Analysis of Semi-Toeplitz Preconditioners for First-order PDEs[1]

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Abstract

A semi-Toeplitz preconditioner for nonsymmetric, nondiagonally dominant systems of equations is studied. The preconditioner solve is based on a Fast Modified Sine Transform. As a model problem we study a system of equations arising from an implicit time-discretization of a scalar hyperbolic PDE. Analytical formulas for the eigenvalues and the eigenvectors of the preconditioned system are derived. The convergence of a minimal residual iteration is shown to depend *only* on the grid ratio in space and *not* on the number of unknowns.

Contents

1 Introduction

We are interested in solving systems of first-order PDEs such as the Euler equations and the Maxwell equations. For the Euler equations, we are mainly interested in the case when there are different time-scales present in the problem, and the fastest time-scale does not have to be resolved. An important application is almost incompressible flow [4], [5], where the sound waves in the medium are much faster than the motion of the fluid. For an explicit discretization in time the restriction on the time-step due to the CFL criterion becomes too severe. For the Maxwell equations, we intend to consider complicated geometries such that the smallest grid-cell in the space-discretization restricts the time-step considerably in an explicit time-discretization. Therefore we use an implicit time-discretization. This leads to a system of equations

$$Au = b, \tag{1}$$

which has to be solved for each time-step. A is nonsymmetric, and since the time-step is large compared to the space-step, it is also strongly nondiagonally dominant.

In this report we theoretically examine the convergence properties when we apply a minimal residual iteration to (1), utilizing a semi-Toeplitz preconditioner. Such preconditioners have shown to be well suited in a domain decomposition setting of the problem [8].

2 The model problem

2.1 The differential equation

In [7] we consider a scalar two-dimensional equation with variable coefficients. Here we will restrict our presentation to constant coefficients in order to be able to derive theoretical properties of the preconditioned system.

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} = g, \quad 0 < x_1 \leq 1, \quad 0 < x_2 \leq 1, \quad t > 0. \tag{2}$$

Problem (2) is well-posed if we prescribe $u(0, x_2, t)$, $u(x_1, 0, t)$, and $u(x_1, x_2, 0)$.

2.2 Discretization

Introduce a uniform grid as

$$x_{d,j} = jh_d, \quad j = 0, \ldots, m_d, \quad h_d = 1/m_d, \quad d = 1, 2.$$

Let $u_{j,k}$ denote the approximate solution at the point $(x_{1,j}, x_{2,k})$. Now we discretize equation (2) in time using the trapezoidal rule with time-step Δt

$$\frac{u^{n+1} - u^n}{\Delta t} + \tfrac{1}{2} \sum_{d=1}^{2} \left(\left(\frac{\partial u}{\partial x_d}\right)^{n+1} + \left(\frac{\partial u}{\partial x_d}\right)^{n} \right) = \tfrac{1}{2}(g^{n+1} + g^n).$$

For the spatial derivatives we use second-order centered differences in the interior of the domain and one-sided first-order differences at the outflow boundaries. We define the following quantities

$$\kappa_d \equiv \frac{\Delta t}{h_d}, \quad d = 1, 2,$$

$$u^n = \begin{pmatrix} u^n_{1,1} & u^n_{2,1} & \dots & u^n_{m_1,1} & u^n_{1,2} & \dots & u^n_{m_1,m_2} \end{pmatrix}^T,$$

and finally write the equations as

$$Au^{n+1} \equiv (I_{m_2} \otimes A_1 + \kappa_2 A_2 \otimes I_{m_1}) u^{n+1} = b, \tag{3}$$

where b contains known quantities and A_1 and A_2 are defined by

$$A_1 = \begin{pmatrix} 4 & \kappa_1 & & & \\ -\kappa_1 & 4 & \kappa_1 & & \\ & \ddots & \ddots & \ddots & \\ & & -\kappa_1 & 4 & \kappa_1 \\ & & & -2\kappa_1 & 4 + 2\kappa_1 \end{pmatrix}, \tag{4}$$

$$A_2 = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -2 & 2 \end{pmatrix}.$$

3 Iterative methods

The matrix A defined in (3) is extremely sparse with five nonzero diagonals and semi-bandwidth m_1. Modern CG-like iterative methods are well suited for nonsymmetric systems of equations. In this report we consider minimal residual iterations, [3], which in each iteration fulfills

$$\|r^{(i)}\|_2 = \min_{p_i \in \mathcal{P}_i,\, p_i(0)=1} \|p_i(M^{-1}A) r^{(0)}\|_2,$$

where $\mathcal{P}_i$ is the set of all polynomials of degree i, M is the left preconditioner, $r^{(i)} \equiv M^{-1}(Au^{(i)} - b)$ and $u^{(i)}$ is the approximation of u obtained in iteration i.

If $M^{-1}A$ is diagonalizable we obtain

$$\frac{\|r^{(i)}\|_2}{\|r^{(0)}\|_2} \leq \mathrm{cond}_2(W_{M^{-1}A}) \min_{p_i \in \mathcal{P}_i,\, p_i(0)=1} \max_{1\leq \ell \leq n} |p_i(\lambda_\ell)| \equiv \mathrm{cond}_2(W_{M^{-1}A}) \cdot \varepsilon_i, \quad (5)$$

where $W_{M^{-1}A}$ is the eigenvector matrix and λ_ℓ are the eigenvalues of $M^{-1}A$. From (5) we conclude that we will have finite termination in n iterations, where n is the number of distinct eigenvalues to the preconditioned system. Moreover, if we can precondition our system such that the eigenvalues of $M^{-1}A$ are contained in k dense clusters, we have a good approximation to the solution in k iterations. Clustering of the eigenvalues may be even more important than a condition number improvement, [1], [2], and [12]. In Section 4 we define a preconditioner that yields a highly clustered spectrum. Since the iterative method includes the solution of

$$Mx = y \quad (6)$$

in each step, we must have a fast solver for this system. The preconditioner solve defined in this report is based on a Fast Modified Sine Transform developed in [6].

