

Strang-Type Preconditioners for Systems of LMF-Based ODE Codes

Raymond H. Chan†

Department of Mathematics, The Chinese University of Hong Kong, Shatin, Hong Kong

Michael K. Ng‡

Department of Mathematics, The University of Hong Kong, Pokfulam Road, Hong Kong

Xiao-Qing Jin§

Faculty of Science and Technology, The University of Macau, Macau

We consider the solution of ordinary differential equations (ODEs) using boundary value methods. These methods require the solution of one or more unsymmetric, large and sparse linear systems. The GMRES method with the Strang-type block-circulant preconditioner is proposed for solving these linear systems. We show that if an A_{k_1, k_2} -stable boundary value method is used for an m -by- m system of ODEs, then our preconditioners are invertible and all the eigenvalues of the preconditioned systems are 1 except for at most $2m(k_1 + k_2)$ outliers. It follows that when the GMRES method is applied to solving the preconditioned systems, the method will converge in at most $2m(k_1 + k_2) + 1$ iterations. Numerical results are given to illustrate the effectiveness of our methods.

1. Introduction

In this paper, we consider the solution of

$$\begin{cases} \frac{d\mathbf{y}(t)}{dt} = J_m \mathbf{y}(t) + \mathbf{g}(t), & t \in (t_0, T], \\ \mathbf{y}(t_0) = \mathbf{z}, \end{cases} \quad (1)$$

by boundary value methods (BVMs), see [5]. Here $\mathbf{y}(t)$, $\mathbf{g}(t) : \mathbb{R} \rightarrow \mathbb{R}^m$, $\mathbf{z} \in \mathbb{R}^m$, and $J_m \in \mathbb{R}^{m \times m}$. BVMs are numerical methods based on the linear multistep formulae (LMF) for solving ordinary differential equations (ODEs). By applying the method, the solution to (1) is given by the solution of a linear system

$$M\mathbf{y} = \mathbf{b}, \quad (2)$$

where M depends on the LMF used. Although initial value methods (IVMs) (where the system of equations can be solved easily by forward recursions) are more efficient

† Research supported in part by Hong Kong Research Grants Council Grant No. CUHK 4207/97P and CUHK DAG Grant No. 2060143.

‡ Research supported in part by Hong Kong Research Grants Council Grant No. HKU 7147/99P and UK/HK Joint Research Scheme Grant No. 20009819.

§ Research supported in part by UM Research Grant No. RG009/98-99S/JXQ/FST.

than BVMs, the advantage in using BVMs over IVMs comes from their stability properties, see for instances [1,4] and [5, p. 79 and Figures 5.1–5.3].

By applying BVMs to the ODE in (1), the matrix M in (2) can be written as

$$M = A \otimes I_m - hB \otimes J_m, \quad (3)$$

where A and B are $(s+1)$ -by- $(s+1)$ matrices with entries depending on the LMF used, I_m is the m -by- m identity matrix and $h = (T - t_0)/s$ is the integration step size. We note that both A and B can be reduced to a sum of a Toeplitz matrix plus a low rank matrix. (A matrix is said to be Toeplitz if its entries are constant along its diagonals.) The size of the matrix M is very large when h is small and/or m is large. If a direct method is used to solve the system, the operation count will be too expensive and slow for practical, large scale applications.

In [2], Bertaccini proposed to use Krylov subspace methods [8] such as the GMRES method and the BiCGstab method to solve (2). In order to speed up the convergence rate of the Krylov subspace methods, he proposed two circulant matrices as preconditioners. (A matrix is called circulant if it is Toeplitz and the last entry of every row is the first entry of its succeeding row.) The use of circulant matrices as preconditioners for solving Toeplitz systems have been studied extensively since 1986. It has been shown that they are good preconditioners for a large class of Toeplitz systems, see [6] and the references therein. The first preconditioner proposed in [2] for the matrix M in (3) is the well-known T. Chan circulant preconditioner, see [6]. The second one is a new preconditioner that he called the P -circulant preconditioner. His numerical results showed that the Krylov subspace methods, when applied to solving both circulant preconditioned systems, converge very quickly. He showed moreover that P is invertible for some special BVMs whereas the T. Chan preconditioners may be singular or very ill-conditioned.

