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Block {ω}-circulant preconditioners for the systems of differential equations

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Abstract. The numerical solution of large and sparse nonsymmetric linear systems of algebraic equations is usually the most time consuming part of time-step integrators for differential equations based on implicit formulas. Preconditioned Krylov subspace methods using Strang block circulant preconditioners have been employed to solve such linear systems. However, it has been observed that these block circulant preconditioners can be very ill-conditioned or singular even when the underlying nonpreconditioned matrix is well-conditioned. In this paper we propose the more general class of the block {ω}-circulant preconditioners. For the underlying problems, ω can be chosen so that the condition number of these preconditioners is much smaller than that of the Strang block circulant preconditioner (which belongs to the same class with $\omega = 1$) and the related iterations can converge very quickly.

1 Introduction

In this paper, we consider a new class of preconditioners based on {ω}-circulant matrices for the iterative solution of the linear equations arising in the numerical solution of ordinary and time-dependent partial differential equations. In particular, these preconditioners are designed for the schemes which generate block-Toeplitz-like structures, i.e., that are small rank perturbations of block-Toeplitz matrices (see [3,4] for more detail).

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We recall that an $n \times n$ matrix $A_n = (a_{j,k})$ is said to be Toeplitz if $a_{j,k} = \alpha_{j-k}$, $j, k = 1, \ldots, n$, i.e., A_n is constant along its diagonals. An $n \times n$ matrix $\breve{A}_n$ is said to be circulant if it is Toeplitz and its diagonals satisfy $\breve{a}_{n-j} = \breve{a}_{-j}$, $j = 1, \ldots, n-1$. The circulant matrices $\breve{A}_n$ are diagonalized by the Fourier matrix $F = (F_{j,k})$, $F_{j,k} = e^{2\pi \mathbf{i} jk/n}/\sqrt{n}$, $j, k = 0, \ldots, n-1$, where $\mathbf{i}$ is the imaginary unit (see [19,15] and their references).

Definition 1 *W is an $n \times n$ $\{\omega\}$-circulant matrix if there exists a number ω such that*

$$W = \begin{pmatrix} a_0 & a_1 & \cdots & a_{n-1} \\ \omega a_{n-1} & a_0 & \cdots & a_{n-2} \\ \omega a_{n-2} & \omega a_{n-1} & \cdots & a_{n-3} \\ \vdots & \vdots & \cdots & \vdots \\ \omega a_1 & \omega a_2 & \cdots & a_0 \end{pmatrix}.$$

Moreover, we recall the following result (see [18]).

Theorem 1 *Let $\omega = \exp(\mathbf{i}\theta)$, $-\pi < \theta \leq \pi$, and W be an $n \times n$ $\{\omega\}$-circulant matrix. Then, the following decomposition holds:*

$$W = \Omega^* F^* \Lambda F \Omega, \tag{1}$$

where $\Omega = \operatorname{diag}(1, \omega^{-1/n}, \ldots, \omega^{-(n-1)/n})$, Λ is a diagonal matrix containing the eigenvalues of W and F is the Fourier matrix.

The numerical solution of an initial value problem (IVP) (or a boundary value problem (BVP)) for ordinary differential equations (ODE) and for time-dependent partial differential equations (PDE), either linear or nonlinear, can be reduced, at each integration step, to the solution of a linear IVP such as

$$\mathbf{y}'(t) = J_m \mathbf{y}(t) + \mathbf{g}(t), \ t \in (t_0, T], \quad \mathbf{y}(t_0) = \mathbf{z}, \tag{2}$$

where $\mathbf{y}(t), \mathbf{g}(t) : \mathbb{R} \to \mathbb{R}^m$, $\mathbf{z} \in \mathbb{R}^m$, and $J_m \in \mathbb{R}^{m \times m}$. Similarly, a nonlinear BVP can be reduced to a linear BVP. We apply to (2) fully implicit methods for differential equations based on linear multistep formulas in boundary value form (see [1,9] and their references). These methods approximate the solution of (2) by means of a discrete boundary value problem. We apply the following μ-step linear multistep formula over a uniform mesh $t_j = t_0 + jh$, for $j = 0, \ldots, s$, $h = (T - t_0)/s$, to (2):

$$\sum_{i=-\nu}^{\mu-\nu} \alpha_{i+\nu} \mathbf{y}_{n+i} = h \sum_{i=-\nu}^{\mu-\nu} \beta_{i+\nu} \mathbf{f}_{n+i}, \quad n = \nu, \ldots, s - \mu + \nu. \tag{3}$$

Here, $\mathbf{y}_n$ is the discrete approximation to $\mathbf{y}(t_n)$, $\mathbf{f}_n = J_m\mathbf{y}_n + \mathbf{g}_n$ and $\mathbf{g}_n = \mathbf{g}(t_n)$. The method in (3) should be used with ν initial conditions and $\mu - \nu$ final conditions. That is, we need the values $\mathbf{y}_0, \ldots, \mathbf{y}_{\nu-1}$ and the values $\mathbf{y}_{s-\mu+\nu+1}, \ldots, \mathbf{y}_s$. For example, the initial condition in (2) provides us only with one value, i.e., with $\mathbf{y}_0$. In order to obtain the other initial and final values, we have to provide $(\mu - 1)$ additional equations. The coefficients $\alpha_i^{(j)}$ and $\beta_i^{(j)}$ of these equations can be chosen so that the truncation errors for these initial and final conditions are of the same order as that in (3) (see [9, p. 132]). By combining (3) with the additional methods, we obtain a discrete boundary value problem. These equations can be restated to give the following linear system of algebraic equations:

$$M\mathbf{y} \equiv (A \otimes I_m - hB \otimes J_m)\mathbf{y} = \mathbf{e}_1 \otimes \mathbf{z} + h(B \otimes I_m)\mathbf{g} \equiv \mathbf{b}, \qquad (4)$$

where

$$\mathbf{e}_1 = (1, 0, \cdots, 0)^t \in \mathbb{R}^{(s+1)},\ \mathbf{y} = (\mathbf{y}_0, \cdots, \mathbf{y}_s)^t \in \mathbb{R}^{(s+1)m},$$

$\mathbf{g} = (\mathbf{g}_0, \cdots, \mathbf{g}_s)^t \in \mathbb{R}^{(s+1)m}$, and A and B are $(s+1)$-by-$(s+1)$ matrices given by

$$A = \begin{pmatrix}
1 & \cdots & 0 & & & & \\
\alpha_0^{(1)} & \cdots & \alpha_\mu^{(1)} & & & & \\
\vdots & \vdots & \vdots & & & 0 & \\
\alpha_0^{(\nu-1)} & \cdots & \alpha_\mu^{(\nu-1)} & & & & \\
\alpha_0 & \cdots & \alpha_\mu & & & & \\
 & \alpha_0 & \cdots & \alpha_\mu & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & \ddots & \ddots & \ddots & \\
 & & & & \alpha_0 & \cdots & \alpha_\mu \\
 & & 0 & & \alpha_0^{(s-\mu+\nu+1)} & \cdots & \alpha_\mu^{(s-\mu+\nu+1)} \\
 & & & & \vdots & \vdots & \vdots \\
 & & & & \alpha_0^{(s)} & \cdots & \alpha_\mu^{(s)}
\end{pmatrix}$$

and B defined similarly. The size of the matrix M can be very large when s or m are large. If a direct method is used to solve the system (4), e.g., for a multidimensional partial differential equation, the operation count can be much higher for practical applications than for that proposed (see the comparisons with a sparse direct solver in [3]).

