l)} \end{bmatrix} \begin{bmatrix} \bar{u}_1^{(l)} \\ \bar{u}_2^{(l)} \\ \bar{u}_3^{(l)} \\ \bar{u}_4^{(l)} \end{bmatrix} = \begin{bmatrix} \bar{f}_1^{(l)} \\ \bar{f}_2^{(l)} \\ \bar{f}_3^{(l)} \\ \bar{f}_4^{(l)} \end{bmatrix}.$$

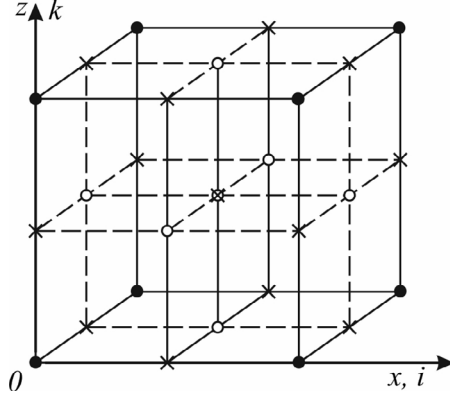


Fig. 1. Nodes of the two-level method on cubic embedded grids.

Here, the right lower block is denoted by $A_{4,4}^{(l)}=A^{(l+1)}$ and is represented in a similar form of block order four. Thus, the original block matrix $A=A^{(1)}$ is defined in a recursive m -stage manner. Since in the representation considered of a SLAE with two-level ordering of variables, corresponding to different numbers of embedded grids and types of nodes in each of them, the notation of the vectors used has an unusual recursive structure:

$$(u^{(l)}) = ((u_1^{(l)})^\top, (u_2^{(l)})^\top, (u_3^{(l)})^\top, (u^{(l+1)})^\top)^\top, \quad l=1, 2, \dots, m-1;$$

moreover, for $l+1=m$ the subvector $u^{(m)}$ is not partitioned.

For the matrix $A^{(l)}=D^{(l)}+L^{(l)}+U^{(l)}$, the preconditioner is defined in the following factorized form (recall that $(C)_1$ denotes the diagonal part of the matrix C):

$$\begin{aligned} B^{(l)} &= (G^{(l)} + U^{(l)})(G^{(l)})^{-1}(G^{(l)} + U^{(l)}) \\ &= \begin{bmatrix} G_{1,1}^{(l)} & 0 & 0 & 0 \\ A_{2,1}^{(l)} & G_2^{(l)} & 0 & 0 \\ 0 & A_{3,2}^{(l)} & G_3^{(l)} & 0 \\ 0 & 0 & A_{4,3}^{(l)} & G_4^{(l)} \end{bmatrix} (G^{(l)})^{-1} \begin{bmatrix} G_1^{(l)} & A_{1,2}^{(l)} & 0 & 0 \\ 0 & G_2 & A_{2,3}^{(l)} & 0 \\ 0 & 0 & G_3^{(l)} & A_{3,4}^{(l)} \\ 0 & 0 & 0 & G_4^{(l)} \end{bmatrix}, \end{aligned} \quad (20)$$

where

$$\begin{aligned} G_1^{(l)} &= A_{1,1}^{(l)}, \quad G_2^{(l)} = A_{2,2}^{(l)} - (A_{2,1}^{(l)}(G_1^{(l)})^{-1}A_{1,2}^{(l)})_1 - \theta_2 S_2^{(l)}, \\ S_2^{(l)} e_2 &= \left[A_{2,1}^{(l)}(G_1^{(l)})^{-1}A_{1,2}^{(l)} - (A_{2,1}^{(l)}(G_1^{(l)})^{-1}A_{1,2}^{(l)})_1 \right] e_2, \\ G_3^{(l)} &= A_{3,3}^{(l)} - \left(A_{3,2}^{(l)}(G_2^{(l)})^{-1}A_{2,3}^{(l)} \right)_1 - \theta_3 S_3^{(l)}, \\ S_3^{(l)} e_3 &= \left[A_{3,2}^{(l)}(G_2^{(l)})^{-1}A_{2,3}^{(l)} - \left(A_{3,2}^{(l)}(G_2^{(l)})^{-1}A_{2,3}^{(l)} \right)_1 \right] e_3, \\ G_4^{(l)} &= A_{4,4}^{(l)} - A_{4,3}^{(l)}(G_3^{(l)})^{-1}A_{3,4}^{(l)}. \end{aligned}$$