In this paper, we propose a preconditioner of the form

$$S = s(A) \otimes I_m - h \cdot s(B) \otimes J_m,$$

for (3). Here $s(A)$ and $s(B)$ are the Strang-type preconditioners for A and B , see [6]. We prove that if an A_{k_1, k_2} -stable BVM is used to discretize (1), then S is invertible and the preconditioned matrix can be decomposed as

$$S^{-1}M = I_{m(s+1)} + L,$$

where the rank of L is at most $2m(k_1 + k_2)$ which is independent of the integration step size h . It follows that the GMRES method applied to the preconditioned system will converge in at most $2m(k_1 + k_2) + 1$ iterations in exact arithmetic. We note that our proposed preconditioner preserves important algebraic properties in the matrix M , such as the invertibility and the tensor and sparsity pattern.

In contrast, Bertaccini [2] showed that with his P -circulant preconditioner P ,

$$P^{-1}M = I_{m(s+1)} + U + V,$$

where the rank of U is equal to $2m(k_1 + k_2)$, but V is a matrix of order $O(1)$. Because of the extra term V , it is not sufficient to guarantee that the GMRES method will

converge in at most $2m(k_1 + k_2) + 1$ iterations. Thus we expect the performance of our preconditioner is better than that of the P -circulant preconditioner. Numerical results in §5 will illustrate the effectiveness of our preconditioners.

Besides BVMs, there is a class of iterative methods for the solution of systems of ODEs known as waveform relaxation methods [9,10,12]. Splitting the matrix J_m in (1) into

$$J_m = N_m - P_m$$

gives the waveform relaxation method:

$$\begin{cases} \frac{d\mathbf{y}_{k+1}(t)}{dt} + P_m \mathbf{y}_{k+1}(t) = N_m \mathbf{y}_k(t) + \mathbf{g}(t), & t \in (t_0, T], \\ \mathbf{y}_{k+1}(t_0) = \mathbf{z}, \end{cases} \quad (4)$$

$k = 0, 1, 2, \dots$, where $\mathbf{y}_0(t)$ is an initial guess usually given by $\mathbf{y}_0(t) = \mathbf{z}$, for $t \in [t_0, T]$. Different choices of P_m lead to different preconditioning techniques for the waveform relaxation methods. We remark that we can use the idea in this paper to precondition the linear system arising from the application of BVMs to (4).

The paper is organized as follows. In §2, we recall the boundary value methods. We introduce the Strang-type block-circulant preconditioner in §3 and give the convergence and cost analysis of our method in §4. Numerical examples are given in §5. Finally, §6 contains some concluding remarks.

2. BVMs and Their Matrix Forms

BVMs are methods based on LMF for solving ODEs, see [5]. Given (1), a BVM approximates its solution by means of a discrete boundary value problem. By using a μ -step LMF over a uniform mesh

$$t_j = t_0 + jh, \quad j = 0, \dots, s,$$

with $h = (T - t_0)/s$, we have

$$\sum_{i=-\nu}^{\mu-\nu} \alpha_{i+\nu} \mathbf{y}_{s+i} = h \sum_{i=-\nu}^{\mu-\nu} \beta_{i+\nu} \mathbf{f}_{s+i}, \quad n = \nu, \dots, s - \mu + \nu. \quad (5)$$

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 BVM in (5) must be used with ν initial conditions and $\mu - \nu$ final conditions. That is, we need the values $\mathbf{y}_0, \dots, \mathbf{y}_{\nu-1}$ and the values $\mathbf{y}_{s-\mu+\nu+1}, \dots, \mathbf{y}_s$. The initial condition in (1) only provides us with one value. In order to obtain the other initial and final values, we have to provide additional $(\mu - 1)$ equations:

$$\sum_{i=0}^{\mu} \alpha_i^{(j)} \mathbf{y}_i = h \sum_{i=0}^{\mu} \beta_i^{(j)} \mathbf{f}_i, \quad j = 1, \dots, \nu - 1, \quad (6)$$

and

$$\sum_{i=0}^{\mu} \alpha_{\mu-i}^{(j)} \mathbf{y}_{s-i} = h \sum_{i=0}^{\mu} \beta_{\mu-i}^{(j)} \mathbf{f}_{s-i}, \quad j = s - \mu + \nu + 1, \dots, s. \quad (7)$$

The coefficients $\alpha^{(j)}$ and $\beta^{(j)}$ in (6) and (7) should be chosen such that the truncation errors for these initial and final conditions are of the same order as that in (5), see [5, p.132]. By combining (5), (6) and (7), we obtain a linear system as in (2). The advantage in using BVMs is that they have much better stability properties than traditional initial value methods, see [5, p.79 and Figures 5.1–5.3].