In [2,3], Krylov subspace methods such as GMRES (Saad et al. [29]) or BiCGStab (van der Vorst [31]), have been proposed to solve (4). In order to speed up the convergence rate of Krylov subspace methods, circulant

matrices as preconditioners were considered there. The first preconditioner proposed in [2,3] for the matrix M in (4) is based on the well-known T. Chan circulant approximation (see [15]). The second one proposed in [2,3] is based on a new preconditioner called the P-circulant preconditioner. Moreover, in [3] and in [16,27] was the generalized Strang preconditioner for (4) was proposed. In these papers, it was shown theoretically and numerically that both the P-circulant and generalized Strang preconditioned iterations can converge very quickly. However, when the Jacobian matrix J_m in (4) has small or zero singular values, e.g., for differential problems with a constant steady-state solution (see [2,5]), the Strang block circulant preconditioner can be singular or severely ill-conditioned. To overcome these shortcomings, a modification of Strang's approximation was suggested in [4].

The main aim of this paper is to extend the preliminary results and the analysis in [7], where we proposed block preconditioners for nonsymmetric matrices based on skew-circulant matrices. In particular, here we propose the more general class of block $\{\omega\}$-circulant preconditioners for linear systems in (4).

We stress that other techniques for banded Toeplitz linear systems can be found, e.g., in [20,10,23,13] but they are very effective in the Hermitian case whereas, in general, the underlying matrices are nonsymmetric.

The approach in [17] is based on T. Chan's preconditioner. As observed in [3,5], this approach can be suitable for certain schemes, but can give ill-conditioned preconditioners even when the original matrices are well-conditioned. The approach described in [25] is based on the application of the preconditioner by using the normal equations. However, in [6] we observed that the related conjugate gradient iterations can converge very slowly.

The approaches in [11,24] are based on the factorization of generating functions of Toeplitz matrices. These preconditioners are not circulant matrices. Therefore, the corresponding preconditioners for the system (4) may not be efficiently inverted.

The paper is organized as follows. In Sect. 2, we introduce and analyze the new class of block preconditioners. In Sect. 3, the convergence of preconditioned iterations and the asymptotic computational cost of using various Krylov accelerators are discussed. Finally, numerical examples, remarks and comparisons are given in Sect. 4.

2 Block $\{\omega\}$-circulant preconditioners

In [2,3] and [16] the following generalized simple circulant (or Strang) preconditioner for (4) was introduced:

$$S = s(A) \otimes I_m - hs(B) \otimes J_m, \tag{5}$$

where $s(A)$, $s(B)$ were simple circulant (or Strang's circulant) approximations for A and B, i.e., $s(A)$ was given by

$$s(A) = \begin{pmatrix} \alpha_\nu & \cdots & \alpha_\mu & & & \alpha_0 & \cdots & \alpha_{\nu-1} \\ \vdots & \ddots & & \ddots & & & \ddots & \vdots \\ \alpha_0 & & \ddots & & \ddots & & & \alpha_0 \\ & \ddots & & \ddots & & \ddots & 0 & \\ & & \ddots & & \ddots & & \ddots & \\ & 0 & & \ddots & & \ddots & & \ddots \\ \alpha_\mu & & & & \ddots & & \ddots & \alpha_\mu \\ \vdots & \ddots & & & & \ddots & & \ddots \\ \alpha_{\nu+1} & \cdots & \alpha_\mu & & & \alpha_0 & \cdots & \alpha_\nu \end{pmatrix},$$

and $s(B)$ was defined similarly. Recall that the eigenvalues ϕ_j, $j = 0, \ldots, s$, of a circulant matrix $\breve{A}$ can be written as linear combinations of the entries $\tilde{\alpha}_j$, $j = 0, \ldots, s$, of its first row (see Davis [19]):

$$\phi_l = \sum_{j=0}^{s} \tilde{\alpha}_j u^{jl}, \quad l = 0, \ldots, s, \quad u = \exp\left(\frac{2\pi \mathbf{i}}{s+1}\right). \tag{6}$$

Notice that, due to the consistency condition $\sum_{j=0}^{\mu} \alpha_j = 0$ on the coefficients of (3) and to (6), $s(A)$ is always singular. If, for simplicity, J_m is diagonalizable, the eigenvalues of (5) are $\phi_j - h\psi_j\mu_r$, where ϕ_j, ψ_j, μ_r are the eigenvalues of $s(A)$, $s(B)$, J_m, respectively. Then, as observed in [4], if J_m has a zero (very small) singular value, then the preconditioner S is singular (can be severely ill-conditioned). In this case, the convergence can be impossible (very slow). The P-circulant approximation was proposed in [2,3] for the problems which have J_m as above and, in general, for other problems generating a preconditioned matrix $P^{-1}M$ which is ill-conditioned and/or which has the convex hull of the spectrum of the eigenvalues enclosing the origin of the complex plane (see [3,5]). The P-circulant preconditioner $p(A)$ is a circulant matrix, the entries of whose first row are given by $p_0, \ldots, p_{n-1}$, where

$$p_j = \frac{(s+1+j)\alpha_{j+\nu} + j\alpha_{j+\nu-(s+1)}}{s+1}, \quad j = 0, \ldots, s. \tag{7}$$

In this paper, we propose the more general class of block {ω}-circulant preconditioners for (4) to overcome the shortcoming mentioned above:

$$C = \tilde{s}(A) \otimes I_m - h\tilde{s}(B) \otimes J_m, \tag{8}$$

where $\tilde{s}(A)$, $\tilde{s}(B)$ are $\{\omega\}$-circulant matrices approximating A and B, respectively.

The $\{\omega\}$-circulant matrices are Toeplitz matrices whose first entry of a row is given by multiplying the last entry of the preceding row by ω (see Definition 1). Note that the $\{1\}$-circulant matrices ($\theta = 0$) are just circulant matrices, while $\{-1\}$-circulant matrices ($\theta = \pi$) are skew-circulant matrices. For instance, the simple (or Strang-type) skew-circulant approximation $\tilde{s}(A)$ for A in (2) is given by

$$\tilde{s}(A) = \begin{pmatrix} \alpha_\nu & \cdots & \alpha_\mu & & & -\alpha_0 & \cdots & -\alpha_{\nu-1} \\ \vdots & \ddots & & \ddots & & & \ddots & \vdots \\ \alpha_0 & & \ddots & & \ddots & & & -\alpha_0 \\ & \ddots & & \ddots & & \ddots & 0 & \\ & & \ddots & & \ddots & & \ddots & \\ & 0 & & \ddots & & \ddots & & \\ -\alpha_\mu & & & & \ddots & & \ddots & \alpha_\mu \\ \vdots & \ddots & & & & \ddots & & \vdots \\ -\alpha_{\nu+1} & \cdots & -\alpha_\mu & & & \alpha_0 & \cdots & \alpha_\nu \end{pmatrix},$$

and $\tilde{s}(B)$ defined similarly. The skew-circulant matrices as preconditioners for Hermitian and skew-Hermitian Toeplitz systems were considered in [12, 22, 14].

