Numerical Linear Algebra with Applications, Vol. 2(1), 51–77 (1995)

Eigenvalue Translation Based Preconditioners for the GMRES(k) Method

S. A. Kharchenko

Computing Center of Russian Academy of Sciences, Vavilov st., 40, 117967 Moscow, Russia

and

A. Yu. Yeremin

Institute of Numerical Mathematics of Russian Academy of Sciences, Leninskij prosp., 32A, 117334 Moscow, Russia

The paper considers a possible approach to the construction of high-quality preconditionings for solving large sparse unsymmetric offdiagonally dominant, possibly indefinite linear systems. We are interested in the construction of an efficient iterative method which does not require from the user a prescription of several problem-dependent parameters to ensure the convergence, which can be used in the case when only a procedure for multiplying the coefficient matrix by a vector is available and which allows for an efficient parallel/vector implementation with only one additional assumption that the most of eigenvalues of the coefficient matrix are condensed in a vicinity of the point 1 of the complex plane. The suggested preconditioning strategy is based on consecutive translations of groups of spread eigenvalues into a vicinity of the point 1. Approximations to eigenvalues to be translated are computed by the Arnoldi procedure at several GMRES(k) iterations. We formulate the optimization problem to find optimal translations, present its suboptimal solution and prove the numerical stability of consecutive translations. The results of numerical experiments with the model CFD problem show the efficiency of the suggested preconditioning strategy.

KEY WORDS Arnoldi procedure Spread and condensed eigenvalues Eigenvalue translations

1. Introduction

Iterative solution of large sparse unsymmetric linear systems comprises the most time-consuming stage when solving many nonlinear industrial problems. Many difficulties occur when constructing high-quality preconditionings for linear systems resulting at each nonlinear Newton iteration since the coefficient matrices are large, unsymmetric, highly

CCC 1070–5325/95/010051–27

Received 1 February 1992
Revised 6 September 1992

offdiagonally dominant and possibly indefinite, moreover their functional properties may significantly vary at each nonlinear iteration. Application to these matrices of standard preconditioning strategies (like ILU, BSSOR, multigrid or other) produces in most cases unpredictable results with respect to the preconditioning quality and, ultimately, with respect to the convergence. Evidently, the properties of these matrices may be considerably improved, for example, by introduction of a large artificial dissipation into the approximation scheme and/or of the artificial time into nonlinear iterations. But such an improvement does not necessary lead to a reduction of the total solution time of the original problem (since it may result in a considerable deterioration of the quality of approximation of the original problem and/or to a significant increase of the required number of nonlinear iterations).

In this paper we consider an approach to the construction of high-quality preconditionings when solving large sparse unsymmetric offdiagonally dominant (possibly indefinite) linear systems by iterative methods. It should be noted that the type of the distribution of the eigenvalues of the preconditioned matrix can be considered as a crucial factor determining the convergence properties of most existing iterative methods, for example, the presence of the spread eigenvalues may extremely slow down the convergence. That is why as a criterion of the quality of the preconditioner we consider in this paper the type of the distribution of the eigenvalues of the preconditioned matrix. We expect (this is a natural heuristic but it is wrong in general) that the smaller the number of bad (spread) eigenvalues lying outside of a vicinity of the point 1 the higher the observed convergence rate of the corresponding iterative method (e.g., of the GMRES method).

We are interested in a procedure for generating a high-quality preconditioner (a) which does not require from the user a prescription of several problem-dependent parameters to ensure the convergence, (b) which can be used in the case when only a procedure for multiplying the coefficient matrix by a vector is available and (c) which allows for an efficient parallel/vector implementation.

Obviously, a solution of this challenging problem is extremely hard and actually we consider it in a relaxed form: we are interested in a procedure for generating a preconditioner which satisfies conditions (a)–(c) assuming that (d) most of eigenvalues of the coefficient matrix are condensed in a vicinity of the point 1 of the complex plane.

The relaxed formulation is quite realistic since due to condition (b) as a coefficient matrix we can consider an already preconditioned matrix, say, using ILU, BSSOR, multigrid or other preconditioning strategies satisfying condition (d).

The main idea of a possible scheme for generating high-quality preconditionings satisfying conditions (a)–(d) can be based on the so-called translations of spread eigenvalues into a vicinity K_0 of the point 1 using low rank transformations of the coefficient matrix A of the form

$$\tilde{A} = A(I_n + u_1 v_1^h) \cdot \ldots \cdot (I_n + u_\ell v_\ell^h) \tag{1.1}$$

where the vectors u_j and v_j, $1 \leq j \leq \ell$ are to be determined and the condensed eigenvalues of $\tilde{A}$ lie in a vicinity of 1.

Similar ideas have already been exploited. In [12] Saad suggested the use of exact invariant subspaces to improve the eigenvalue distribution. Unfortunately, several difficulties arise when applying this approach to the considered class of matrices. First, the number of spread eigenvalues can be sufficiently large and cannot be estimated *a priori*. Even if the number of spread eigenvalues is known the computation of the required approximations to the corresponding eigenpairs (using, for example, the Arnoldi procedure) may require

enormous arithmetic costs (when exploiting the Arnoldi procedure with a very large value of k). Actually in this case the construction of a high-quality preconditioner reduces to the solution of the partial eigenvalue problem for A which is much harder to solve than a linear algebraic system with the coefficient matrix A.

In [6] the authors suggested the low-rank updating scheme for constructing high-quality preconditioners to improve the convergence of the Richardson iterations. The main drawback of this scheme is related to the fact that rank-one updates improve the distribution of singular values of the preconditioned matrix while the convergence of the Richardson iterations is determined by the distribution of eigenvalues of the preconditioned matrix and thus we cannot expect a substantial improvement of the convergence rate when the number of low-rank updates is significantly smaller than the size of the linear system.

In this paper we consider another approach to the construction of high-quality eigenvalue translation based preconditioners. We suggest translating spread eigenvalues consecutively group by a group using low-rank transformations constructed at several global cycles of the Arnoldi procedure to perform a step-by-step spectrum condensation. Since the Arnoldi procedure is the most cost-consuming stage of the restarted GMRES(k) method it is natural to combine eigenvalue translation technique and the restarted GMRES(k) method. A possible eigenvalue translation preconditioned GMRES(k) method can be described as follows. At the current GMRES(k) iteration (parameter k is assumed to be relatively small) we extract approximations only to some spread eigenvalues of A, perform translations of the detected spread eigenvalues into a vicinity of the point 1 and go to the next global GMRES(k) iteration but with transformed matrix (1.1). Since the Arnoldi procedure provides for inexpensive and relatively accurate approximations to spread eigenvalues lying near the boundary of the convex hull of the spectrum a step-by-step spectrum condensation can lead to a substantial reduction of the arithmetic costs for computing approximations to spread eigenvalues. But in this case we must pay a special attention to ensure the monotonicity of spectrum condensation at consecutive global GMRES(k) iterations. Moreover, the vectors u_j and v_j from (1.1) must be determined to ensure the numerical stability of consecutive translations of groups of spread eigenvalues, i.e., when translating we must minimize a possible deterioration of the accuracy of already approximated but not yet translated spread eigenvalues and of already translated and of condensed eigenvalues.

In a sense the Eigenvalue Translation preconditioned GMRES(k) (ET-p-GMRES(k)) [1] method can be considered as a compromise between the preconditioned full GMRES method and the preconditioned restarted GMRES(k) method. Thus it seems natural to compare the suggested approach with the former.

It is well known that the full GMRES method is the optimal iterative scheme (in the exact arithmetic) with respect to minimization of the residual over the computed Krylov subspace and to the arithmetic complexity measured by the number of the preconditioned matrix vector multiplications. Unfortunately, the quickly growing (like $O(k^2n)$, where k is the size of the computed Krylov subspace while n is the problem size) arithmetic complexity for making orthogonal the direction vectors may soon become much larger than the arithmetic costs for multiplying the preconditioned matrix by a vector. Hence, we have to make restarts due to the arithmetic complexity considerations. Moreover, the recent theoretical and numerical investigations [8] show that an increase of the dimension k of the Krylov subspace can lead (due to rounding errors in a procedure for multiplying the preconditioned matrix

[1] The notation '-p' means that eigenvalue translation preconditioning can be applied to an already preconditioned linear system, e.g. an ILU preconditioned linear system (ET-ILU-GMRES(k) method), a BSSOR preconditioned linear system (ET-BSSOR-GMRES(k) method) and so on.

by a vector and in the orthogonalization scheme) to a considerable increase of rounding errors in the matrix relations of the Arnoldi procedure which may cause the jump of the computed residual in the standard realizations ([13] and [17]) of the full GMRES method (by the jump of the computed residual we mean the situation when the norm of the final residual computed for the new guess to the solution is larger than the estimate of the norm of the residual computed by the standard technique). So we have to make restarts of the full GMRES method also due to the numerical stability considerations. In reality an application of the full GMRES makes sense only if a very high quality preconditioner is available which can ensure the convergence in a relatively small number of the Arnoldi iterations. On the other hand, application of the restarted GMRES(k) method when the preconditioned matrix is not sufficiently well-conditioned can lead to a very slow convergence. Therefore an opportunity to improve the preconditioning quality during iterations to accelerate the convergence of the restarted GMRES(k) method and to reduce the costs as compared with the full GMRES method seems to be promising.

The paper is organized as follows. Section 2 contains theoretical results underlying the eigenvalue translation construction. In section 3 we consider the construction of eigenvalue translation based preconditioners and prove the numerical stability of consecutive translations of several groups of spread eigenvalues. To find optimal vectors u_j and v_j we also formulate the optimization problem and describe its suboptimal solution. Section 4 discusses some realization aspects of the eigenvalue translation based preconditioned GMRES(k) method. Section 5 contains the result of numerical experiment, while concluding remarks are presented in section 6.

We conclude this section by introducing the notation utilized throughout the paper.

Let Z be an arbitrary rectangular matrix with complex entries.