The discrete problem (2) generated by (5)–(7) is given by

$$M\mathbf{y} \equiv (A \otimes I_m - hB \otimes J_m)\mathbf{y} = \mathbf{e}_1 \otimes \mathbf{z} + h(B \otimes I_m)\mathbf{g}, \quad (8)$$

where $\mathbf{e}_1 = (1, 0, \dots, 0)^t \in \mathbb{R}^{(s+1)}$, $\mathbf{y} = (\mathbf{y}_0, \dots, \mathbf{y}_s)^t \in \mathbb{R}^{(s+1)m}$, $\mathbf{g} = (\mathbf{g}_0, \dots, \mathbf{g}_s)^t \in \mathbb{R}^{(s+1)m}$, and A and B are $(s+1)$ -by- $(s+1)$ matrices given by:

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

and

$$B = \begin{pmatrix} 0 & \cdots & 0 & & & & & & & & \\ \beta_0^{(1)} & \cdots & \beta_\mu^{(1)} & & & & & & & & \\ \vdots & \vdots & \vdots & & & & & & & & \\ \beta_0^{(\nu-1)} & \cdots & \beta_\mu^{(\nu-1)} & & & & & & & & \\ \beta_0 & \cdots & \beta_\mu & & & & & & & & \\ & & \beta_0 & \cdots & & & \beta_\mu & & & & \\ & & & \ddots & & & \ddots & \ddots & & & \\ & & & & \ddots & & \ddots & \ddots & & & \\ & & & & & & \beta_0 & \cdots & & \beta_\mu & \\ & & & & & & \beta_0^{(s-\mu+\nu+1)} & \cdots & & \beta_\mu^{(s-\mu+\nu+1)} & \\ & & & & & & \vdots & \vdots & & \vdots & \\ & & & & & & \beta_0^{(s)} & \cdots & & \beta_\mu^{(s)} & \end{pmatrix}.$$

3. Construction of the Preconditioner

In [2], Bertaccini proposed to use Krylov subspace methods with block-circulant preconditioners for solving (8). Two preconditioners were considered. The first one is the T. Chan block-circulant preconditioner T . It is defined as

$$T = c(A) \otimes I_m - hc(B) \otimes J_m \quad (9)$$

where $c(A)$ is the minimizer of $\|A - C\|_F$ over all $(s + 1)$ -by- $(s + 1)$ circulant matrices C under the Frobenius norm $\|\cdot\|_F$, see [6], and $c(B)$ is defined similarly. More precisely, the diagonals $\hat{\alpha}_j$ and $\hat{\beta}_j$ of $c(A)$ and $c(B)$ are given by

$$\hat{\alpha}_j = \left(1 - \frac{j}{s+1}\right) \alpha_{j+\nu} + \frac{j}{s+1} \alpha_{j+\nu-(s+1)}, \quad j = 0, 1, \dots, s,$$

and

$$\hat{\beta}_j = \left(1 - \frac{j}{s+1}\right) \beta_{j+\nu} + \frac{j}{s+1} \beta_{j+\nu-(s+1)}, \quad j = 0, 1, \dots, s,$$

respectively.

The second preconditioners proposed in [2] is called the P -circulant preconditioner. It is defined as

$$P = \tilde{A} \otimes I_m - h\tilde{B} \otimes J_m \quad (10)$$

where the diagonals $\tilde{\alpha}_j$ and $\tilde{\beta}_j$ of \tilde{A} and \tilde{B} are given by

$$\tilde{\alpha}_j = \left(1 + \frac{j}{s+1}\right) \alpha_{j+\nu} + \frac{j}{s+1} \alpha_{j+\nu-(s+1)}, \quad j = 0, 1, \dots, s,$$

and

$$\tilde{\beta}_j = \left(1 + \frac{j}{s+1}\right) \beta_{j+\nu} + \frac{j}{s+1} \beta_{j+\nu-(s+1)}, \quad j = 0, 1, \dots, s,$$

respectively. The numerical results in [2] show that the GMRES method converges very fast for both preconditioners. For some special BVMs, Bertaccini has proved that the preconditioner P is invertible, but the preconditioner T may be singular or very ill-conditioned.