We observe that various trigonometric approximations can be combined. For example, $\{\omega\}$-P-circulant preconditioners can be defined by using (7) to give the first row of the related $\{\omega\}$-circulant approximation. A similar combination can be made by using T. Chan's optimal circulant matrices. However, for brevity, here we will focus mainly on Strang-type $\{\omega\}$-circulant preconditioners, giving some hints on extending the properties to other approximations. Moreover, it is straightforward to observe that P-circulant approximations can be seen as $\{\omega\}$-circulant preconditioners with $\omega = \exp(\mathbf{i}\theta)$, $\theta = 0$, whose entries are defined as in (7).

We prove that, under suitable assumptions on the formula (3), the block $\{\omega\}$-circulant preconditioner C in (8) is invertible.

The stability of a boundary value method is closely related to the two characteristic polynomials

$$\rho(z) = \sum_{j=0}^{\mu} \alpha_j z^j \quad \text{and} \quad \sigma(z) = \sum_{j=0}^{\mu} \beta_j z^j. \tag{9}$$

Note that they are polynomials of degree μ. A polynomial $p(z)$ of degree μ is an $N_{\nu,\mu-\nu}$-polynomial if

$$|z_1| \leq |z_2| \leq \cdots \leq |z_\nu| \leq 1 < |z_{\nu+1}| \leq \cdots \leq |z_\mu|,$$

and the roots z_j on the unit circle $|z| = 1$ are simple.

Definition 2 [9] *Consider the formula (3) with the characteristic polynomial $\rho(z)$ given by (9). The formula is said to be $0_{\nu,\mu-\nu}$-stable if $\rho(z)$ is an $N_{\nu,\mu-\nu}$-polynomial.*

Definition 3 [9] *Consider the formula (3) with the characteristic polynomials $\rho(z)$ and $\sigma(z)$ given by (9). The region*

$$\mathcal{D}_{\nu,\mu-\nu} = \{q \in \mathbb{C} : \rho(z) - q\sigma(z) \text{ has } \nu \text{ zeros inside } |z| = 1 \text{ and } \mu - \nu \text{ zeros outside } |z| = 1\}$$

is called the **region of $A_{\nu,\mu-\nu}$-stability** *of the formula. Moreover, the method is said to be $A_{\nu,\mu-\nu}$-stable if*

$$\mathbb{C}^- \equiv \{q \in \mathbb{C} : Re(q) < 0\} \subseteq \mathcal{D}_{\nu,\mu-\nu}.$$

It can be observed that the above definitions are a generalization of the well-known definitions of 0-stability and of A-stability for a linear multistep formula (see, e.g., [26, Chapter 3]).

We stress that the methods considered here are consistent, $0_{\nu,\mu-\nu}$-stable, $A_{\nu,\mu-\nu}$-stable and have as boundary locus a regular Jordan curve, where the boundary locus Γ of an LMF is given by

$$\Gamma = \left\{ q \in \mathbb{C} : q = \frac{\rho(z)}{\sigma(z)}.\ |z| = 1 \right\}, \tag{10}$$

$\rho(z)$, $\sigma(z)$ defined in (9) (see, e.g., [26, Sect. 3.8]). Methods which are consistent, $0_{\nu,\mu-\nu}$-stable, $A_{\nu,\mu-\nu}$-stable and which have as boundary locus a regular Jordan curve, are such that $\rho(z)$ has only the root $z = 1$ and $\sigma(z)$ has at most the root $z = -1$ on the unit circle $|z| = 1$ (see [9, Sect. 4.7]).

2.1 Boundary locus techniques for block circulant preconditioners

Recall that the eigenvalues of the underlying block preconditioner can be written as

$$\epsilon_j^{-\nu} \left(\tilde{\rho}(\epsilon_j) - h\, \lambda_r(J_m) \tilde{\sigma}(\epsilon_j) \right),\ r = 1, \ldots, m,\ j = 0, \ldots, s, \tag{11}$$

where

$$\tilde{\rho}(z) = \sum_{j=0}^{\mu} \tilde{\alpha}_j z^j, \quad \tilde{\sigma}(z) = \sum_{j=0}^{\mu} \tilde{\beta}_j z^j. \tag{12}$$

The coefficients of $\tilde{\rho}(z), \tilde{\sigma}(z)$ are derived from the characteristic polynomials (9). The argument ϵ_j in (11), $j = 0, \ldots, s$, is a point on the unit circle $|z| = 1$. For example, when $\epsilon_j = u_j$, $u_j = u^j$, then circulant matrices, and when $\epsilon_j = \tilde{u}_j$,

$$\tilde{u}_j = u^j \cdot \exp\left(\frac{\mathbf{i}\theta}{s+1}\right) = \exp\left(\mathbf{i}\frac{\theta + 2\pi j}{s+1}\right), \quad j = 0, \ldots, s,$$

then $\{\omega\}$-circulant matrices are considered in the expression (11), respectively. We also observe that the block skew-circulant and the simple circulant preconditioners are considered for $\tilde{\alpha}_j = \alpha_j, \tilde{\beta}_j = \beta_j, j = 0, \ldots, \mu$, in (12). On the other hand, an $\{\omega\}$-P-circulant-based preconditioner can be defined by taking coefficients as

$$\tilde{\alpha}_j = \alpha_j \left(1 + \frac{j-\nu}{s+1}\right), \ \tilde{\beta}_j = \beta_j \left(1 + \frac{j-\nu}{s+1}\right), \ j = 0, \ldots, \mu,$$

for the $\{\omega\}$-circulant matrices and similarly for T. Chan's optimal circulant preconditioners.

According to (11), a block preconditioner

$$R = c(A) \otimes I_m - h\, c(B) \otimes J_m, \tag{13}$$

where $c(G)$ is a $\{\omega\}$-circulant approximation for the matrix G, is nonsingular if the points $h\,\lambda_r(J_m)$, $r = 1, \ldots, m$, $h > 0$, do not belong to the set

$$\Sigma = \left\{ q \in \mathbb{C} : q = \frac{\tilde{\rho}(z)}{\tilde{\sigma}(z)}, \ z = \epsilon_j, \ j = 0, \ldots, s \right\}. \tag{14}$$

We call the finite set Σ the *discrete boundary locus* of the underlying block preconditioner. It is worth noting that the boundary locus Γ of formula (3) is a continuous set in $\mathbb{C}$. Thus Σ is a finite set of points in Γ. The last property does not hold for P-circulant and optimal circulant-based preconditioners. However, there exist classes of LMF such that the set Σ is in $\mathbb{C}^+ = \{z \in \mathbb{C} : \Re(z) \geq 0\}$ with $\Re(z) \neq 0$ for the P-circulant approximations of the matrices A, B of their coefficients (see [5]).