$\Re(Z)$ denotes the real part of the matrix Z;
$\Im(Z)$ denotes the imaginary part of the matrix Z;
$\bar{Z}$ denotes the complex conjugate matrix to Z;
Z^t denotes the transpose matrix to Z;
Z^h denotes the transpose and complex conjugate matrix to Z;
$\{Z\}_{ij}$ denotes the (i, j)th entry of Z;
$\{Z\}_{*i}$ (respectively $\{Z\}_{i*}$) denotes the ith column (row) of Z;
for a square matrix Z $\lambda(Z)$ denotes an eigenvalue of Z;
for a square Hermitian matrix Z $\lambda_{min}(Z)$ denotes its minimal eigenvalue while $\lambda_{max}(Z)$ denotes the maximal eigenvalue;
$\sigma_{min}(Z)$ (respectively $\sigma_{max}(Z)$) denotes the minimal (maximal) singular value of Z, i.e., $\sigma_{min}(Z) = \sqrt{\lambda_{min}(Z^h Z)}$ and $\sigma_{max}(Z) = \sqrt{\lambda_{max}(Z^h Z)}$;
$\| Z \|$ denotes the Euclidean norm of Z, i.e., $\| Z \| = \sigma_{max}(Z)$.

For a square matrix Z the set of its eigenvalues is denoted by $Spec(Z)$, while $Cond(Z)$ stands for the condition number of a square nonsingular matrix Z with respect to the Euclidean norm, i.e.,

$$Cond(Z) = \sigma_{max}(Z)/\sigma_{min}(Z)$$

The scalar product of two vectors z_1 and z_2 is defined by the standard relation:

$$(z_1, z_2) = z_2^h z_1$$

Let B be a $k \times k$ matrix and $\lambda(B)$ be an eigenvalue of B. By $x(B)$ and $y(B)$ we denote, respectively, the right and the left eigenvectors corresponding to $\lambda(B)$. We will assume in

what follows that the eigenvectors are normalized according to the following equalities:

$$\begin{cases} \| x(B) \| & = 1 \\ (x(B), y(B)) & = 1 \end{cases} \tag{1.2}$$

By $\mathcal{S}_{\lambda(B)}(B)$ we denote the condition number [18] of a simple eigenvalue $\lambda(B)$ of B defined according to the following equality:

$$\mathcal{S}_{\lambda(B)}(B) = \frac{\| x(B) \| \| y(B) \|}{| (x(B), y(B)) |}$$

Taking into account normalization (1.2) the above definition can be rewritten in the form

$$\mathcal{S}_{\lambda(B)}(B) = \| y(B) \|$$

To establish the correspondence between matrices, eigenvalues, and eigenvectors we utilize subscripts. For example, $x_j(B)$ denotes the right eigenvector of a matrix B corresponding to $\lambda_j(B)$, while y denotes the left eigenvector corresponding to λ.

Let M be a set of elements. By $Car(M)$ we denote the number of elements of the set M.

2. Estimating spectral characteristics of an unsymmetric matrix via the Arnoldi procedure

For the block pair $\{\Lambda, X\}$ we define the block eigenresidual $R(B)$ with respect to a matrix B by the equality

$$R(B) = BX - X\Lambda \tag{2.1}$$

Let us establish the relation between the pair $\{\Lambda, X\}$ and the corresponding exact block eigenpair of B. To this end we need the following result.

Lemma 2.1 ([3]) *Let B be a square matrix and $\lambda(B)$ be a simple eigenvalue. Let E be a square perturbation matrix. Then there exists an eigenvalue $\lambda(B + E)$ of the matrix $B + E$ which satisfies the following inequality*

$$|\lambda(B + E) - \lambda(B)| \leq \| E \| \mathcal{S}_{\lambda(B)}(B) + O(\| E \|^2)$$

The following statement is valid.

Lemma 2.2. *Let $R(B)$ be the block eigenresidual of the pair $\{\Lambda, X\}$ with respect to the matrix B and assume that the columns of the matrix X are linearly independent. Then the pair $\{\Lambda, X\}$ is the block eigenpair of the matrix $B + E$, where $E = -R(B)(X^h X)^{-1} X^h$ and*

$$\| E \| \leq \frac{\| R(B) \|}{\sigma_{min}(X)}$$

Let $y(B)$ be the left eigenvector of the matrix B corresponding to an eigenvalue $\lambda(B)$. Then the following inequality is satisfied:

$$\| X^h y(B) \| \leq \max_{\lambda \in Spec(\Lambda)} \frac{1}{| \lambda - \lambda(B) |} \| R(B) \| \| y(B) \|$$

Proof Let us proof the second statement of the lemma. Taking into account the identity

$$y(B)^h BX = \lambda(B)y(B)^h X = y(B)^h(R(B) + X\Lambda)$$

we obtain the equality

$$y(B)^h X(\lambda(B)I - \Lambda) = y(B)^h R(B)$$

Now the second statement of the lemma is a straightforward corollary of this equality. ■

After k steps of the Arnoldi procedure [1] the following relations hold true:

$$\begin{cases} AP &= PH + \beta w e_k^h, \ \| w \| = 1 \\ P^h P &= I_k \\ w^h P &= 0 \end{cases} \tag{2.2}$$

where P is the real $n \times k$ matrix whose columns form the orthonormal basis of the computed Krylov subspace, H is the real $k \times k$ Arnoldi matrix, $\beta \geq 0$ is a real number, w is the $k+1$th direction vector, I_k is the $k \times k$ identity matrix, and e_k is its kth column.

Remark Here and in what follows we assume that all computations are performed in exact arithmetic.

Remark Throughout the paper we assume that the eigenvalues of the Arnoldi matrix H are simple.

Let $\{\lambda_j(H), x_j(H)\}$, $\| x_j(H) \| = 1$, $j = 1, ..., k$, be the eigenpairs of the Arnoldi matrix H.

Let M be a subset of the set $\{1, ..., k\}$, $Car(M) = m$. Let $\Lambda_M(H)$ be the diagonal $m \times m$ matrix whose diagonal entries are equal to $\lambda_j(H)$, $j \in M$. Let $X_M(H)$ be the $k \times m$ matrix made up with eigenvectors $x_j(H)$, $j \in M$, arranged according to the numbering of the eigenvalues $\lambda_j(H)$ in the matrix $\Lambda_M(H)$. Denote $\Lambda_M = \Lambda_M(H)$, $X_M = PX_M(H)$.

Lemma 2.3. *The block eigenresidual $R_M(A)$ of the block pair $\{\Lambda_M, X_M\}$ with respect to the matrix A can be presented as follows:*

$$R_M(A) = w\alpha_M$$

where $\alpha_M = \beta e_k^h X_M(H)$. In particular, $\| R_M(A) \| = \| \alpha_M \|$.

Combining the statements of the Lemmata 2.1–2.3, one can estimate the relation between the block pair $\{\Lambda_M, X_M\}$ and the corresponding exact block eigenpair of A.

Let us estimate other spectral characteristics of the matrix A via iteration data of the Arnoldi procedure. We will exploit the following lemma.

Lemma 2.4. *Let the matrices $V \in \mathcal{R}^{n \times n}$ and $T \in \mathcal{R}^{k \times k}$ be Hermitian. If the equalities*

$$\begin{cases} T &= P^h V P \\ P^h P &= I_k \end{cases}$$

are satisfied with $P \in \mathcal{R}^{n \times k}$, then eigenvalues of the matrices T and V, ordered in the

nondecreasing order, satisfy the Cauchy interlacing inequalities

$$\lambda_j(V) \leq \lambda_j(T) \leq \lambda_{n-\ell+j}(V)$$

Proof Let P_1 be the complement of P to an orthonormal basis in $\mathcal{R}^n$. Denote $U = [P, P_1]$. Then we have

$$VU = V[P, P_1] = [P, P_1]\begin{bmatrix} T & C^h \\ C & W \end{bmatrix} = U\tilde{V}$$

for some matrices C and W. The matrix $\tilde{V}$ is similar to V and hence has the same eigenvalues. The matrices $\tilde{V}$ and T satisfy the Cauchy interlacing theorem [10]. Lemma 2.4 is thus proved. ∎

Denote $\hat{P} = [P, w]$ and

$$\hat{H} = \begin{bmatrix} H \\ \beta e_k^h \end{bmatrix}$$

From (2.2) we obtain the equalities:

$$\begin{cases} AP &= \hat{P}\hat{H} \\ H &= P^h AP \\ \hat{H} &= \hat{P}^h AP \end{cases} \tag{2.3}$$

Lemma 2.5. *(a) Eigenvalues of the pairs of the matrices* $\{A + A^h, H + H^h\}$, $\{i(A-A^h), i(H-H^h)\}$ *and* $\{A^hA, \hat{H}^h\hat{H}\}$ *satisfy the interlacing inequalities of Lemma* 2.4

(b) Let equalities (2.2) *be satisfied for* $\beta = 0$ *and* λ *be a simple eigenvalue of the matrices A and H. Then the inequality is valid*

$$\mathcal{S}_\lambda(H) \leq \mathcal{S}_\lambda(A)$$

(c) If equalities (2.2) *are satisfied with* $\beta = 0$, *then singular values of the eigenvector matrix of H and the kernel eigenvector matrix of A under a similar scaling satisfy inequalities of the Cauchy interlacing theorem.*

Proof (a) From equalities (2.3) we have

$$\begin{cases} H + H^h &= P^h(A + A^h)P \\ H - H^h &= P^h(A - A^h)P \\ \hat{H}^h\hat{H} &= P^hA^hAP \end{cases}$$

Applying Lemma 2.4 to these equalities and observing that the matrices $i(H - H^h)$ and $i(A - A^h)$ are Hermitian we obtain the statement (a) of the lemma.