In this paper, we propose the following preconditioner for (8):

$$S = s(A) \otimes I_m - hs(B) \otimes J_m, \quad (11)$$

where $s(A)$ and $s(B)$ are given by

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

and

$$s(B) = \begin{pmatrix} \beta_\nu & \cdots & \beta_\mu & & \beta_0 & \cdots & \beta_{\nu-1} \\ \vdots & \ddots & & & & \ddots & \vdots \\ \beta_0 & & & & & & \beta_0 \\ & \ddots & & & & & 0 \\ & & 0 & & & & \\ & & & \ddots & & & \\ \beta_\mu & & & & & & \beta_\mu \\ \vdots & \ddots & & & & \ddots & \vdots \\ \beta_{\nu+1} & \cdots & \beta_\mu & & \beta_0 & \cdots & \beta_\nu \end{pmatrix}.$$

Here $\{\alpha_i\}_{i=0}^\mu$ and $\{\beta_i\}_{i=0}^\mu$ are the coefficients in (5). We note that $s(A)$ and $s(B)$ are the generalized Strang-type circulant preconditioners of A and B respectively, see [6].

We now prove that S is invertible provided that the given BVM is stable and the eigenvalues of J_m are in the negative half of the complex plane \mathbb{C} . The stability of a BVM is closely related to two characteristic polynomials defined as follows:

$$\rho(z) \equiv z^\nu \sum_{j=-\nu}^{\mu-\nu} \alpha_{j+\nu} z^j \quad \text{and} \quad \sigma(z) \equiv z^\nu \sum_{j=-\nu}^{\mu-\nu} \beta_{j+\nu} z^j. \quad (12)$$

Note that they are μ -degree polynomials.

DEFINITION 1 [5, p.101] Consider a BVM with the characteristic polynomials $\rho(z)$ and $\sigma(z)$ given by (12). 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 given BVM. Moreover, the BVM is said to be *$A_{\nu, \mu-\nu}$ -stable* if

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

THEOREM 1 If the BVM for (2) is $A_{\nu, \mu-\nu}$ -stable and $h\lambda_k(J_m) \in \mathcal{D}_{\nu, \mu-\nu}$ where $\lambda_k(J_m)$ ($k = 1, \dots, m$) are the eigenvalues of J_m , then the preconditioner S in (11) is nonsingular.

Proof. Since $s(A)$ and $s(B)$ are circulant matrices, their eigenvalues are given by

$$g_A(z) \equiv \alpha_\mu z^{\mu-\nu} + \dots + \alpha_\nu + \alpha_{\nu-1} \frac{1}{z} + \dots + \alpha_0 \frac{1}{z^\nu} = \frac{\rho(z)}{z^\nu}$$

and

$$g_B(z) \equiv \beta_\mu z^{\mu-\nu} + \dots + \beta_\nu + \beta_{\nu-1} \frac{1}{z} + \dots + \beta_0 \frac{1}{z^\nu} = \frac{\sigma(z)}{z^\nu},$$

evaluated at $\omega_j = e^{2\pi i j / (s+1)}$ for $j = 0, \dots, s$, see [6]. The eigenvalues $\lambda_{jk}(S)$ of S are therefore given by

$$\lambda_{jk}(S) = g_A(\omega_j) - h\lambda_k(J_m)g_B(\omega_j), \quad j = 0, \dots, s, \quad k = 1, \dots, m.$$

Since the BVM is $A_{\nu, \mu-\nu}$ -stable, if $h\lambda_k(J_m) \in \mathcal{D}_{\nu, \mu-\nu}$, the μ -degree polynomial $\rho(z) - h\lambda_k(J_m)\sigma(z)$ will have no roots on the unit circle $|z| = 1$. Thus for all $k = 1, \dots, m$,

$$g_A(z) - h\lambda_k(J_m)g_B(z) = \frac{1}{z^\nu} \{\rho(z) - h\lambda_k(J_m)\sigma(z)\} \neq 0, \quad \forall |z| = 1.$$

It follows that $\lambda_{jk}(S) \neq 0$ for all $j = 0, \dots, s$, and $k = 1, \dots, m$. \square

In particular, we have

COROLLARY 1 If the BVM is $A_{\nu, \mu-\nu}$ -stable and $\lambda_k(J_m) \in \mathbb{C}^-$, then the preconditioner S is nonsingular.