We consider problems whose Jacobian matrices have their eigenvalues in the left half-plane, including the imaginary axis.

Definition 4 *An A-stable ($A_{\nu,\mu-\nu}$-stable if $\mu > \nu$) linear multistep formula is AP-stable ($AP_{\nu,\mu-\nu}$-stable if $\mu > \nu$) for the preconditioner (13) if*

$$\Sigma \subseteq \mathbb{C}^+ \ \textit{and} \ \tilde{\rho}(\epsilon_j) \neq 0, \ j = 0, \ldots, s.$$

Note that the AP-stability of formula (3) can be easily verified by drawing the boundary locus Ω directly. A sample for generalized Adams methods (see [9] for the coefficients) is shown in Fig. 1.

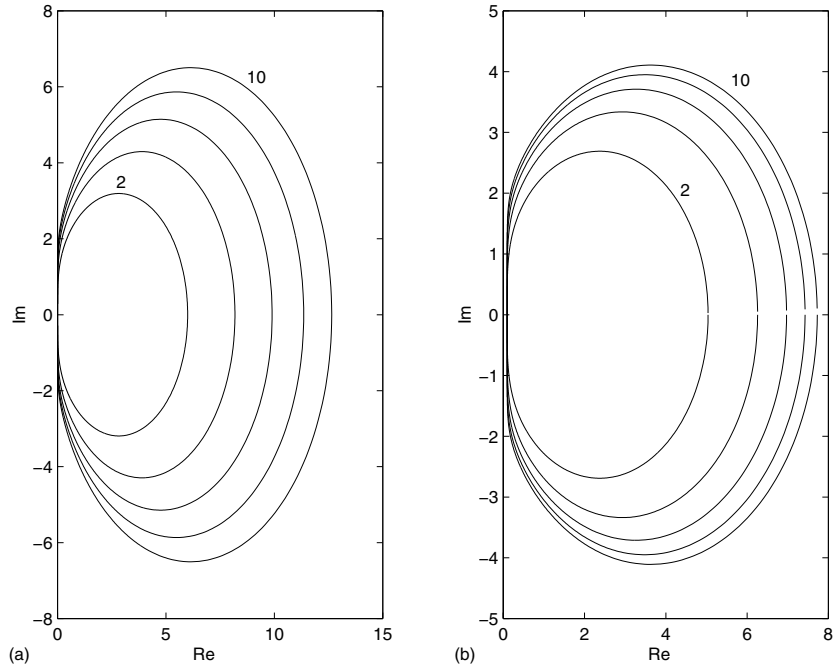

Fig. 1. Boundary locus of skew-circulant **(a)** and P-circulant **(b)** block preconditioners for generalized Adams method, $\mu = 2, 4, 6, 8, 10$, $s = 10$. Note that the formulas above are $AP_{\nu,\mu-\nu}$-stable for these preconditioners

Theorem 2 *For problem (2) with $\Re(\lambda_r(J_m)) \leq 0$, $r = 1, \ldots, m$, a block preconditioner (13) for an $AP_{\nu,\mu-\nu}$-stable formula (3) is invertible for all step-sizes $h > 0$.*

Corollary 1 *There exist no $AP_{\nu,\mu-\nu}$-stable formulas (3) for the simple block circulant preconditioner in (5).*

Proof It is enough to observe that, in (5), we have $\tilde{\rho}(1) = \rho(1) = 0$. □

Theorem 3 *An $A_{\nu,\mu-\nu}$-stable formula (3), whose boundary locus Γ in (10) is a regular Jordan curve, is $AP_{\nu,\mu-\nu}$-stable for block {ω}–(simple)–circulant preconditioners, $\omega = \exp(\mathbf{i}\theta)$ and $\theta \neq 2n\pi$, n an integer.*

Proof An $A_{\nu,\mu-\nu}$-stable LMF whose boundary locus is a regular Jordan curve is such that $\Gamma \in \mathbb{C}^+$ (see [9]). Therefore, $\Sigma \in \mathbb{C}^+$ for {ω}-circulant preconditioners based on the simple circulant matrices. However, if $\lambda_k(J_m) = 0$ for some k, then $\min_r \Re(\lambda_r(C)) > 0$. Indeed, expressions of the eigenvalues of the block preconditioner based on the {ω}-circulant matrix C as in (8) are given (see (6) and (1)) by

$$\tilde{u}_j^{-\nu} \left(\rho(\tilde{u}_j) - h\,\lambda_k(J_m)\sigma(\tilde{u}_j)\right), \quad j = 0, \ldots, s, \quad k = 1, \ldots, m, \qquad (15)$$

i.e., they are equal to the values assumed by the rational function

$$\frac{1}{z^{\nu}}\left(\rho(z) - h\,\lambda_k(J_m)\sigma(z)\right)$$

evaluated at

$$z = \tilde{u}_j = u^j \cdot \exp\left(\frac{\mathbf{i}\theta}{s+1}\right) = \exp\left(\mathbf{i}\frac{\theta + 2\pi j}{s+1}\right), \quad j = 0, \ldots, s,$$

where $\omega = \exp(\mathbf{i}\theta)$. We note that, by arguments similar to those for the block preconditioner based on Strang's circulant as in [16], if $h\lambda_k(J_m) \in \mathcal{D}_{\nu,\mu-\nu}$, then the polynomial

$$p(z) = \rho(z) - h\,\lambda_k(J_m)\sigma(z)$$

of degree μ has no roots on the unit circle $|z| = 1$. Therefore, the expressions (15), i.e., the eigenvalues of the block preconditioner C, cannot be zero. Note that, if $\Re(\lambda_k(J_m)) < 0$, then $h\lambda_k(J_m) \in \mathcal{D}_{\nu,\mu-\nu}$, and the $\{\omega\}$-circulant preconditioner is nonsingular.

If $\lambda_k(J_m) = 0$ for some k, then (15) gives

$$\frac{1}{\tilde{u}_j^{\nu}}\rho(\tilde{u}_j), \;\; j = 0, \ldots, s.$$

From the hypotheses, the only zero of $\rho(z)$ of unit modulus for the underlying methods is at $z = 1$, but $\tilde{u}_j \neq 1$ for all j if $\theta \neq 0$, $-\pi < \theta \leq \pi$. Therefore, (15) cannot be zero if the Jacobian matrix J_m is such that $\Re(\lambda_k(J_m)) \leq 0$, $k = 1, \ldots, m$. □

Similar results can be stated for P-circulant preconditioners by using the results on the eigenvalues of P-circulant matrices that can be found in [5] by observing that the minimum eigenvalue of an $\{\omega\}$-P-circulant matrix is now such that

$$\tilde{\rho}(1) \geq \sum \tilde{\alpha}_j \geq \frac{1}{s+1} > 0,$$

i.e., can be bounded below independently of θ. Note that a similar bound for $\{\omega\}$–(simple)–circulant matrices cannot be stated.