(b) Let P_1 be the complement of P from (2.2) to an orthonormal basis in $\mathcal{R}^n$. Denote $U = [P, P_1]$, where U is a unitary matrix whose columns form a basis in $\mathcal{R}^n$. Let us construct an expansion of the columns of AP_1 over the basis U:

$$\begin{cases} AP &= PH \\ AP_1 &= PH_1 + P_1H_2 \end{cases} \tag{2.4}$$

where H_1 and H_2 are matrices of the appropriate sizes. Equalities (2.4) can be rewritten in

the form $AU = U\breve{H}$, where

$$\breve{H} = \begin{bmatrix} H & H_1 \\ 0 & H_2 \end{bmatrix}$$

Now to prove the statement (b) of the lemma it remains to show the inequality $\mathcal{S}_\lambda(H) \leq \mathcal{S}_\lambda(\breve{H})$, where by the hypothesis λ is not an eigenvalue of H_2. Let X be the matrix made up with the right eigenvectors of the Arnoldi matrix H. Then the columns of the matrix $[X^h; 0]^h$ coincide with the right eigenvectors of the matrix $\breve{H}$. Let the columns of the matrix $[X_1^h; X_2^h]^h$ coincide with the remaining right kernel vectors of $\breve{H}$. Evidently, the left kernel vectors of the matrix $\breve{H}$ coincide with the columns of the matrix

$$\begin{bmatrix} X & X_1 \\ 0 & X_2 \end{bmatrix}^{-h} = \begin{bmatrix} Y & 0 \\ Y_1 & Y_2 \end{bmatrix}$$

The equality $YX^h = I_k$ means that the columns of the matrix Y coincide with the left eigenvectors of the Arnoldi matrix H. Then we obtain

$$\mathcal{S}_\lambda(\breve{H}) = \left\| \begin{matrix} X_{(i)} \\ 0 \end{matrix} \right\| \cdot \left\| \begin{matrix} Y_{(i)} \\ Y_{1(i)} \end{matrix} \right\| \geq \| X_{(i)} \| \cdot \| Y_{(i)} \| = \mathcal{S}_\lambda(H)$$

where the subscript (i) indicates the eigenvector number (the column number) corresponding to the eigenvalue λ. This completes the proof of the statement (b) of the lemma.

(c) Matrix $\breve{H}$ from the proof of statement (b) is unitary similar to the matrix A. Hence, singular values of the kernel eigenvector matrix of A are equal to the square roots of eigenvalues of the matrix

$$\begin{bmatrix} X & X_1 \\ 0 & X_2 \end{bmatrix}^h \begin{bmatrix} X & X_1 \\ 0 & X_2 \end{bmatrix} = \begin{bmatrix} X^hX & X^hX_1 \\ X_1^hX & X_1^hX_1 + X_2^hX_2 \end{bmatrix} \tag{2.5}$$

The square roots of eigenvalues of the left upper block of block 2×2 matrix (2.5) are equal to the singular values of the matrix made up with the eigenvectors of H. Now the statement (c) of the lemma follows immediately from the Cauchy interlacing theorem. ■

Remark Several scaling strategies of eigenvector matrices were considered (see, for example, [2], [18]) which are close to optimal one (in the sense of minimization of the condition number of the matrix). In this paper we utilize the scaling strategy from [2]. Let $x(H)$ be an eigenvector of the Arnoldi matrix H and $\beta = 0$. Let $x(H)$ be scaled so that $\| x(H) \| = 1$. Then by Lemma 2.2, $Px(H)$ is an eigenvector of A and $\| Px(H) \| = 1$. Therefore, this scaling strategy of eigenvectors of A and of H is compatible in the sense of equality (2.5) and is close to optimal one for both matrices.

Let us consider Lemmata 2.1–2.3. The first term in the right-hand side of the inequality of Lemma 2.1 can be considered as the first-order eigenvalue perturbation. With $r_j(A) = w\beta(x_j(H), e_k)$, $B = A - r_j(A)x_j^h$ and $E = r_j(A)x_j^h$, Lemmata 2.1–2.3 imply that the evaluation of the radius of the circle containing an eigenvalue of A detected by the Arnoldi procedure requires the estimation of the quantity

$$\mathcal{S}_{\lambda_j(H)}(A - r_j(A)x_j^h)$$

From statement (b) of the Lemma 2.5 we can conclude that the condition number of the eigenvalue of the matrix H approximates from below the condition number of the corre-

sponding eigenvalue of the matrix A when $\beta = 0$. Thus we can expect that the term

$$\| r_j(A) \| \mathcal{S}_{\lambda_j(H)}(H) \tag{2.6}$$

can be considered as the lower estimate for the first-order perturbation term of the eigenvalue. The following statement is valid.

Lemma 2.6. *Quantity* (2.6) *can be considered as an upper probabilistic estimate of the first-order eigenvalue perturbation term from Lemma* 2.1.

Proof Let $\lambda(H)$ be an eigenvalue of H and $x(H)$, $\| x(H) \| = 1$, be the corresponding eigenvector. Denote $\lambda = \lambda(H)$ and $x = Px(H)$ and compute also the residual $r(A)$ of the pair $\{\lambda, x\}$ with respect to the matrix A. Then denoting $G = A - r(A)x^h$ we obtain from Lemma 2.2 that $\{\lambda, x\}$ is an eigenpair of G. Let us estimate the first-order perturbation term of an eigenvalue λ of the matrix G. We have

$$\begin{cases} Gx & = & \lambda x \\ G^h y(G) & = & \bar{\lambda} y(G) \end{cases}$$

for a vector $y(G)$. Let ΔG be a perturbation of the matrix G, then

$$(G + \Delta G)(x + \Delta x) = (\lambda + \Delta\lambda)(x + \Delta x)$$

or

$$G\Delta x + \Delta G(x + \Delta x) = \lambda\Delta x + \Delta\lambda(x + \Delta x) \tag{2.7}$$

In our case we choose $\Delta G = r(A)x^h$. Then multiplying (2.7) by $y^h(G)$ and preserving in the resulting equality the first-order terms only we get the relation

$$(\Delta\lambda)_1 = \frac{(\, r(A), y(G)\,)}{(\, x, y(G)\,)}$$

where $(a)_1$ denotes the first-order perturbation of a number a.

Let P_1 be the complement of the matrix $[P, w]$ to an orthogonal matrix in $\mathcal{R}^n$. Present the eigenvector $y(G)$ as a direct sum of three orthogonal projections

$$y(G) = y_P + y_w + y_{P_1}$$

where t_Z denotes an orthogonal projection of a vector t onto a subspace spanned by the columns of a matrix Z.

Then we have

$$|(\Delta\lambda)_1| = \frac{\| r(A) \| \| y_w \|}{|\, (x, y_P)\,|} = \| r(A) \| \frac{\| y_P \|}{|\, (x, y_P)\,|} \frac{\| y_w \|}{\| y_P \|}$$

The vector $y = Py(H)$ can be considered as an accurate approximation to y_P since $y(H)$ is an eigenvector of the matrix $H^h \equiv P^h G^h P$, which is a Galerkin projection of the matrix G^h onto the subspace, spanned by the columns of the matrix P.

Therefore, we can expect that the relation

$$|(\Delta\lambda)_1| \approx \frac{\| r(A) \| \| Py(H) \|}{| (Px(H), Py(H)) |} \frac{\| y_w \|}{\| y_P \|} = \| r(A) \| \mathcal{S}_\lambda(H) \frac{\| y_w \|}{\| y_P \|}$$

is valid. Since the greater is the order k of the Arnoldi matrix H the smaller is the probability of

$$\frac{\| y_w \|}{\| y_P \|} > 1$$

(because y_w lies in the subspace of dimension 1, while y_P belongs to the subspace of dimension k) and thus we derive the upper probabilistic estimate

$$| (\Delta\lambda)_1 | \leq \| r(A) \| \mathcal{S}_\lambda(H)$$

which completes the proof of the lemma. ■

3. Eigenvalue translations

The asymptotic convergence rate of the iterative GMRES(k) method is highly dependent [13] on the distribution of the coefficient matrix eigenvalues. We can expect that the smaller is the number of eigenvalues of the coefficient matrix lying outside of a neighborhood of the point 1 of the complex plane the higher is the convergence rate. Thus, it seems natural to partition all eigenvalues into 'good' eigenvalues condensed around the point 1 which do not significantly affect the actual convergence rate and 'bad' eigenvalues lying outside this vicinity which may cause stagnation of the convergence. Evidently, some 'bad' eigenvalues may be clustered.

In this paper for the sake of convenience 'good' eigenvalues are said to be condensed eigenvalues, while the domain containing all condensed eigenvalues is said to be the cluster, and 'bad' eigenvalues are said to be 'spread' eigenvalues.

There may be given several definitions of the condensed and the spread eigenvalues, for example, in terms of the so-called ϵ-pseudoeigenvalues [9]. In this paper we assume that the vicinity K_0 of the point 1 of the complex plane, containing all condensed eigenvalues of the matrix (i.e. the cluster), is a prescribed, simply connected domain of the complex plane (say a rectangle or an ellipse) which contain the point 1 and which does not contain the origin.

Definition 3.1. *An eigenvalue $\lambda_j(H)$ of the Arnoldi matrix H is said to be an approximation to the spread eigenvalue of the matrix A if $\lambda_j(H) \notin K_0$.*

Assume that after k steps of the Arnoldi procedure we have computed the Arnoldi matrix H.

Let M be a subset of the set $\{1, ..., k\}$, $Car(M) = m \leq k$, such that $\lambda_j(H)$, $j \in M$ are approximations to spread eigenvalues of A (we emphasize that H does not necessarily contain approximations to all spread eigenvalues of A).

The main idea of the suggested preconditioning strategy of the GMRES(k) method consists in the so-called translations of spread eigenvalues into the cluster using right multiplicative rank-one transformations of the matrix A of the form

$$\tilde{A} = A(I_n + u_1 v_1^h) \cdot \ldots \cdot (I_n + u_\ell v_\ell^h), \quad \ell \leq k$$

where the vectors u_j and v_j, $1 \leq j \leq \ell$ are chosen to satisfy the following conditions:

(1) the transformed matrix $\tilde{A}$ must be real;
(2) after all transformations the condensed and the translated eigenvalues must belong to a slightly perturbed cluster $\tilde{K}_0$;
(3) when translating consecutively several groups of spread eigenvalues approximated by the Arnoldi procedure we require that the current translation does not lead to a considerable deterioration of the accuracy of already approximated but not yet translated eigenvalues;
(4) the growth of the condition number of the eigenvector matrix under translation must be minimal.