Proof. We just note that $h\lambda_k(J_m) \in \mathbb{C}^- \subseteq \mathcal{D}_{\nu, \mu-\nu}$. \square

4. Spectra of Preconditioned Matrices and Operation Cost

In this section, we show that all the eigenvalues of the preconditioned matrix $S^{-1}M$ are 1 except for at most $2m\mu$ outliers and hence the GMRES method applied to the preconditioned system will converge in at most $2m\mu + 1$ iterations in exact arithmetic.

THEOREM 2 All the eigenvalues of the preconditioned matrix $S^{-1}M$ are 1 except for at most $2m\mu$ outliers.

Proof. Let $E = M - S$, we have by (8) and (11),

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

It is easy to check that L_A and L_B are $(s+1)$ -by- $(s+1)$ matrices with nonzero entries only 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 $\mu > \nu$, $\text{rank}(L_A) \leq \mu$ and $\text{rank}(L_B) \leq \mu$. Thus, we have

$$\text{rank}(L_A \otimes I_m) = \text{rank}(L_A) \cdot m \leq m\mu$$

and

$$\text{rank}(L_B \otimes J_m) = \text{rank}(L_B) \cdot m \leq m\mu.$$

Therefore

$$S^{-1}M = I_{m(s+1)} + S^{-1}E = I_{m(s+1)} + L,$$

where the rank of L is at most $2m\mu$. \square

We now show that the GMRES method for the system $S^{-1}M\mathbf{y} = S^{-1}\mathbf{b}$ will converge fast. We first note that given a linear system $A\mathbf{x} = \mathbf{b}$, the GMRES method, in the k -th iteration, will seek an approximation of \mathbf{x} from the affine subspace $\mathbf{x}_0 + \text{span}\{\mathbf{r}_0, A\mathbf{r}_0, A^2\mathbf{r}_0, \dots, A^{k-1}\mathbf{r}_0\}$. Here \mathbf{x}_0 is the initial guess and \mathbf{r}_0 is the initial residual. Thus if $A = I + L$, where I is the identity matrix, then the GMRES method will converge in at most $\text{rank}(L) + 1$ iterations in exact arithmetic. Hence we have

COROLLARY 2 When the GMRES method is applied to solving the preconditioned system $S^{-1}M\mathbf{y} = S^{-1}\mathbf{b}$, the method will converge in at most $2m\mu + 1$ iterations in exact arithmetic.

In contrast, Bertaccini [2] showed that with his P -circulant preconditioner P ,

$$P^{-1}M = I_{m(s+1)} + U + V,$$

where the rank of U is equal to $2m\mu$ and $\|V\|_2 = O(1)$ (the right hand side of (46) in [2] is bounded by $O(1/(hs)) = O(1)$). Because of the extra term V , one can not conclude that the GMRES method will converge in at most $2m\mu + 1$ iterations.

Regarding the cost per iteration, the main work in each iteration for the GMRES method is the matrix-vector multiplication

$$S^{-1}M\mathbf{z} = (s(A) \otimes I_m - hs(B) \otimes J_m)^{-1}(A \otimes I_m - hB \otimes J_m)\mathbf{z}$$

see for instance Saad [11]. Since A and B are banded matrices and J_m is assumed to be sparse, the matrix-vector multiplication $M\mathbf{z} = (A \otimes I_m - hB \otimes J_m)\mathbf{z}$ can be done very fast.

To compute $S^{-1}(M\mathbf{z})$, since $s(A)$ and $s(B)$ are circulant matrices, we have the following decompositions

$$s(A) = F\Lambda_A F^* \quad \text{and} \quad s(B) = F\Lambda_B F^*$$

where Λ_A and Λ_B are diagonal matrices containing the eigenvalues of $s(A)$ and $s(B)$ respectively and F is the Fourier matrix, see [6]. It follows that

$$S^{-1}(M\mathbf{z}) = (F^* \otimes I_m)(\Lambda_A \otimes I_m - h\Lambda_B \otimes J_m)^{-1}(F \otimes I_m)(M\mathbf{z}).$$

This product can be obtained by using Fast Fourier Transforms and solving s linear systems of order m . Since J_m is sparse, the matrix

$$\Lambda_A \otimes I_m - h\Lambda_B \otimes J_m$$

will also be sparse. Thus $S^{-1}(M\mathbf{z})$ can be obtained by solving s sparse linear systems of order m . It follows that the total number of operations per iteration is $\gamma_1 ms \log s + \gamma_2 smn$, where n is the number of nonzeros of J_m , and γ_1 and γ_2 are some positive constants.