2.2 The choice of ω

Remark 1 We observe that the $\{\omega\}$-circulant simple approximation which gives the "best" block preconditioners (8) has $\omega = -1$, i.e., $\theta = \pi$ (see Definition 1 and Theorem 1) and then is skew-circulant.

Indeed, a good ({ω}-circulant) preconditioner using a certain ({ω}-circulant) approximation $a_n(T)$ for an $n \times n$ (small rank perturbation of a) Toeplitz matrix T_n can be expected if $a_n(T)$ has the following properties:

1) there exist matrices E, R such that $a_n(T) - T_n = E + R$, $\mathrm{rank}(E) = e$ is small with respect to n, independent of n and $||R|| = \delta$, $\delta \ll ||a_n(T)||$, where $||\cdot||$ is a p-norm or the Frobenius norm (note that $e = e(\omega)$ and $\delta = \delta(\omega)$ for {ω}-circulant matrices);
2) $a_n(T)$ is nonsingular and well-conditioned;
3) $a_n(T)$ is easy and cheap to compute from T and the linear system $a_n(T)v = \hat{v}$ is easy and cheap to solve.

The above claims are well-known for circulant matrices and, more generally, for trigonometric preconditioners (see [30,3,4]), and can be easily adapted for {ω}-circulant matrices. A more detailed discussion can be found in [5].

We observe that the conditions 1) and 3) above can be satisfied by any choice of $\theta \in (-\pi, \pi]$ for $\omega = \exp(\mathbf{i}\theta)$ (recall Definition 1 and Theorem 1). To this end, if $c_1, \ldots, c_n$ are the entries of the first row of the matrix $F^* \Lambda F$ in (8) and $t_0, \ldots, t_{n_1}, t_0, \ldots, t_{-n_2}$, $n_1, n_2 < \lceil n/2 \rceil$, are the entries of the first row and column of T, respectively, the following conditions must be satisfied:

$$c_1 = t_0, c_2\omega^{-1/n} = t_2, \ldots, c_{n_1}\omega^{-(n_1-1)/n} = t_{n_1},$$

$$c_n\omega^{1/n} = t_{-1}, c_{n-1}\omega^{2/n} = t_{-2}, \ldots, c_{n-n_2+1}\omega^{n_2/n} = t_{-n_2}.$$

Note that, if $\theta = 0$ or if $\theta = \pi$, T is a banded matrix and the {ω}-circulant approximation is of generalized Strang-type, then the parameters characterizing $a_n(T)$ need not be computed each time we change n (i.e., for (3), the time-step discretization), $n \geq \mu + 1$. However, condition 2) above requires that $\theta \neq 0$ (i.e., $\omega \neq 1$, as otherwise $a_n(T)$ is the standard Strang's circulant approximation of T). Finally, if $-\pi < \theta \leq \pi$,

$$\min_{\theta=\pi} \sigma_j(a_n(T)) > \min_{\theta\neq\pi} \sigma_j(a_n(T)) \geq 0, \tag{16}$$

where the $\sigma_j(\cdot)$, $j = 1, \ldots, n$, are the singular values of the underlying matrix, i.e., the absolute values of its eigenvalues (because A_n in our case is normal). Therefore, the condition number of A_n is minimum for $\theta = \pi$ and for that value we have experienced the better performances. However, property (16) can have a moderate influence on the behavior of the preconditioned iterations if the Jacobian matrix in (4) does not have small singular values or eigenvalues whose imaginary parts are much greater than their real parts (see the numerical experiments in [3,16,27]). Finally, note that a different choice of θ could yield more convenient values for $e = e(\omega)$ and $\delta = \delta(\omega)$, improving the convergence rate.

3 Convergence of preconditioned iterations

The spectrum of the preconditioned system is clustered around $(1, 0) \in \mathbb{C}$ and hence the convergence of a Krylov subspace method can be faster if the underlying preconditioner is used. By using arguments similar to those used in [3, Theorem 4.2], we obtain the following result.

Theorem 4 *If the block $\{\omega\}$-circulant preconditioner C is such that $\omega = \exp(\mathbf{i}\theta)$, $-\pi < \theta \leq \pi$, $\theta \neq 0$ and $\Re(\lambda_r(J_m)) \leq 0$, $r = 1, \ldots, m$, then the eigenvalues of the preconditioned matrix $C^{-1}M$ are equal to $1 \in \mathbb{C}$ except for at most $2m\mu$ outliers.*

Proof Let $E = M - C$; by (8),

$$E = ((A - \tilde{s}(A)) \otimes I_m) - h(B - \tilde{s}(B)) \otimes J_m) = L_A \otimes I_m - hL_B \otimes J_m.$$

It is easy to check that L_A and L_B are $(s + 1)$-by-$(s + 1)$ matrices with nonzero entries at most in the following four corners: a ν-by-$(\mu + 1)$ block in the upper left; a ν-by-ν block in the upper right; a $(\mu - \nu)$-by-$(\mu + 1)$ block in the lower right; and a $(\mu - \nu)$-by-$(\mu - \nu)$ block in the lower left. Since $\mu > \nu$, $\operatorname{rank}(L_A) \leq \mu$ and $\operatorname{rank}(L_B) \leq \mu$. Thus, we have

$$\operatorname{rank}(L_A \otimes I_m) \leq m\mu \quad \text{and} \quad \operatorname{rank}(L_B \otimes J_m) \leq m\mu.$$

The result follows. □

We remark that often the pattern of the matrices A, $\tilde{s}(A)$, B and $\tilde{s}(B)$ is such that the rank of E is $m\mu$. Therefore, in these cases, there are at most $m\mu$ outliers for the eigenvalues of $C^{-1}M$. For example, consider the linear multistep formulas used in boundary value form such that $B = \tilde{s}(B) = s(B) = I$. The generalized backward differentiation formulas or those for the midpoint method used in boundary value form as in [9] belong to this class. In that case, it is straightforward to observe that $L_A \otimes I_m$ has rank $m\mu$ and L_B is the null matrix. Therefore, for these classes of formula, the rank of E is $m\mu$.

As a consequence of Theorem 4, for the formulas (3) such that $C^{-1}M$ is diagonalizable and nonsingular, GMRES converges (in infinite precision arithmetic) in at most $2m\mu + 1$ iterations, independently of s ($m\mu + 1$ iterations for suitable patterns of the above mentioned matrices). However, this result need not be very useful, e.g., in the case of semidiscretization of PDEs. Indeed, we observe that m can be very large there and the number of preconditioned iterations can be (approximately) equal to a constant, usually much lower than $2m\mu$ (see Sect. 4 (numerical experiments and related remarks) and [3,4]). Indeed, there are many classes of PDEs which, after semidiscretization, lead to a preconditioned spectrum whose outliers

are clustered into a few clusters outside the main one in $(1, 0) \in \mathbb{C}$, as the spatial discretization is refined (see, e.g., [5]). Therefore, in these cases, a sharper analysis as in [8] may give more detailed information on the convergence process (see [5] also).