It should be noted that we use the right transformation of the matrix in order to preserve monotonicity of the norms of the residuals when passing from one to another global GMRES(k) iteration.

The eigenvalue translation based preconditioned GMRES(k) method with transformations satisfying conditions (1)–(4) can be described as follows.

Assume that at the current global GMRES(k) iteration we have computed the spectral characteristics of the Arnoldi matrix H. Then:

(a) According to the eigenvalues of H we determine approximations to spread eigenvalues of A, i.e., according to a prescribed cluster K_0 we partition all eigenvalues of H into spread and condensed eigenvalues. Here we emphasize that the Arnoldi matrix H does not necessarily contain approximations to all spread eigenvalues of A.
(b) We try to translate spread eigenvalues group by group. Each group of spread eigenvalues is translated into the cluster K_0 using the rank one transformation of the form

$$\tilde{A} = A \, (\, I_n \, + \, X_U u v^h Y_U^h \,) \tag{3.1}$$

where X_U and Y_U are $n \times m_j$ real matrices, $1 \leq m_j \leq k, 1 \leq j \leq \ell$, constructed using the right and the left eigenvectors of the Arnoldi matrix H corresponding to the spread eigenvalues from the group to be translated, while the vectors u and v of length m_j are determined to satisfy stability conditions (2)–(4). If the stability conditions cannot be satisfied we either reorganize the group or even do not translate some spread eigenvalues.
(c) Go to the next global GMRES(k) iteration with the transformed matrix $\tilde{A}$. It should be noted that we may need several global GMRES(k) iterations in order to translate all spread eigenvalues of A into the cluster K_0. After translating all spread eigenvalues we may expect the required fast convergence.

Now let us consider the construction and the numerical stability of eigenvalue translations in more detail.

3.1. Construction of transformation (3.1)

Let, after k steps of the Arnoldi procedure, equalities (2.2) be valid. Let $\{\lambda_j(H), x_j(H), y_j(H)\}$, $j = 1, ..., k$ be the eigentriples of the nonsingular Arnoldi matrix H.

Let M be a subset of the set $\{1, ..., k\}$, $Car(M) = m$. Let $\Lambda_M(H)$ be the diagonal $m \times m$ matrix whose diagonal entries are equal to $\lambda_j(H)$, $j \in M$. Since H is a real matrix its

eigenvalues are real or form complex conjugate pairs. We will assume in what follows that the eigenvalues with nonzero imaginary parts appear in the subset M also by complex conjugate pairs.

Let $X_M(H)$ be the $k \times m$ matrix made up with the right eigenvectors $x_j(H)$, $j \in M$, and $Y_M(H)$ be the $k \times m$ matrix made up with the left eigenvectors $y_j(H)$, $j \in M$, and let the columns of these matrices be arranged according to a numbering of the eigenvalues $\lambda_j(H)$ in the matrix $\Lambda_M(H)$. Since the right and the left eigenvectors of the matrix corresponding to different eigenvalues are orthogonal we normalize the matrices $X_M(H)$ and $Y_M(H)$ according to equalities (1.2) as follows:

$$\begin{cases} \| x_j(H) \| & = & 1, \ j \in M \\ Y_M(H)^h X_M(H) & = & I_m \end{cases} \tag{3.2}$$

Denote $\Lambda_M = \Lambda_M(H)$, $X_M = PX_M(H)$ and $Y_M = PY_M(H)$, where P is the matrix from (2.2).

Let us transform the matrices Λ_M, X_M and Y_M to a form involving only real quantities. To this end let us consider the unitary matrix

$$U_* = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$$

where i is the imaginary unity.

Let $\lambda_j(H)$, $j \in M$, be an eigenvalue of H with a nonzero imaginary part. Denote $\lambda = \lambda_j(H)$, $x = x_j(H)$, and $y = y_j(H)$. Then it can be easily shown that the following equalities hold true:

$$U_* \begin{bmatrix} \lambda & 0 \\ 0 & \bar{\lambda} \end{bmatrix} U_*^h = \begin{bmatrix} \Re(\lambda) & -\Im(\lambda) \\ \Im(\lambda) & \Re(\lambda) \end{bmatrix}$$

$$[x, \ \bar{x}] U_*^h = [\, \Re(x) + \Im(x), \ \Re(x) - \Im(x) \,]$$

$$[y, \ \bar{y}] U_*^h = [\, \Re(y) + \Im(y), \ \Re(y) - \Im(y) \,]$$

The right-hand sides of these equalities contain only real matrices. Let U be the unitary block-diagonal $m \times m$ matrix with nonzero 1×1 and 2×2 diagonal blocks. The diagonal 1×1 blocks correspond to real eigenvalues from Λ_M and are equal to 1, while the diagonal 2×2 blocks correspond to the eigenvalues with nonzero imaginary parts and are equal to U_*. Let us denote

$$\begin{cases} D_U(H) & = & U \Lambda_M(H) U^h \\ X_U(H) & = & X_M(H) U^h \\ Y_U(H) & = & Y_M(H) U^h \end{cases}$$

The matrices $D_U(H)$, $X_U(H)$, and $Y_U(H)$ are real. Denote $D_U = D_U(H)$, $X_U = PX_U(H)$ and $Y_U = PY_U(H)$. Therefore, the matrices X_U and Y_U from transformation (3.1) can be correctly constructed.

To determine the optimal vectors u and v suppose that

$$R_M(A) = AX_M - X_M \Lambda_M = 0$$

Thus, we have the equalities

$$\begin{cases} AX_U &= X_U D_U \\ Y_U^h X_U &= I_m \end{cases} \tag{3.3}$$

Let $\tilde{\Lambda}_M$ be a diagonal matrix made up with the closed with respect to the complex conjugation set of eigenvalues from the cluster K_0. Suppose that the matrix $\tilde{\Lambda}_M$ has no multiple eigenvalues. For the matrix $\tilde{\Lambda}_M$ we construct the unitary matrix $\tilde{U}$ similarly as we did for Λ_M. We define real matrix $\tilde{D}_U$ by the following equality:

$$\tilde{D}_U = \tilde{U}\tilde{\Lambda}_M\tilde{U}^h \tag{3.4}$$

When translating a block eigenvalue Λ_M into the block eigenvalue $\tilde{\Lambda}_M$ belonging to the cluster K_0 we should satisfy the following equality which is similar to the first equality in (3.3):

$$\tilde{A}X_U S = X_U S\tilde{D}_U \tag{3.5}$$

where S is an unknown real matrix. Substituting equalities (3.1) and (3.3) into (3.5) we derive the relations:

$$\tilde{A}X_U S = X_U D_U S + X_U D_U u v^h S = X_U S\tilde{D}_U$$

or

$$(\ D_U\ +\ D_U u v^h\ )\ S = S\ \tilde{D}_U \tag{3.6}$$

To find the vectors u and v we proceed as follows: we choose vectors f and g and we show that there is a nonsingular matrix S for which

$$D_U S\ -\ S\tilde{D}_U = f g^h \tag{3.7}$$

Then we compute u and v from $u = -D_U^{-1} f$ and $v^h = g^h S^{-1}$.

Thus we have to solve the following

Problem 3.1. *For given $m \times m$ matrices D_U and $\tilde{D}_U$ and given vectors f and g find an $m \times m$ matrix S satisfying matrix equation* (3.7).

Consider first the problem of solvability of matrix equation (3.7).

Definition 3.2. ([5]) *The pair (Z, z), where Z is a square $\ell \times \ell$ matrix and z is a vector of the length ℓ, is said to be controllable if $dim\{z, Zz, \ldots, Z^{\ell-1}z\} = \ell$.*

The following theorem is valid.

Theorem 3.1. ([5]) *Problem* 3.1 *has a unique nonsingular solution S if the following conditions are satisfied:*

- *the matrices D_U and $\tilde{D}_U$ have no common eigenvalues;*
- *the pairs (D_U, f) and $(\tilde{D}_U^h, g)$ are controllable.*

In the considered case the matrices D_U and $\tilde{D}_U$ have no common eigenvalues since the spectrum of $\tilde{D}_U$ belongs to the cluster K_0, while the spectrum of D_U lies outside the cluster K_0.

Lemma 3.1. *The pair (D_U, f) is controllable if:*

- *the matrix D_U has no multiple eigenvalues;*
- *all components of the vector $\hat{f} \equiv U^h f$ are nonzero.*

Proof By the hypothesis of the lemma we have:

$$dim\{f, D_U f, \ldots, D_U^{m-1} f\} = dim\{\hat{f}, \Lambda_M \hat{f}, \ldots, \Lambda_M^{m-1} \hat{f}\} = m$$

since all coefficients of the expansion of the vector $\hat{f}$ over the eigenbasis of the matrix Λ_M are nonzero and the degree of the minimal polynomial of the matrix Λ_M is equal to m. ■

By construction the matrices D_U and $\tilde{D}_U$ have no multiple eigenvalues. Applying Lemma 3.1 to the pairs (D_U, f) and $(\tilde{D}_U^h, g)$ we conclude that equation (3.7) has a nonsingular solution S if the vectors $U^h f$ and $\tilde{U} g$ have no zero components. A nonsingular solution S to matrix equation (3.7) being found one can compute the vectors u and v due to the nonsingularity of the matrix D_U. The solution S to matrix equation (3.7) depends on the choice of vectors f and g. These additional degrees of freedom allows us to formulate the problem for determining optimal vectors f and g in the following form:

Problem 3.2. *For a given matrix D_U and given cluster K_0 find real vectors f and g and a matrix $\tilde{D}_U$ which minimize the condition number of the matrix S determined from matrix equation* (3.7).

This formulation of Optimization Problem 3.2 seems to be quite natural because as it will be shown below the estimate of the growth of the condition number of eigenvector matrix when passing from A to $\tilde{A}$ and all perturbation estimates for the translated and the condensed eigenvalues in the case $R_M(A) \neq 0$ involve the term $Cond(S)$ (cf. Lemmata 3.2–3.3).