Here, $G_1^{(l)}, G_2^{(l)}, G_3^{(l)}$ are diagonal matrices, and $G_4^{(l)}$ is a seven-diagonal matrix with the same matrix portrait as $A^{(l+1)}$, which is the matrix of the SLAE corresponding to the next-level grid. The compensation parameters $\theta_2^{(l)}, \theta_3^{(l)} \in [0, 1]$ are considered distinct for generality, and the trial vectors $e_2^{(l)}, e_3^{(l)}$ have dimensions $N_2^{(l)}, N_3^{(l)}$. In order to specify the preconditioning matrix $B^{(l)}$, we also need to represent the matrix $G_4^{(l)}$ in factorized form. We consider two

factorizations. If $l + 1 = \overline{m}$ is the number of the last grid, then the exact triangular decomposition $G_4^{(l)} = A^{(l+1)} = L^{(l+1)}U^{(l+1)}$ is used. Otherwise, the matrix $A^{(l+1)} = G_4^{(l)}$ in (20) is replaced by the preconditioner $B^{(l+1)}$ defined by the same formula. The use of the preconditioner of the form (20) formally corresponds to the Incomplete Factorization Implicit Method, IFIM, see [22], with coefficient (based on the row sum criterion).

Note that if $\theta_2^{(l)} = \theta_3^{(l)} = 1$ (the full compensation mode), then the generalized row sum criterion is applied to the initial and preconditioning matrices in the form $Ae = Be$, where

$$e = e^{(l)} = ((e_1^{(l)})^\top, (e_2^{(l)})^\top, (e_3^{(l)})^\top, (e_4^{(l)})^\top)^\top,$$

$e^{(l)} \in \mathcal{R}^{N_l}$ is defined recursively in the same way as $u^{(l)}$; the vectors $e_2^{(l)}, e_3^{(l)}$ are defined in accordance with (20), whereas the vectors $e_1^{(l)}, e_4^{(l)}$ are chosen arbitrarily. In this case, the preconditioned iterative method converges in one iteration, provided that the initial error vector is equal to $u - u^0 = e^{(l)}$. Optimization of the compensation parameters θ and estimates of the resulting convergence rate for some particular cases can be found in [22] and in the references therein. In general, the problem of choosing the iterative parameters is still open. A possible approach is to determine the values of $\theta_q^{(l)}$, $q = 2, 3$, $l = 1, \dots, m$, in (18) from the condition $(Be, e) = (Ae, e)$, which leads to expressions of the form

$$\theta_q^{(l)} = \mu_q^{(l)} / (\nu_q^{(l)} - \mu_q^{(l)}), \quad (21)$$

where

$$\mu_q^{(l)} = \left(A_{q,q-1}^{(l)} (G_{q-1}^{(l)})^{-1} A_{q-1,q}^{(l)} e_q^{(l)}, e_q^{(l)} \right), \quad \nu_q^{(l)} = \left(\left(A_{q,q-1}^{(l)} (G_{q-1}^{(l)})^{-1} A_{q-1,q}^{(l)} \right)_1 e_q^{(l)}, e_q^{(l)} \right).$$

In order to choose an appropriate number m of embedded grids, it is necessary to estimate the computational complexity of the direct algorithm for solving the l th SLAE of dimension $N_l \equiv CN_1 \times 2^{-3(l-1)}$, $l = 1, 2, \dots, m$, where C is a constant. Since the triangular decomposition method requires $Q_l \approx CN_l^3$ arithmetic operations, we have $Q_m/Q_1 \approx 2^{3(1-m)}$. This means, for example, that the costs of using the direct algorithm in the two-grid method are $512 = 2^9$ times less and for $m = 3$ they are 2^{18} times less than in solving the original SLAE by a direct method. And since the preconditioning quality deteriorates and convergence rate slows down as the number of grids grows, we conclude that in practice the choice of a multigrid method reduces to choosing between $m = 2$ and $m = 3$.

Application of a preconditioning matrix B in computing approximate solutions u^n is based on solving the auxiliary SLAEs

$$Bv^n = r^n \equiv f - Au^n, \quad (22)$$

where

$$B = (G + L)G^{-1}(G + U), \quad v^n = (v_1^n, v_2^n, v_3^n, v_4^n),$$

and u^0 is an arbitrary initial vector.