We observe that the underlying block preconditioner can also be applied to a normal equation approach to solve (4). However, we have found that GMRES usually gives better results (see [6]). The analysis of the convergence rate for the conjugate gradients for the normal equation can be easily adapted for {ω}-circulant preconditioners from [6]. It is worth noting that the computational cost of the various preconditioners described in the previous sections is $O(ms \log s)$ if J is banded, say. Details on the implementation and the computational complexity of using block circulant preconditioners can be found in [3]. Finally, it is worth mentioning that most of the results in the previous sections can be easily adapted for the numerical integration of (multi) delay differential equations, boundary value problems, differential algebraic equations (see [27]) and the other classes of problem described in [9].

4 Numerical tests

In this section, we consider differential problems originating from the semi-discretization of model problems from partial differential equations. We compare the number of iterations needed to converge for GMRES for different preconditioners. The initial guess for the iterative solver is the zero vector. The stopping criterion is $\|\mathbf{r}_j\|_2 < 10^{-6}\|\mathbf{b}\|_2$, $\mathbf{r}_j$ being the true residual after j iterations. All experiments are performed in MATLAB.

In [3,4] it was observed that a high condition number for the (preconditioner) matrix can give an ineffective delayed convergence of the Krylov accelerator (see [21] also). To this end, we list a lower bound for the condition number of the matrices of the underlying linear systems and for the related preconditioners by the LINPACK estimated 1-norm procedure. We see that the condition numbers of the original system, P-circulant, modified Strang as in [4] (denoted by "MS-circ" in the tables) and {ω}-circulant based on Strang's (i.e., using a skew-circulant approximation for A and B) preconditioners, are often comparable, in contrast to what happens for the preconditioner based on the Strang approximation. We observe that the underlying nonpreconditioned matrices are well-conditioned (see [6]), but this property is lost if the preconditioner chosen is ill-conditioned. Therefore, the convergence of preconditioned GMRES iterations gets slower. As expected, this is confirmed by all the numerical experiments as well.

Example 1 We consider the advection equation of first order with periodic boundary conditions:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \dfrac{\partial u}{\partial x} = 0, \\ u(x,0) = x(\pi - x), & x \in [0,3], \\ u(\pi,t) = u(0,t), & t \in [0,6]. \end{cases}$$

We discretize the partial derivative $\partial/\partial x$ using central differences and step size $\delta x = 3/m$. We obtain a family of systems of initial value problem with the $m \times m$ Jacobian matrix

$$J_m = \frac{1}{2\delta x} \begin{pmatrix} 0 & -1 & & & -1 \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \ddots \\ & & \ddots & \ddots & \ddots & -1 \\ 1 & & & 1 & 0 \end{pmatrix}.$$

Note that J_m has pure imaginary eigenvalues and the underlying discretization gives a stable scheme (see, e.g., [28]). The generalized Adams method with $\mu = 3$ (order 4, see [9] for the coefficients), is used to solve the above differential equation. The numbers of matrix-vector products required to solve the related linear system are given in Table 1. The unpreconditioned and preconditioned spectrum of eigenvalues of M are displayed in Fig. 2 (except for two outliers that are in quite a "safe" region in the right half plane).

Table 1. Advection equation (Example 1). Number of matrix-vector multiplications required for convergence of full GMRES. The $*$ denotes that the preconditioner cannot be used and its condition number is undefined.

		No precond.		Strang-circ		P-circ		Skew-circ		MS-circ	
m	s	It.	Cond.	It.	Cond.	It.	Cond.	It.	Cond.	It.	Cond.
25	8	157	170	*	*	23	130	30	150	26	1900
	16	136	280	*	*	22	200	28	1700	24	6300
	32	98	480	*	*	21	340	21	840	23	9600
50	8	301	330	23	5700	20	230	36	570	23	5750
	16	327	530	28	40000	23	340	30	7900	28	39000
	32	233	770	34	69000	28	580	24	2500	34	69000
75	8	>500	450	*	*	20	330	38	9100	27	6800
	16	>500	660	*	*	25	500	31	590	51	65000
	32	430	1200	*	*	26	780	43	3400	42	156300

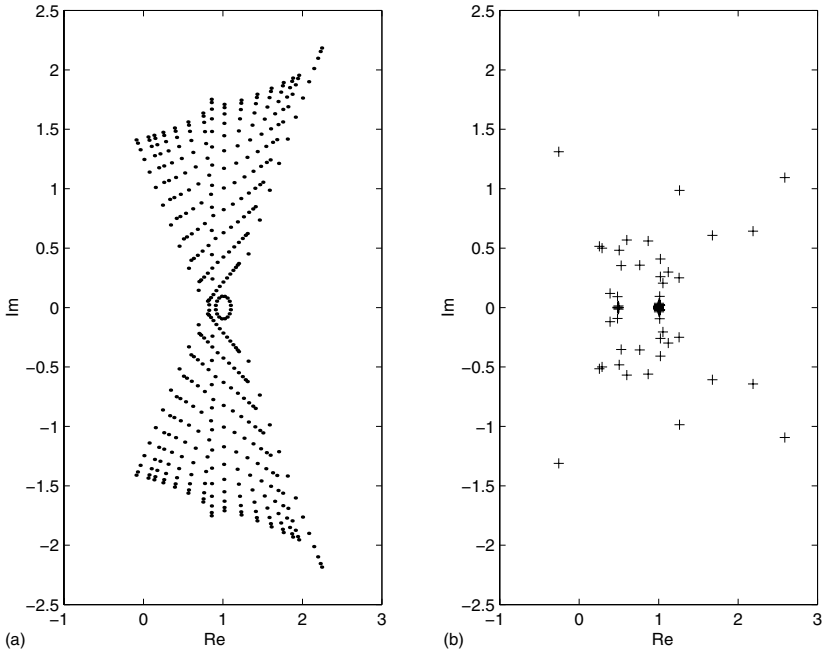

Fig. 2. Advection equation (Example 1). Eigenvalue distribution of the matrix M before and after skew-circulant preconditioning ($s = 16$, $m = 25$)

The spectrum of the P-circulant preconditioned matrix for Example 1 can be found in Fig. 4(a).

It can be observed that the skew-circulant-based block preconditioned iterations usually converge fast, while the Strang-based one cannot be used for odd m because the Jacobian matrix has an eigenvalue equal to zero. For even values of m, the above preconditioner is nonsingular but can be very ill-conditioned. Notice that, for m odd, the condition number of the preconditioner based on the modified Strang approximation can be greater with respect to the P-circulant and to the skew-circulant block preconditioners.