In section 3.4 we present an approach to a suboptimal solution of Optimization Problem 3.2. Now we suppose that for given D_U and K_0 we have found a solution ($\tilde{D}_U$, f, g and S) to Optimization Problem 3.2.

3.2. Numerical stability of eigenvalue translations

Let the vectors u and v from (3.1) be found for $R_M(A) = 0$ as described in section 3.1. We will utilize these vectors when translating a group of spread eigenvalues into the cluster also in the case $R_M(A) \neq 0$. Hence, we need now to investigate the numerical stability of translations of the spread eigenvalues, i.e., to estimate perturbations of condensed and translated eigenvalues with respect to the case $R_M(A) = 0$.

Definition 3.3. *We call translations of the spread eigenvalues numerically stable if the radii of the circles containing perturbed eigenvalues tend to zero when $\| R_M(A) \|$ tends to zero.*

To estimate the radii of the circles containing perturbed eigenvalues we will exploit Lemmata 2.1, 2.2, 2.3 and 2.6.

In order to prove the numerical stability of eigenvalue translations we present, according to Lemma 2.1, estimates of the norms of the equivalent perturbations of the matrix $\tilde{A}$ after which the corresponding block pair becomes the exact block eigenpair of the perturbed matrix.

Equalities (3.4) and (3.5) imply that the approximation to the right block eigenvector corresponding to the translated eigenvalues is of the form

$$\tilde{X}_M = X_M \hat{S}$$

where $\hat{S} = U^h S \tilde{U}$.

Lemma 3.2. *(a) There exists matrix E_{tr} such that the block pair $\{\tilde{\Lambda}_M, \tilde{X}_M\}$ is the block eigenpair of the matrix $\tilde{A} + E_{tr}$ and*

$$\| E_{tr} \| \leq \| R_M(A) \| \frac{(1 + \| uv^h \|)}{\sigma_{min}(X_M(H))}$$

(b) Let $\lambda(A)$ be an eigenvalue of A and $y(A)$ be the corresponding left eigenvector. Then there exists a matrix E_{cl} such that the pair $\{\bar{\lambda}(A), y(A)\}$ is the eigenpair of the matrix $(\tilde{A} + E_{cl})^h$ and such that

$$\| E_{cl} \| \leq \| R_M(A) \| \, |\lambda(A)| \, \| Y_M(H) \| \, \| uv^h \| \max_{\lambda \in Spec(D_U)} \frac{1}{|\lambda - \lambda(A)|}$$

Proof (a) Let $R_M(\tilde{A})$ be the block eigenresidual of the block pair $\{\tilde{\Lambda}_M, \tilde{X}_M\}$ with respect to the matrix $\tilde{A}$. Then, according to the first statement of the Lemma 2.2, the block pair $\{\tilde{\Lambda}_M, \tilde{X}_M\}$ is the exact block eigenpair of the matrix $\tilde{A} + E_{tr}$, where

$$E_{tr} = -R_M(\tilde{A})(\tilde{X}_M^h \tilde{X}_M)^{-1} \tilde{X}_M^h$$

Since

$$R_M(\tilde{A}) = A(I_n + X_U uv^h Y_U^h)\tilde{X}_M - \tilde{X}_M \tilde{\Lambda}_M = R_M(A)(I_m + U^h uv^h U)\hat{S}$$

we have

$$\begin{aligned} E_{tr} &= -R_M(A)(I_m + U^h uv^h U)\hat{S}(\hat{S}^h X_M^h X_M \hat{S})^{-1} \hat{S}^h X_M^h \\ &= -R_M(A)(I_m + U^h uv^h U)(X_M^h X_M)^{-1} X_M^h \end{aligned}$$

This equality implies the statement a) of the Lemma.

(b) Let $r(\tilde{A}^h)$ be the eigenresidual of the pair $\{\bar{\lambda}(A), y(A)\}$ with respect to the matrix $\tilde{A}^h$. We have

$$E_{cl} = -r(\tilde{A}^h) y(A)^h / \| y(A) \|^2$$

The equality

$$\tilde{A}^h y(A) - \bar{\lambda}(A) y(A) = \bar{\lambda}(A) Y_U v u^h X_U^h y(A)$$

implies that

$$\| E_{cl} \| \leq |\lambda(A)| \, \| Y_U \| \, \| uv^h \| \frac{\| X_U^h y(A) \|}{\| y(A) \|}$$

Now the statement (b) of the lemma follows from Lemma 2.2. ∎

Let us estimate the term $\| uv^h \|$ of the inequalities of Lemma 3.2.

Lemma 3.3. *The following inequality holds true:*

$$\| uv^h \| \leq \min_d \left[Cond(S) \max_{\tilde{\lambda} \in K_0} | \tilde{\lambda} - d | \max_{\lambda \in Spec(D_U)} \left| \frac{1}{\lambda} \right| + \max_{\lambda \in Spec(D_U)} \left| \frac{d}{\lambda} - 1 \right| \right].$$

Proof From equality (3.6) we obtain the equalities

$$D_U uv^h S = S\tilde{D}_U - D_U S = S(\tilde{D}_U - dI_m) - (D_U - dI_m)S$$

and hence

$$uv^h = D_U^{-1} S(\tilde{D}_U - dI_m)S^{-1} + dD_U^{-1} - I_m$$

which implies the statement of the lemma. ∎

Remark Strictly speaking, Lemma 3.2 describes only the numerical stability of the simple eigenvalues of the matrix A under transformation (3.1). The numerical stability of multiple eigenvalues of the matrix A can be proved in a similar way.

Let us estimate the condition numbers of eigenvalues of the matrix $\tilde{A}$. Equalities (2.2) and (3.1) imply the relation

$$\tilde{A}P = P\tilde{H} + \beta w \tilde{e}_k^h \tag{3.8}$$

where

$$\begin{aligned} \tilde{H} &= H(I_k + X_U(H)uv^h Y_U(H)^h) \\ \tilde{e}_k^h &= e_k^h(I_k + X_U(H)uv^h Y_U(H)^h) \end{aligned} \tag{3.9}$$

Equality (3.8) is similar to the first equality in (2.2). We have thus derived an *a posteriori* estimate of the spectral characteristics of the matrix $\tilde{A}$ (see Section 2). It should be emphasized that relation (3.8) provides an efficient procedure for numerical verification of the quality of constructed translations (3.1).

Equality (3.9) implies that condition number of the matrix made up with right eigenvectors of the matrix $\tilde{H}$ increase in at most $Cond(S)$ times as compared to the condition number of the matrix made up with right eigenvectors of the matrix H. Moreover, the above perturbation estimates contain the term $Cond(S)$ which justifies the suggested formulation of Optimization Problem 3.2.

3.3. Translation of different groups of spread eigenvalues

Let us justify the opportunity of consecutive translations of different groups of spread eigenvalues approximated by the Arnoldi procedure.

Lemma 3.4. *Under transformation* (3.1) *of the matrix A the eigenresidual of the pair* $\{\lambda_j(H), Px_j(H)\}$, $j \notin M$ *remains unchanged.*

Proof We have

$$r_j(\tilde{A}) = \tilde{A}Px_j(H) - \lambda_j(H)Px_j(H) = APx_j(H) - \lambda_j(H)Px_j(H) = r_j(A)$$

because $Y_U^h(H)x_j(H) = UY_M^h(H)x_j(H) = 0$ if $j \notin M$. ■

From Lemma 3.4 it follows that transformation (3.1) does not lead to any deterioration of the approximation accuracy of already approximated but not yet translated eigenvalues since the corresponding eigenresidual remains unchanged. It means that we can translate different groups of spread eigenvalues in an arbitrary order.

3.4. Suboptimal solution of Optimization Problem

In this subsection we describe an approach to a suboptimal solution of Optimization Problem 3.2.

Recall the formulation of Optimization Problem 3.2. We need to find a solution S to the matrix equation

$$D_U S - S\tilde{D}_U = fg^h \tag{3.10}$$

of the minimal condition number $Cond(S)$ assuming that the matrix D_U and the simply connected domain K_0 containing eigenvalues of the matrix $\tilde{D}_U$ are given.

Unfortunately, up to now we have not been able to present an optimal solution to Optimization Problem 3.2. In this paper we describe a suboptimal solution which allows us to obtain a successful numerical result (see section 5).

We split the solution of Optimization Problem 3.2 into the two different stages:

- *Stage 1.* For a specific choice of vectors f and g find an optimal distribution of the eigenvalues of the matrix $\tilde{D}_U$ in the cluster K_0.
- *Stage 2.* For the given matrix $\tilde{D}_U$ find the optimal vectors f and g which minimize $Cond(S)$.

To find the solution to Stage 1 of Optimization Problem 3.2 we first premultiply equality (3.10) by U^h and then postmultiply the result by $\tilde{U}$. Thus we get the equality

$$\Lambda_M \hat{S} - \hat{S}\tilde{\Lambda}_M = \hat{f}\hat{g}^h \tag{3.11}$$

where $\hat{S} = U^h S\tilde{U}$, $\hat{f} = U^h f$ and $\hat{g}^h = g^h\tilde{U}$.

The solution $\hat{S}$ to matrix equation (3.11) with the given Λ_M, $\tilde{\Lambda}_M$, $\hat{f}$ and $\hat{g}$ is the Cauchy type matrix [15] of the form

$$\{\hat{S}\}_{ij} = \frac{\{\hat{f}\}_i \{\bar{\hat{g}}\}_j}{\lambda_i - \tilde{\lambda}_j} \tag{3.12}$$

Moreover, let $\hat{\xi}$ and $\hat{\eta}$ be vectors of the length m and be the solutions to the linear systems

$$\begin{cases} \hat{S}\hat{\xi} = \hat{f} \\ \hat{\eta}^h\hat{S} = \hat{g}^h \end{cases} \tag{3.13}$$

Then the matrix $\hat{S}^{-1}$ takes the following form [15]

$$\{(\hat{S})^{-1}\}_{ij} = \frac{\{\hat{\xi}\}_i \{\bar{\hat{\eta}}\}_j}{\lambda_j - \tilde{\lambda}_i} \tag{3.14}$$

Unfortunately, in the general case of arbitrary vectors $\hat{f}$ and $\hat{g}$ we cannot estimate the condition number of the matrix $\hat{S}$ since the vectors $\hat{\xi}$ and $\hat{\eta}$ are unknown.