Next let us compare the computational cost of our method with a direct solver for the linear system (2). Consider first the simple case where J_m is diagonalizable: $J_m = Q_m^{-1}\Phi_m Q_m$. In general, the number of operations required to compute Q_m , Q_m^{-1} and Φ_m is $O(m^3)$, see [7]. The solution to (2) can be obtained by multiplying the matrices $I_s \otimes Q_m$ and $I_s \otimes Q_m^{-1}$ to some vectors, and solving m banded linear systems of order s and bandwidth μ . Hence the total number of operations for direct solvers is $\gamma_3 m^3 + \gamma_4 sm^2 + \gamma_5 ms\mu^2$, where γ_3 , γ_4 and γ_5 are some positive constants. If the number of iterations required for convergence of our method is smaller than

$$\frac{\gamma_3 \left(\frac{m}{s}\right) m + \gamma_4 m + \gamma_5 \mu^2}{\gamma_1 \log s + \gamma_2 n},$$

then the complexity of our method is better than that of direct solvers. In particular, when m is larger than s or the bandwidth of the matrices A and B are very large (i.e., when we employ higher order BVMs), our method will be more efficient.

In the case where the Jacobian matrix J_m is not diagonalizable, then direct solvers will not be able to make use of the block structure of M and hence will be very expensive. Example 3 in [3] shows that the preconditioned GMRES method with circulant preconditioners can still be very effective though. Moreover, for nonlinear problems, J_m will be different at each Newton iteration and therefore the cost of diagonalization of these J_m will be very expensive.

5. Numerical Tests

In this section, we illustrate the efficiency of our preconditioner over other circulant preconditioners by solving the test problems given in [2]. All the experiments were performed in MATLAB. We used the MATLAB-provided M-file “gmres” (see MATLAB on-line documentation) to solve the preconditioned systems. In our tests, the zero vector is the initial guess and the stopping criterion is $\|\mathbf{r}_q\|_2 / \|\mathbf{r}_0\|_2 < 10^{-6}$, where \mathbf{r}_q is the residual after q iterations. In the examples, the BVM we used is the third order generalized Adam’s method which has $\mu = 2$. Its formulae and the additional initial and final conditions can be found in [5, p.153].

Example 1. Heat equation:

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \\ u(0, t) = \frac{\partial u}{\partial x}(\pi, t) = 0, & t \in [0, 2\pi], \\ u(x, 0) = x, & x \in [0, \pi]. \end{cases}$$

We discretize the partial differential operator $\partial^2/\partial x^2$ with central differences and step size equals to $\pi/(m+1)$. The system of ODEs obtained is:

$$\begin{cases} \frac{d\mathbf{y}(t)}{dt} = T_m \mathbf{y}(t), & t \in [0, 2\pi] \\ \mathbf{y}(0) = [x_1, x_2, \dots, x_m]^t, \end{cases}$$

where T_m is a scaled discrete Laplacian matrix

$$T_m = \frac{(m+1)^2}{\pi^2} \begin{pmatrix} -2 & 1 & & & & \\ & 1 & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -1 \end{pmatrix}. \quad (13)$$

Example 2. Wave equation:

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \\ u(0, t) = \frac{\partial u}{\partial x}(\pi, t) = 0, & t \in [0, 2\pi], \\ u(x, 0) = x, & x \in [0, \pi], \\ \frac{\partial u}{\partial t}(x, 0) = 0, & x \in [0, \pi]. \end{cases}$$

We again discretize $\partial^2/\partial x^2$ with central differences and step size equals to $\pi/(m+1)$. The resulting system of ODEs is:

$$\begin{cases} \frac{d\mathbf{y}(t)}{dt} = H_m \mathbf{y}(t), & t \in [0, 2\pi] \\ \mathbf{y}(0) = [x_1, x_2, \dots, x_{m/2}, 0, \dots, 0]^t, \end{cases}$$

where H_m is a Hamiltonian matrix

$$H_m = \begin{pmatrix} 0_{m/2} & I_{m/2} \\ T_{m/2} & 0_{m/2} \end{pmatrix},$$

with T_m given in (13).