We remark that the performance of other block {ω}-circulant preconditioners is about the same as that of block skew-circulant preconditioners, but deteriorates when $|\theta|$ is small. In particular, this happens when there exist eigenvalues of the Jacobian matrix J_m that are zero (or very small in modulus), positive or complex such that the convex hull of the spectrum of the preconditioned matrix encloses the origin of the complex plane (see [5]). Therefore, we only present the results of block skew-circulant preconditioners in the paper.

Example 2 We consider the diffusion equation in a rectangular domain with a variable diffusion coefficient:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \nabla(c\nabla u), & (x, y) \in \mathbf{R} = [0, 3] \times [0, 3], \\ u((x, y), t) = 0, & (x, y) \in \partial\mathbf{R}, \quad t \in [0, 6], \\ u((x, y), 0) = x\, y, & (x, y) \in \mathbf{R}, \end{cases}$$

where $c = c(x, y)$ is a suitable smooth function. If we discretize the differential operator with centered differences and step-size $\delta x = 3/(m + 1)$, we obtain a system of m^2 ordinary differential equations whose $m^2 \times m^2$ Jacobian matrix J_m is block tridiagonal (Toeplitz if and only if $c(x, y)$ is constant). Here we assume that

$$c(x, y) = \exp(-x^\beta - y^\beta), \quad \beta \geq 0. \tag{17}$$

We note that the underlying Jacobian matrix has real and strictly negative eigenvalues.

The generalized Adams method with $\mu = 4$ (order 5, see [9] for the coefficients) is used to solve the above differential problem.

The numbers of matrix-vector products needed to solve the related linear system, when $\beta = 3$, are given in Table 2. The unpreconditioned and skew-circulant preconditioned spectrums of eigenvalues of M are displayed in Fig. 3; compare this with the block preconditioner using P-circulant matrices (see Fig. 4(b)).

Table 2. Diffusion equation (Example 2), $\beta = 3$ in (17). Number of matrix-vector multiplications required for the convergence of full GMRES. The † denotes that the preconditioner cannot be used because severely ill-conditioned and its condition number is greater than 10^{30}

		No precond.		Strang-circ		P-circ		Skew-circ		MS-circ	
m	s	It.	Cond.	It.	Cond.	It.	Cond.	It.	Cond.	It.	Cond.
8	8	56	500	51	10^{21}	13	400	9	200	12	340
	16	67	500	51	10^{21}	13	400	9	200	13	340
	24	75	500	52	10^{21}	14	400	9	200	13	340
16	8	161	2500	>300	10^{24}	13	1600	9	1100	13	1660
	16	182	2500	>300	10^{24}	14	1600	9	1100	13	1660
	24	190	2500	>300	10^{24}	14	1600	9	1100	13	1660
24	8	>300	5600	†	†	13	3900	10	2700	13	3900
	16	>300	5600	†	†	14	3900	9	2700	13	3900
	24	>300	5600	†	†	14	3900	9	2700	14	3900

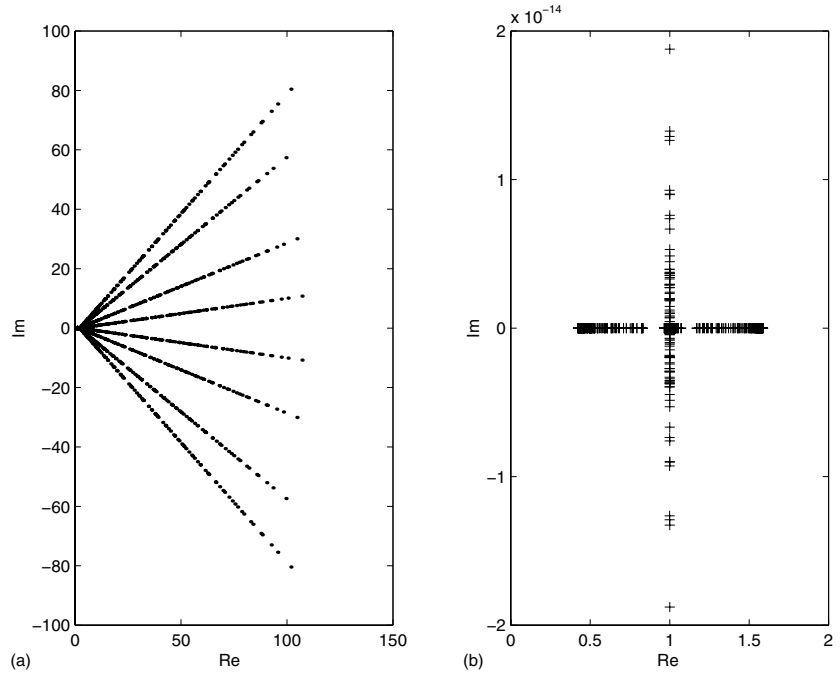

Fig. 3. Diffusion equation (Example 2), $\beta = 3$ in (17). Eigenvalue distribution of the matrix M before and after skew-circulant preconditioning ($s = 8$, $m = 16$)

We observe that the Strang preconditioner and {ω}-circulant preconditioners with $\omega = \exp(\mathbf{i}\theta)$ and $|\theta|$ small, can be safely used only if β is between 0 and 1 and the width of the spatial grid is not too small. For instance, when $\beta = 1$ or $\beta = 2$, the number of iterations of GMRES using the preconditioner based on Strang's circulant matrices increases significantly when m increases. Moreover, we find that the ill-conditioning of the Strang approximation (i.e., $\theta = 0$) can already give polluted numerical results when m is of the order of 50 and $\beta < 3$. For $\beta \geq 3$, the Strang block preconditioner (and then {ω}-circulant preconditioners with small $|\theta|$) cannot be used at all because it is severely ill-conditioned (see Table 2). However, the new skew-circulant preconditioner for this example performs well, slightly faster than the MS-circulant, independently of how large m is.

We have observed that {ω}-P-circulant preconditioners perform similarly to the P-circulant for the two model problems considered in this section. However, the former can be useful when, e.g., J_m is ill-conditioned and the given formula (3) is not $AP_{\nu,\mu-\nu}$-stable for {ω}-circulant preconditioners, while it is $AP_{\nu,\mu-\nu}$-stable for the {ω}-P-circulant preconditioners.