With account for the structure of the preconditioner B and given the residual vector r^n , the solution of SLAE (22) is carried out using the relations

$$(G + L)w^n = r^n, \quad (G + U)v^n = Gw^n, \quad G = \text{diag} \{G_k\}, \quad (23)$$

which, in block form, are as follows:

$$\begin{aligned} G_1 w_1^n &= r_1^n; & k = 2, 3, 4: & \quad G_k w_k^n = r_k^n - A_{k,k-1} w_{k-1}^n; \\ v_4^n &= w_4^n; & k = 3, 2, 1: & \quad v_k = w_k - G_k^{-1} A_{k,k+1} w_{k+1}^n. \end{aligned} \quad (24)$$

It is important to observe that solution of the auxiliary SLAE with the matrix G_4 from (24) actually means solution of the system on the coarse grid Ω_2 , having the same seven-diagonal structure as the matrix $A^{(2)}$; formulas (24) for $k = 2, 3, 4$ correspond to the reduction

(restriction) stage of the two-grid method, whereas for $k=3, 2, 1$ they describe the prolongation stage, and solution of the SLAE with the coefficient matrix G_4 is the coarse grid correction.

Note that in accordance with (14), formulas (22)–(24) determine an incomplete factorization method. In the simpler case where $G=\omega^{-1}D$, they represent either a symmetric (if A is a symmetric matrix) or an unsymmetric method of successive over-relaxation, SSOR or USSOR, respectively. If $\omega=1$ and A is a Stieltjes matrix, then the SSOR method (which coincides with the symmetric Seidel method), gives rise to a monotone preconditioning matrix. Moreover, the factors of the triangular decomposition of this matrix,

$$B_1=L_1U_1, \quad L_1=(D+U)U_D^{-1}=U_1^\top, \quad D=L_DU_D, \quad (25)$$

also are monotone, i.e., the inverse matrices $B_1^{-1}, L_1^{-1}, U_1^{-1}$ are nonnegative. Therefore, when multiplied by vectors, the latter matrices possess certain smoothing properties (see [8, 12]), whence the preconditioner (25) can be used as a smoothing operator. More exactly, one can use the “double” preconditioning with the matrix

$$\overline{B}=L_1L_2U_2U_1=\overline{B}^\top, \quad (26)$$

where L_2U_2 is an IFIM or a SSOR type preconditioner. In this case, at every iteration inversion of the matrices L_1 and U_1 in formulas (23) corresponds to the stages of preliminary and final smoothing, respectively. It is not difficult to show that if $\theta_2, \theta_3 \in (0, 1)$ and $\omega \in (0, 2)$, then all the considered preconditioning matrices, including those of the form (25) in the case of smoothing, are positive definite. This ensures the convergence of all the proposed iterative multigrid incomplete factorization methods in Krylov subspaces.

5. POSSIBLE EXTENSIONS OF THE ALGORITHMS

The multigrid approaches considered above remain applicable to the seven-point grid equations whenever the computational domain is composed of parallelepipeds, and the boundary conditions of mixed type are allowed, provided that the coefficient matrix of the SLAE being solved remains a Stieltjes matrix. Naturally, the grid can be parallelepipedal not literally, but topologically. However, if it becomes irregular and/or unstructured, then the construction of the algorithms proposed needs additional investigation. The same applies to the higher-order schemes, in which, for example, to every node, edge, and face several unknowns correspond. In such a case, possible block generalizations of multigrid methods not only result in a much more complicated computational process but also make its analysis significantly more difficult.

Reducing the dimension of the boundary-value problem significantly simplifies the approaches under consideration both for rectangular and triangular grids. Transition to a 3D computational domain with a tetrahedral grid neither implies essential difficulties because in this case as well the recursive vector structure of embedded grids gives rise to SLAEs with block tridiagonal matrices. This makes it possible to use preconditioners and conjugate direction methods of the same types at different grid levels. Yet another possible generalization of the AMG approach consists in passing to nonuniform matrix structures in the algebraic systems obtained on a sequence of embedded grids. Finally, we note that the algorithms can be generalized to the unsymmetric case by using the preconditioned generalized minimal residual method (GMRES), see the surveys [7, 20].

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