Let the vectors $\hat{f}$ and $\hat{g}$ be of the form

$$\hat{f}^h = \hat{g}^h = [1, \ldots, 1] \tag{3.15}$$

For these vectors $\hat{S}$ takes the form of the Cauchy matrix $\hat{C}$ [16]

$$\{ \hat{C} \}_{ij} = \frac{1}{\lambda_i - \tilde{\lambda}_j} \tag{3.16}$$

As in [16] we introduce the polynomials $\mathcal{L}(t)$ and $\tilde{\mathcal{L}}(t)$:

$$\mathcal{L}(t) = (t - \lambda_1) \cdots (t - \lambda_m), \ \tilde{\mathcal{L}}(t) = (t - \tilde{\lambda}_1) \cdots (t - \tilde{\lambda}_m)$$

Theorem 3.2 ([16]) *The inverse to the matrix $\hat{C}$ can be presented in the following form:*

$$\hat{C}^{-1} = -D\hat{C}^t F$$

where D and F are diagonal matrices with the diagonal entries

$$\{ F \}_{jj} = \frac{\tilde{\mathcal{L}}(\lambda_j)}{\mathcal{L}'(\lambda_j)}$$

and

$$\{ D \}_{jj} = \frac{\mathcal{L}(\tilde{\lambda}_j)}{\tilde{\mathcal{L}}'(\tilde{\lambda}_j)}$$

(here by $Z'(t)$ we denote the derivative of a polynomial $Z(t)$).

Therefore, the inequality

$$Cond(\hat{C}) \leq \| \hat{C} \|^2 \| D \| \| F \|$$

is valid. Denote

$$R = \min_{\substack{i,j \\ i \neq j}} | \lambda_i - \lambda_j |; \quad r = \min_{\substack{i,j \\ i \neq j}} | \tilde{\lambda}_i - \tilde{\lambda}_j |$$

$$R_K = \max_i | \tilde{\lambda}_i |; \quad R_O = \max_i | \lambda_i |$$

Now, we have

$$\| F \| = \max_i | \{ F \}_{ii} | \leq \frac{(R_K + R_O)^m}{R^{m-1}}$$

and

$$\| D \| = \max_i | \{ D \}_{ii} | \leq \frac{(R_K + R_O)^m}{r^{m-1}}$$

By construction there exists some constant d such that

$$\min_{\substack{\tilde{\lambda}\in K_0 \\ \lambda\in Spec(D_U)}} \quad |\,\tilde{\lambda}-\lambda\,| \geq d > 0.$$

From (3.16) we obtain the estimate $\| \hat{C} \| \leq m/d$.
Taking into account all derived estimates we get the final bound of the form

$$Cond(\hat{C}) \leq \left[\frac{(R_K + R_O)^2}{Rr}\right]^m m^2 \frac{Rr}{d^2} \tag{3.17}$$

It can be easily shown that the vectors $\hat{f}$ and $\hat{g}$ from equality (3.15) are the eigenvectors of the matrices U and $\tilde{U}$, respectively, corresponding to the eigenvalue equal to unity and hence the vectors f and g are real. Now from estimate (3.17) it is possible to choose a distribution of the eigenvalues of the matrix $\tilde{\Lambda}_M$ in the cluster K_0 to minimize the upper bound of the condition number of the matrix S under special choice (3.15) of the vectors $\hat{f}$ and $\hat{g}$.

Consider the solution of Stage 2 of Optimization Problem 3.2. Denote by $Diag(\hat{f})$ the diagonal matrix whose (j, j)th diagonal entry is equal to $\{\hat{f}\}_j$. For arbitrary vectors $\hat{f}$ and $\hat{g}$ the matrix $\hat{S}$ can be presented as follows:

$$\hat{S} = Diag(\hat{f})\hat{C}Diag(\bar{\hat{g}}) \tag{3.18}$$

It can be easily seen that $C = U\hat{C}\tilde{U}^h$ is a real matrix. Premultiplying equation (3.18) by U and postmultiplying the result by $\tilde{U}^h$ we obtain

$$S = UDiag(\hat{f})U^h C\tilde{U}Diag(\bar{\hat{g}})\tilde{U}^h \tag{3.19}$$

By the definition the vectors $f = U\hat{f}$ and $g = \tilde{U}\hat{g}$ are real. Now to find the solution to Stage 2 to Optimization Problem 3.2 we must find vectors f and g such that the two-sided block-diagonal scaling of form (3.19) reduces as much as possible the condition number of the matrix S. In our numerical experiments we use the scaling from [2] and the scaling with the vectors $\hat{f}$ and $\hat{g}$ determined from equality (3.15). Actually when translating a group of eigenvalues we compute condition numbers of S for both scalings and utilize the scaling leading to the smallest condition number.

4. Realizing eigenvalue translation preconditioned GMRES(k) algorithm

There may exist many implementations of the eigenvalue translation preconditioned GMRES(k) method which may take into account particular properties of coefficient matrices. However, being mainly interested in construction of a black box iterative solver (see condition (a) from the 'Introduction') by minimizing user-prescribed problem-dependent parameters we will not pay any attention to comparison of different implementations. To demonstrate potential capabilities of the eigenvalue translation technique we describe in this paper only one algorithm which can be exploited as an almost black box for efficient iterative solution of large, sparse offdiagonally dominant possibly indefinite unsymmetric linear

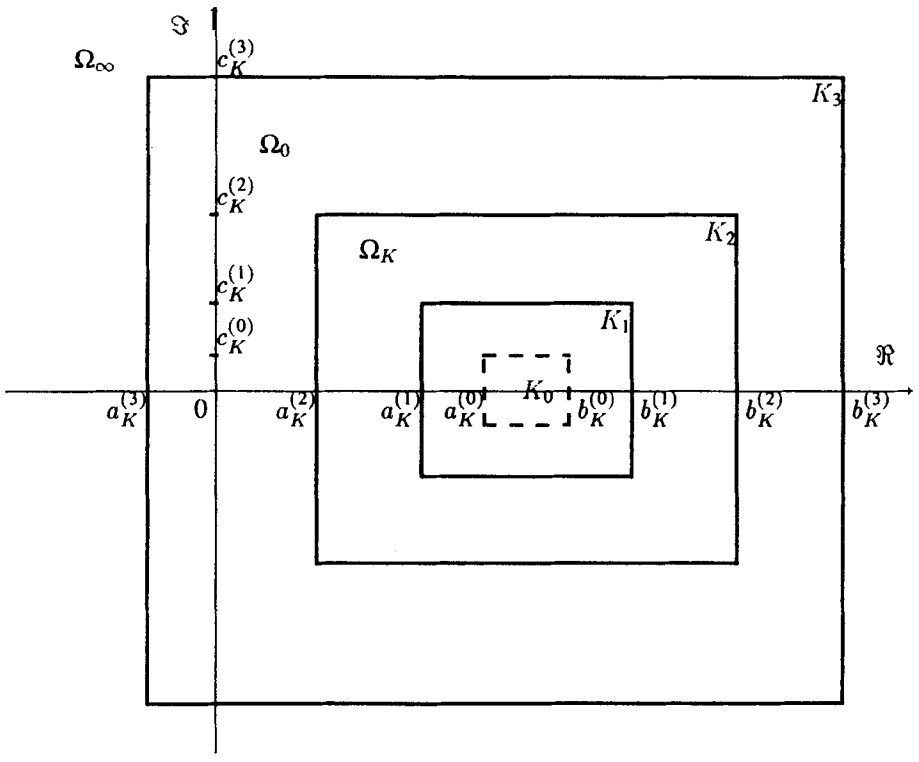

Figure 1. Translation domains for different translation stages

systems. Optimization of eigenvalue translation based preconditionings and comparison of their implementations will be considered in more detail in a forthcoming paper.

In section 3 we derived Optimization Problem 3.2 and described its suboptimal solution to construct the vectors u and v required when translating into a cluster K_0 a block spread eigenvalue Λ_M. Now in order to describe a numerical algorithm realizing the eigenvalue translation preconditioned GMRES(k) method we need to specify how to make a proper choice of Λ_M. When choosing a strategy of eigenvalue translations in the GMRES(k) method we should take into account that the Arnoldi procedure provides sufficiently accurate approximations only for the eigenpairs corresponding to the eigenvalues which lie near the boundary of the convex hull containing the spectrum and which are well separated from other eigenvalues [11]. Hence, all these eigenvalues being treated as spread can be easily translated into the cluster.

To this end for a given cluster K_0 not containing the origin (a rectangle $K_0(a_K^{(0)}, b_K^{(0)}, c_K^{(0)})$, say, see Figure 1) let us prescribe three larger rectangles $K_1(a_K^{(1)}, b_K^{(1)}, c_K^{(1)})$, $K_2(a_K^{(2)}, b_K^{(2)}, c_K^{(2)})$ and $K_3(a_K^{(3)}, b_K^{(3)}, c_K^{(3)})$, $K_0 \supset K_1 \supset K_2 \supset K_3$ (see Figure 1). We require that at the first translation stage all spread eigenvalues from Ω_∞ lying outside K_3 must be translated first. Only after translating all these eigenvalues we translate at the second translation stage all spread eigenvalues from Ω_0. Finally, at the third translation stage we

translate all spread eigenvalues from Ω_K. This translation strategy seems to be quite natural since, due to the approximation property of the Arnoldi procedure at each translation stage, we try to translate only better-approximated spread eigenvalues. However, there may exist eigenvalues close the origin lying near the boundary of the convex hull which are not well separated from other eigenvalues and hence which cannot be sufficiently accurately approximated by the Arnoldi procedure. These eigenvalues may cause a very slow convergence of the GMRES(k) method. In this case we may only try to improve approximations to such eigenpairs by increasing the parameter k of the GMRES(k) method since we cannot expect that at the next cycle of the Arnoldi procedure with the transformed matrix $\tilde{A}$ considerably more accurate approximations to these eigenpairs will be computed. Note that we may need several GMRES(k) iterations to complete one translation stage.