Table 1 lists the numbers of iterations required for convergence of the GMRES method for different m and s . In the table, I means no preconditioner is used, and T , P and S denote that the T. Chan, Bertaccini and Strang-type block-circulant preconditioners are used respectively. These preconditioners are defined in (9)–(11). We see that the number of iterations required for convergence when a circulant preconditioner is used is always less than that when no preconditioner is used. Moreover, the Strang-type preconditioner performs better than T. Chan's and Bertaccini's preconditioners in all cases. As expected from Theorem 2, the numbers under column S stay roughly constant for increasing s when m is fixed; and for fixed s , the numbers grow with m .

m	s	I	S	T	P	m	s	I	S	T	P
24	6	121	31	58	60	24	6	117	54	87	90
	12	222	33	54	56		12	192	59	87	90
	24	269	35	53	53		24	157	71	95	100
	48	302	38	52	52		48	128	95	123	127
	96	363	41	51	51		96	162	143	175	176
48	6	241	43	84	85	48	6	236	88	152	158
	12	476	46	79	82		12	426	103	153	158
	24	605	48	75	76		24	406	119	157	161
	48	684	53	76	76		48	291	134	161	173
	96	838	54	74	73		96	289	180	223	228
96	6	481	59	115	117	96	6	475	124	235	240
	12	998	62	109	115		12	927	167	259	267
	24	>1000	65	103	105		24	>1000	197	263	268
	48	>1000	75	112	114		48	738	210	253	266
	96	>1000	68	95	96		96	656	246	276	291

TABLE 1. NUMBER OF ITERATIONS REQUIRED FOR CONVERGENCE IN EXAMPLES 1 (LEFT) AND 2 (RIGHT).

6. Concluding Remarks

In summary, we have shown that the GMRES method with the Strang-type preconditioner is efficient for solving ODEs from BVMs. We note that the results obtained here can be extended to nonlinear ODEs. Indeed, by linearization, nonlinear problems can be solved iteratively by solving a discrete system (2) in each step. Thus a fast algorithm for solving (2), such as the one proposed here, will be of greater importance in these cases.

We finally remark that Bertaccini has included our results in this paper on the Strang-type preconditioners in the revised edition of [3], which is the journal version of [2].

Acknowledgments: We would like to thank Drs. M.C. Yeung and Q. Ye for their help in the preparation of this paper. We also like to thank the referees for providing additional references.

REFERENCES

- [1] AMODIO, P., MAZZIA, F., and TRIGIANTE, D., 1993. Stability of Some Boundary Value Methods for the Solution of Initial Value Problems. *BIT* **33**, 434–451.
- [2] BERTACCINI, D., A Circulant Preconditioner for the Systems of LMF-Based ODE Codes, preprint, 1999.
- [3] BERTACCINI, D., A Circulant Preconditioner for the Systems of LMF-Based ODE Codes. *SIAM J. Sci. Comput.* to appear.
- [4] BRUGNANO, L., and TRIGIANTE, D., 1993. Stability Properties of Some BVM Methods. *Appl. Numer. Math.* **13**, 291–304.

- [5] BRUGNANO, L., and TRIGIANTE, D., 1998. *Solving Differential Problems by Multistep Initial and Boundary Value Methods*. Gordon and Breach Science Publishers, Amsterdam.
- [6] CHAN, R., and NG, M., 1996. Conjugate Gradient Methods for Toeplitz Systems. *SIAM Review* **38**, 427–482.
- [7] GOLUB, G., and VAN LOAN, C., 1996. *Matrix Computations*. 3rd Edition. Baltimore: The Johns Hopkins University Press.
- [8] GREENBAUM, A., 1997. *Iterative Methods for Solving Linear Systems*, SIAM, Philadelphia.
- [9] LUMSDAINE, A., and WU, D., 1997. Spectra and Pseudospectra of Waveform Relaxation Operators. *SIAM J. Sci. Comput.* **18**, 286–304.
- [10] NEVANLINNA, O., 1989. Remarks on Picard-Lindelöf Iteration, Part I. *BIT* **29**, 328–346.
- [11] SAAD, Y., and SCHULTZ, M., 1996. GMRES: a Generalized Minimal Residual Algorithm for Solving Non-Symmetric Linear Systems. *SIAM J. Sci. Stat. Comput.* **7**, 856–869.
- [12] VANDEWALLE, S., and PIESSENS, R., 1993. On Dynamic Iteration Methods for Solving Time-Periodic Differential Equations. *SIAM J. Num. Anal.* **30**, 286–303.