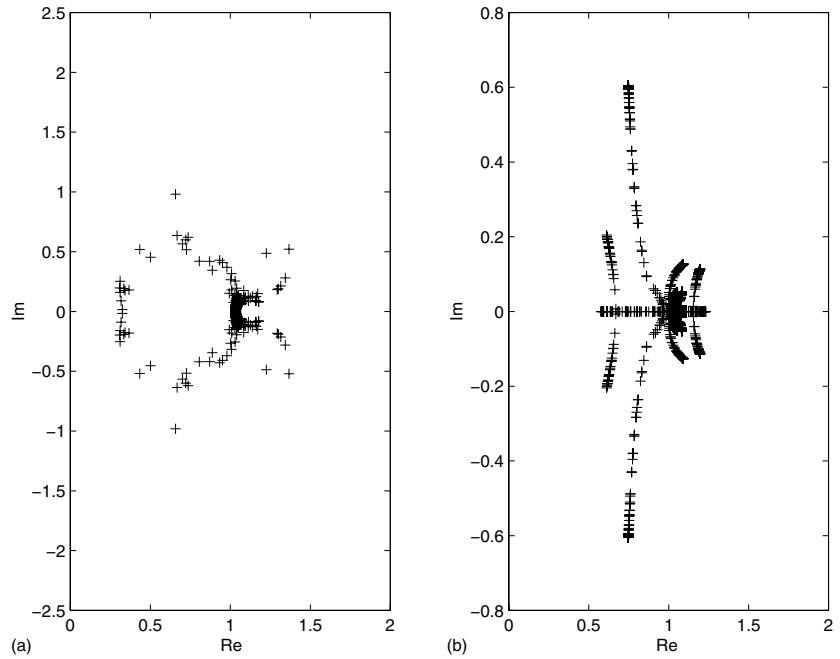

Fig. 4. Eigenvalue distribution of the preconditioned matrix but using the preconditioner based on P-circulant matrices. **(a)**: Parameter as in Fig. 2(b); **(b)**: parameter as in Fig. 3(b)

It is worth noting that the solution of the linear system (4) related to Example 2 with $s = 24$ and $m = 16$ (see Table 2) by MATLAB's built-in sparse direct solver (P-circulant or MS-circulant preconditioners for GMRES) requires roughly more than 20 (1.5) times more flops than using the skew-circulant preconditioned GMRES.

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References

[1] Axelsson, A.O.H., Verwer, J.G.: Boundary value techniques for initial value problems in ordinary differential equations. Math. Comp. **45**, 153–171 (1985)

[2] Bertaccini, D.: P-circulant preconditioners and the systems of the ODE codes. In: Kincaid, D. (ed.): Iterative methods in scientific computation. IV. New Brunswick, NJ: IMACS 1999, pp. 179–193

[3] Bertaccini, D.: A circulant preconditioner for the systems of LMF-based ODE codes. SIAM J. Sci. Comput. **22**, 767–786 (2000)

[4] Bertaccini, D.: Reliable preconditioned iterative linear solvers for some numerical integrators. Numer. Linear Algebra Appl. **8**, 111–125 (2001)

[5] Bertaccini, D.: The spectrum of circulant-like preconditioners for some general linear multistep formulas for linear boundary value problems. SIAM J. Numer. Anal. **40**, 1798–1822 (2002)
[6] Bertaccini, D., Ng, M.K.: The convergence rate of block preconditioned systems arising from LMF-based ODE codes. BIT **41**, 433–450 (2001)
[7] Bertaccini, D., Ng, M.K.: Skew-circulant preconditioners for systems of LMF-based ODE codes. In: Vulkov, L. et al. (eds.): Numerical analysis and its applications. (Lecture Notes in Computer Science **1988**). Berlin: Springer 2001, pp. 93–101
[8] Bertaccini, D., Wen, Y.W., Ng, M.K.: The eigenvalues of nonsymmetric preconditioned block-Toeplitz matrices. Preprint, 2002
[9] Brugnano, L., Trigiante, D.: Solving differential problems by multistep initial and boundary value methods. Amsterdam: Gordon and Breach 1998
[10] Chan, R.H.: Toeplitz preconditioners for Toeplitz systems with nonnegative generating functions. IMA J. Numer. Anal. **11**, 333–345 (1991)
[11] Chan, R.H., Ching, W.-K.: Toeplitz-circulant preconditioners for Toeplitz systems and their applications to queueing networks with batch arrivals. SIAM J. Sci. Comput. **17**, 762–772 (1996)
[12] Chan, R.H., Jin, X.-Q.: Circulant and skew-circulant preconditioners for skew-Hermitian type Toeplitz systems. BIT **31**, 632–646 (1991)
[13] Chan, R.H., Jin, X.-Q.: A family of block preconditioners for block systems. SIAM J. Sci. Statist. Comput. **13**, 1218–1235 (1992)
[14] Chan, R.H., Ng, M.K.: Toeplitz preconditioners for Hermitian Toeplitz systems. Linear Algebra Appl. **190**, 181–208 (1993)
[15] Chan, R.H., Ng, M.K.: Conjugate gradient methods for Toeplitz systems. SIAM Rev. **38**, 427–482 (1996)
[16] Chan, R.H., Ng, M.K., Jin, X.-Q.: Circulant preconditioners for solving ordinary differential equations. In: Bini, D.A. et al. (eds): Structured matrices: recent advances and applications. Huntington, NY: Nova Science 2001, pp. 157–164
[17] Chan, R.H., Yeung, M.-C.: Circulant preconditioners for complex Toeplitz matrices. SIAM J. Numer. Anal. **30**, 1193–1207 (1993)
[18] Cline, R.E., Plemmons, R.J., Worm, G.: Generalized inverses of certain Toeplitz matrices. Linear Algebra Appl. **8**, 25–33 (1974)
[19] Davis, P.J.: Circulant matrices. New York: Wiley 1979
[20] Di Benedetto, F., Fiorentino, G., Serra, S.: CG preconditioning for Toeplitz matrices. Comput. Math. Appl. **25**, 35–45 (1993)
[21] Driscoll, T.A., Toh, K.-C., Trefethen, L.N.: From potential theory to matrix iterations in six steps. SIAM Rev. **40**, 547–578 (1998)
[22] Huckle, T.: Circulant and skewcirculant matrices for solving Toeplitz matrix problems. SIAM J. Matrix Anal. Appl. **13**, 767–777 (1992)
[23] Huckle, T.: Some aspects of circulant preconditioners. SIAM J. Sci. Comput. **14**, 531–541 (1993)
[24] Ku, T., Kuo, C.-C.J.: A minimum-phase LU factorization preconditioner for Toeplitz matrices. SIAM J. Sci. Statist. Comput. **13**, 1470–1487 (1992)
[25] Ku, T., Kuo, C.-C.J.: Spectral properties of preconditioned rational Toeplitz matrices: the nonsymmetric case. SIAM J. Matrix Anal. Appl. **14**, 521–544 (1993)
[26] Lambert, J.D.: Numerical methods for ordinary differential systems. Chichester: Wiley 1991
[27] Lei, S.-L., Jin, X.-Q.: Strang-type preconditioners for differential-algebraic equations. In: Vulkov, L. et al. (eds.): Numerical analysis and its applications. (Lecture Notes in Computer Science **1988**). Berlin: Springer 2001, pp. 505–512

[28] Richtmyer, R.D., Morton, K.W.: Difference methods for initial-value problems. Second edition. New York: Wiley Interscience 1967
[29] Saad, Y., Schultz, M.H.: GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems. SIAM J. Sci. Statist. Comput. **7**, 856–869 (1986)
[30] Tyrtyshnikov, E.E.: A unifying approach to some old and new theorems on distribution and clustering. Linear Algebra Appl. **232**, 1–43 (1996)
[31] van der Vorst, H.A.: Bi-CGSTAB: a fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems. SIAM J. Sci. Statist. Comput. **13**, 631–644 (1992)