When assembling some spread eigenvalues corresponding to the current translation stage into a block eigenvalue Λ_M to be translated we are mainly interested in maintaining the numerical stability. To this end according to estimates of Lemma 3.2 and condition (4) on the transformation we should assemble into Λ_M those spread eigenvalues which minimize the norm of the transformation matrix $(I_n + X_U u v^h Y_U^h)$ and $Cond(S)$ of the matrix solution to (3.7). Actually, minimization may lead to a reduction of the number of spread eigenvalues to be translated by one group and hence to an increase of the number of transformations (3.1). To find a constructive compromise we fix maximal allowable values $cond_{max}$ and $trnorm_{max}$ of $Cond(S)$ and of the norm of the transformation matrix, respectively.

Now we describe our Eigenvalue Translation preconditioned GMRES(k) algorithm:

The ET-p-GMRES(k) Algorithm:

Initialization:

Set

an initial guess to the solution x_0;
the number k_{min} of the Arnoldi iterations to be performed at each GMRES(k) iteration and the maximal number k_{max} of the Arnoldi iterations to be performed if necessary to improve approximations to spread eigenpairs;
the geometric parameters of the translation stages $a_K^{(i)}, b_K^{(i)}, c_K^{(i)}, i = 0, 1, 2, 3$;
the maximal numbers m_i , $i = 1, ..., 3$ of spread eigenvalues to be translated in one group at each translation stage.

Global p-GMRES(k) loop: iterate until convergence

Step 1. Set $k = k_{min}$.

Step 2. Perform k iterations of the Arnoldi procedure.

Step 3. Compute the required spectral characteristics of the Arnoldi matrix H and determine the translation stage; if the spectrum of the matrix H corresponds to the second translation stage and $k = k_{min}$ then set $k = k_{max}$ and continue Step 2.

Step 4. Arrange all real and complex conjugate spread eigenvalues to be translated at this stage into the list in order to maximize the minimal distance between eigenvalues translated by one group (due to estimate (3.17) it may lead to a reduction of $Cond(S)$).

Step 5. Take $m = m_i$. Choose the first m spread eigenvalues from the list (we translate first all real eigenvalues and next all complex conjugate eigenvalues), compute for the

chosen group $Cond(S)$ and $\|I_n + X_U u v^h Y_U^h\|$, if they satisfy the stability criterion for the given $cond_{max}$ and $trnorm_{max}$ go to Step 6, else reduce the number m of spread eigenvalues in the group such that they satisfy the stability criterion; if none of spread eigenvalues satisfies the stability criterion then do not translate any eigenvalue and go to Step 7, else go to Step 6.

Step 6. Perform transformation (3.1) and remove the translated eigenvalues from the list, if all required spread eigenvalues are already translated go to Step 7, else go to Step 5.

Step 7. Complete the current GMRES(k) iteration and check the accuracy, if not accurate enough then go to Step 1 with the transformed coefficient matrix.

Note that it may happen that we can not find at the current translation stage any spread eigenvalue to be translated according to the given values of $cond_{max}$ and $trnorm_{max}$. In this case we do not translate any eigenvalue and perform only restarted GMRES(k) iterations. In our numerical experiment we have used the standard realization of the GMRES(k) method suggested in [13] for which translation of spread eigenvalues with large $Cond(S)$ or $\|I_n + X_U u v^h Y_U^h\|$ may produce jumps of the residuals when passing from one to another global GMRES(k) iteration, due to relatively large rounding errors (see the 'Introduction').

When performing numerical experiment we fix $m_1 = 2$, $m_2 = 4$, $m_3 = 6$, $a_0 = 0.75$, $b_0 = 1.25$, $c_0 = 0.25$, $a_1 = 0.6$, $b_1 = 1.4$, $c_1 = 0.4$, $a_2 = 0.3$, $b_2 = 1.7$, $c_2 = 0.7$, $a_3 = -0.2$, $b_3 = 3.0$, $c_3 = 2.0$, $cond_{max}$ =5.D+5, $trnorm_{max}$ =5.D+5 (it should be emphasized that in most cases variations of these parameters only slightly affect the resulting convergence of the ET-p-GMRES(k)).

Remark The ET-p-GMRES(k) method was extensively exploited when solving many industrial problems (some numerical results can be found in [7]). We emphasize that in all cases the above set of parameters remains unchanged.

5. The numerical experiment

Owing to the lack of space we describe here only one numerical experiment with the ET-ILU-GMRES(k) algorithm from section 4 when solving the sample linear system coming from the model CFD problem governed by the fully coupled 2-D Navier–Stokes equations. The Model Problem describes the steady-state essentially transonic flow with a subcritical Mach number close to 1 over a profile (a detailed description of the model problem can be found in [7]).

The Model Problem was approximated on the 61×81 highly nonuniform curvilinear mesh. The resulting system of nonlinear equations was solved by the Newton method. At each nonlinear iteration it results in the extremely ill-conditioned Jacobian of order 19 764 with 689 296 nonzero entries. As the test matrix A we have chosen

$$A = \partial F / \partial X B^{-1}$$

where $B = LU$ is the incomplete triangular decomposition by positions of the Jacobian $\partial F / \partial X = LU + R$.

It should be emphasized that when computing the incomplete triangular factorization we did not pay any attention to signs and values of its pivots. The resulting restarted ILU-GMRES(k) does not converge even with $k = k_{max} = 50$ due to spread eigenvalues with

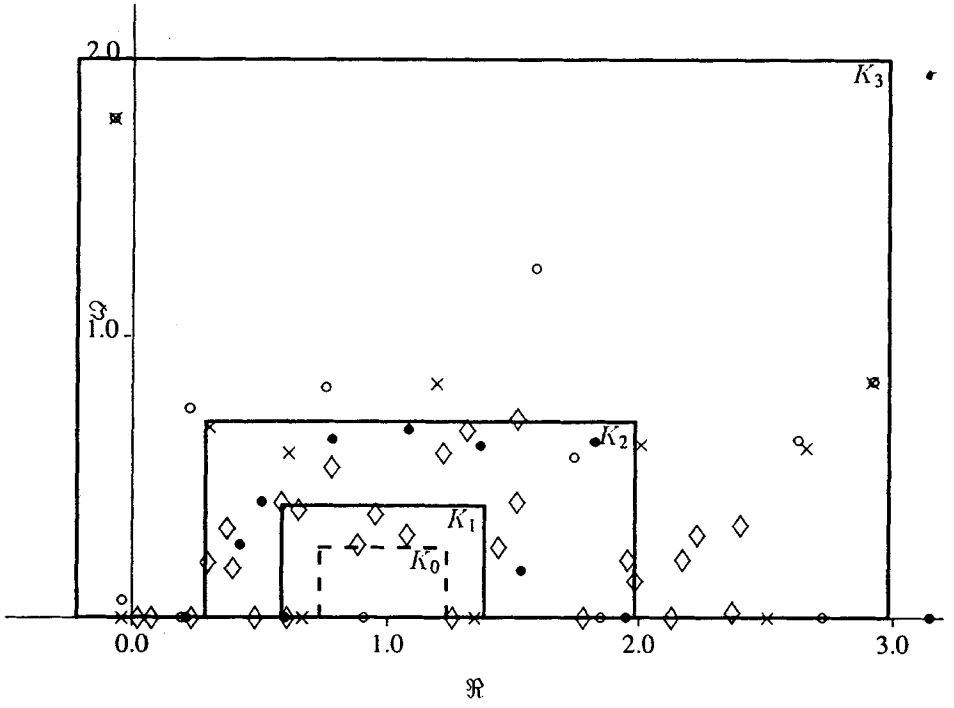

Figure 2. Spectra of the Arnoldi matrices H_i, $i = 1, 2, 3, 4$ at consecutive ET-ILU-GMRES(k) iterations: eigenvalues of H_1 are denoted by '$\times$', eigenvalues of H_2 are denoted by '$\circ$', eigenvalues of H_3 are denoted by '$\diamond$', and eigenvalues of H_4 are denoted by '$\bullet$'

negative real parts of the preconditioned matrix. These eigenvalues appear at each restarted ILU-GMRES(k) iteration and cannot be approximated with the sufficient accuracy even with this large value of k. Any attempt to compute the modified ILU factorization taking into account signs and values of pivots did not lead to any improvement of the convergence.

We solve the system of linear equations

$$Ax = b$$

by the ET-ILU-GMRES(k) method with parameters $k_{min} = 20$, $k_{max} = 50$. In this numerical experiment we utilize the following stopping criterion:

$$\| r_i \| / \| r_0 \| \leq 10^{-8}$$

where $r_i = b - Ax_i$ is the true residual.

Four ET-ILU-GMRES(k) iterations with 1 transformation (3.1) after the first iteration, with 7 transformations (3.1) after the second iteration and with 13 transformations (3.1) after the third iteration were required to satisfy the above stopping criterion (the total number of translated spread eigenvalues is equal to 44 and the total number of translations is equal to 21). The total arithmetic costs for constructing and realizing the ET preconditioned

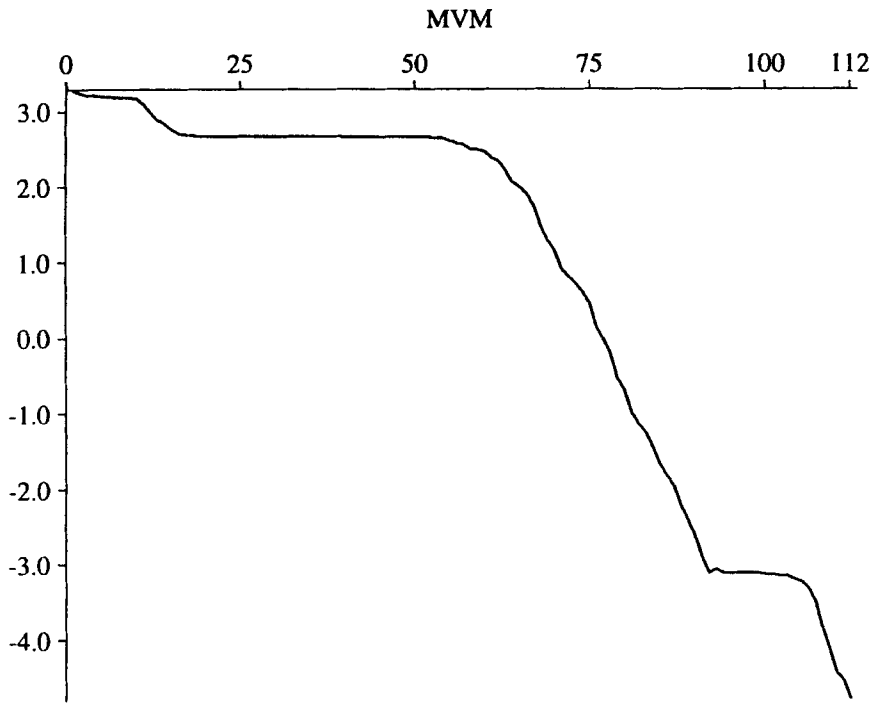

Figure 3. The convergence history of the residuals of the ET-ILU-GMRES(k)

GMRES(k) method (including the costs for computing the orthonormal basis of the Krylov subspace, the costs for solving the local minimization problem and the costs for constructing and realizing the eigenvalue translation preconditioning, i.e., everything except the costs for multiplying the preconditioned matrix by a vector) comprise 24% of the total arithmetic costs (including the costs for constructing the ILU preconditioner) for computing the iterative solution by the ET-ILU-GMRES(k) algorithm.

In Figure 2 we show spectrum condensations at consecutive ET-ILU-GMRES(k) iterations (to make Figure 2 more comprehensible not all eigenvalues of the Arnoldi matrices are marked). In Tables 1–2 we present some eigenvalues of the Arnoldi matrices H_1 and H_4, their condition numbers and the eigenresiduals of the corresponding eigenpairs. In Figure 3 we present the convergence history of norms of the residuals of the ET-ILU-GMRES(k) method in terms of the number of the preconditioned matrix–vector multiplications.

6. Conclusion

In this paper we suggested an approach to construction of high-quality preconditionings via iteration data of the Arnoldi procedure and described an application of this technique to preserve the information when realizing the restarted GMRES(k) method.

The efficiency of the presented ET-p-GMRES(k) algorithm was demonstrated numeri-

Table 1. Eigenvalues of the Arnoldi matrix H_1 at the first ET-ILU-GMRES(k) iteration, their condition numbers and eigenresiduals of the corresponding approximations to the eigenpairs of A

j	$\Re(\lambda_j(H))$	$\Im(\lambda_j(H))$	$\mathcal{S}_{\lambda_j(H)}(H)$	$\| r_j(A) \|$
1	$-0.1361D+02$	$0.0000D+00$	$0.787D+01$	$0.692D-17$
2	$-0.2583D+01$	$0.0000D+00$	$0.572D+01$	$0.967D-07$
3	$-0.1001D+00$	$0.1790D+01$	$0.271D+01$	$0.202D-03$
4	$-0.1001D+00$	$-0.1790D+01$	$0.271D+01$	$0.202D-03$
5	$-0.6713D-01$	$0.0000D+00$	$0.283D+01$	$0.212D+00$
6	$0.2750D+00$	$0.6844D+00$	$0.632D+01$	$0.679D-01$
7	$0.2750D+00$	$-0.6844D+00$	$0.632D+01$	$0.679D-01$
19	$0.2890D+01$	$0.8471D+00$	$0.176D+01$	$0.523D-01$
20	$0.2890D+01$	$-0.8471D+00$	$0.176D+01$	$0.523D-01$

Table 2. Eigenvalues of the Arnoldi matrix H_4 at the fourth ET-ILU-GMRES(k) iteration, their condition numbers and eigenresiduals of the corresponding approximations to the eigenpairs of A

j	$\Re(\lambda_j(\tilde{H}))$	$\Im(\lambda_j(\tilde{H}))$	$\mathcal{S}_{\lambda_j(\tilde{H})}(\tilde{H})$	$\| r_j(\tilde{A}) \|$
1	$0.1850D+00$	$0.0000D+00$	$0.152D+04$	$0.630D-04$
2	$0.3928D+00$	$0.2592D+00$	$0.369D+04$	$0.225D-03$
3	$0.3928D+00$	$-0.2592D+00$	$0.369D+04$	$0.225D-03$
17	$0.1924D+01$	$0.0000D+00$	$0.176D+04$	$0.805D-04$
18	$0.3120D+01$	$0.0000D+00$	$0.144D+05$	$0.112D-09$
19	$0.7458D+01$	$0.0000D+00$	$0.128D+05$	$0.349D-18$

cally when solving the practical CFD problem. However, we believe that the performance of this algorithm can be significantly improved especially by improving the quality of the solution of Optimization Problem 3.2.

When analyzing the above results of the numerical experiment the following conclusions can be made:

1. The eigenvalue translation technique provides a promising approach to construction of efficient and reliable iterative methods for solving large sparse unsymmetric offdiagonal dominant ill-conditioned matrices.
2. It should be noted that the high convergence rate is achieved even in the case when not all spread eigenvalues are translated into the cluster while the number of transformations (3.1) is much smaller than the number of spread eigenvalues of the preconditioned matrix.
3. Efficient application of the eigenvalue translation technique does not require from the user a prescription of several problem dependent parameters (see Remark 4).
4. The serial arithmetic extra costs for computing all transformations (3.1) and for realizing eigenvalue translation preconditioning are relatively small. Moreover, the eigenvalue translation technique can be applied in the case when only a procedure for multiplying the coefficient matrix by a vector is available.
5. It should be emphasized that according to the estimates of Lemma 3.2 we may expect numerically stable translations of only spread eigenvalue with sufficiently small eigenresiduals. Numerical experiments show that actually we can successfully translate spread eigenvalues with relatively large eigenresiduals.

The authors plan to develop the suggested eigenvalue translation technique in the following directions:

- Construction of block transformation (3.1) and reformulation of the Optimization Problem to compute the eigenvalue translations in order to increase the number of spread eigenvalues to be translated simultaneously.
- The eigenvalue translation technique being considered as a method for approximating matrices can be efficiently applied for solving the Partial Pole Assignment Problem.

Acknowledgements

The authors would like to express their deep gratitude to Professor Biswa Nath Datta for introducing them into Partial Pole Assignment problematic. The authors also thank Dr. A. Nikishin for many helpful discussions and Professor Ju. Lifshitz, Dr. O. Zaytsev and Dr. I. Babaev for assistance when choosing the model CFD problems and performing numerical experiments.

REFERENCES

1. W. Arnoldi. The principle of minimized iterations in the solution of the matrix eigenvalue problems. *Quart. Appl. Math.*, 9, 17–29, 1951.
2. Z. Bai, J. Demmel, and A. McKenney. On the conditioning of the nonsymmetric eigenproblems: theory and software. Technical Report 469, Courant Mathematical Institute, 1989.
3. F. Chatelin. *Spectral Approximation of Linear Operators.* Academic Press, New York, 1983.
4. B. Datta. Observer matrix equations and eigenvalue assignment problem. Technical report, 1989.
5. E. de Souza and S. Bhattacharyya. Controllability, observability and the solution of $AX - XB = C$. *Lin. Alg. Appl.*, 39, 167–188, 1981.

6. T. Eirola and O. Nevanlinna. Accelerating with rank-one updates. *Lin. Alg. Appl.*, 121, 511–520, 1989.
7. S. Kharchenko and A. Yeremin. Eigenvalue translation based preconditioners for the GMRES(k) method. Research Report EM-RR-2/92, Elegant Mathematics, Inc. (USA), 1992.
8. S. Kharchenko and A. Yeremin. Stabilized multilevel variable block GMRES(k) method with block eigenvalue/singular value translation technique for solving extremely ill-conditioned unsymmetric linear systems on parallel computers. Research Report EM-RR-8/93, Elegant Mathematics, Inc. (USA), 1993.
9. N. Nachtigal, L. Reichel, and L. Trefethen. A hybrid GMRES algorithm for nonsymmetric linear systems. Technical report, 1991.
10. B. Parlett. *The Symmetric Eigenvalue Problem.* Prentice Hall, Englewood Cliffs, NJ, 1980.
11. Y. Saad. Variations on Arnoldi's method for computing eigenelements of unsymmetric matrices. *Lin. Alg. Appl.*, 34, 269–295, 1980.
12. Y. Saad. Projection and deflation methods for partial pole assignment in linear state feedback. *IEEE Trans. Automat. Contr.*, 33(3), 290–297, 1988.
13. Y. Saad and M. Schultz. GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Stat. Comput.*, 7, 856–869, 1986.
14. W. Shmidt, A. Jameson, and D. Whitfield. Finite volume solution to the Euler equations in transonic flow. *J. Aircraft*, 20(2), 127–133, 1983.
15. E. Tyrtyshnikov. *Toeplitz matrices, their analogues and applications.* Dept. Num. Math. of the USSR Academy of Sciences, 1989.
16. E. Tyrtyshnikov. Cauchy-Toeplitz matrices and some applications. *Lin. Alg. Appl.*, 149, 1–18, 1991.
17. H. Walker. Implementation of the GMRES method using Housholder transformations. *SIAM J. Sci. Stat. Comput.*, 9(1), 152–163, 1988.
18. J. Wilkinson. Sensitivity of eigenvalues. *Utilitas Math.*, 25, 5–76, 1984.
19. I. Yegorov and O. Zaytsev. On an approach to a numerical solution of 2D Navier-Stokes equation. *J. of Comput. Math. & Math. Phys.*, 3(2), 300–313, 1991.