4 Preconditioning

In this report we consider the semi-Toeplitz preconditioner M defined by

$$M = I_{m_2} \otimes \hat{A}_1 + \kappa_2 A_2 \otimes I_{m_1}, \quad \hat{A}_1 = \begin{pmatrix} 4 & \kappa_1 & & \\ -\kappa_1 & \ddots & \ddots & \\ & \ddots & \ddots & \kappa_1 \\ & & -\kappa_1 & 4 \end{pmatrix}. \quad (7)$$

In [7] it is shown that M can be decomposed as

$$M = (I_{m_2} \otimes S_{m_1}) T (I_{m_2} \otimes S_{m_1}^H),$$

where T is block-tridiagonal with diagonal blocks as

$$T = I_{m_2} \otimes \Lambda_1 + \kappa_2 A_2 \otimes I_{m_1},$$

where

$$\Lambda_1 = \mathrm{diag}(\lambda_{1,1}, \ldots, \lambda_{1,m_1}), \quad \lambda_{1,j} = 4 + 2i\kappa_1 \cos\left(\frac{j\pi}{m_1+1}\right). \quad (8)$$

S_{m_1} is the modified sine matrix defined by

$$S_{m_1}(j,k) = \sqrt{\frac{2}{m_1+1}}\, i^{j+k+1} \sin\left(\frac{jk\pi}{m_1+1}\right), \quad j,k = 1,\ldots,m_1. \quad (9)$$

By rearranging the unknowns the solution of

$$Tx = y$$

decouples into m_1 independent tridiagonal systems of order m_2. In [6] it is shown how the modified sine transforms can be evaluated using Fourier transforms of vectors $y \in \mathcal{C}^{\frac{m_1+1}{2}}$. By symmetry we can also reduce the intermediate solution of the tridiagonal systems to the solution of only the first $\frac{m_1+1}{2}$ systems.
To sum up this section we present the different steps in the solution of (6):

- m_2 Fourier transforms of vectors $y \in \mathcal{C}^{\frac{m_1+1}{2}}$
- $\frac{m_1+1}{2}$ solutions of tridiagonal systems of order m_2
- m_2 Fourier transforms of vectors $y \in \mathcal{C}^{\frac{m_1+1}{2}}$

5 Spectral analysis

By defining

$$E \equiv A - M = I_{m_2} \otimes E_1,$$

where E_1 is defined by

$$E_1 = \begin{pmatrix} 0 & \cdots & 0 & 0 & 0 \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & -\kappa_1 & 2\kappa_1 \end{pmatrix},$$

we get

$$M^{-1}A = I + M^{-1}(I_{m_2} \otimes E_1). \tag{10}$$

Otto [9] shows how to compute the eigenvalues and the eigenvectors of (10) when M is a semicirculant preconditioner, i.e., each block is circulant. We use a similar technique here. We will make use of a lemma in [9], which we restate for readability. Let $\mathcal{E}(a, b)$ denote the closed ellipse centered at the origin with semimajor axis b oriented along the imaginary axis and semiminor axis a. Also, let $\mathcal{E}^+(a, b)$ denote the region $\{z | z \in \mathcal{E}(a, b) \text{ and } \Re e(z) \geq 0\}$.

Lemma 5.1 *The eigenvalues $\lambda_{2,k}$, $k = 1, \ldots, m_2$, of A_2 satisfy:*

- $\lambda_{2,k} \neq \lambda_{2,j}$, $k \neq j$
- $\lambda_{2,k} \in \mathcal{E}^+(4m_2^{-3/4}, 2 + 4m_2^{-3/2})$

From Lemma 5.1 we conclude that there exists a nonsingular matrix V_2 such that

$$V_2^{-1} A_2 V_2 = \Lambda_2 = \mathrm{diag}(\lambda_{2,1}, \ldots, \lambda_{2,m_2}).$$

By defining

$$D \equiv (V_2^{-1} \otimes S_{m_1}^H) M (V_2 \otimes S_{m_1}),$$

where S_{m_1} is the modified sine matrix of order m_1 defined in (9), we get

$$\begin{aligned} D &= (V_2^{-1} \otimes S_{m_1}^H)(I_{m_2} \otimes \hat{A}_1 + \kappa_2 A_2 \otimes I_{m_1})(V_2 \otimes S_{m_1}) = \\ &= I_{m_2} \otimes S_{m_1}^H \hat{A}_1 S_{m_1} + \kappa_2 V_2^{-1} A_2 V_2 \otimes I_{m_1} = I_{m_2} \otimes \Lambda_1 + \kappa_2 \Lambda_2 \otimes I_{m_1}, \end{aligned}$$

where Λ_1 is defined in (8). From Lemma 5.1 we get that

$$\Re e(\lambda_{1,j} + \kappa_2 \lambda_{2,k}) = 4 + \kappa_2 \Re e(\lambda_{2,k}) \geq 4,$$

which implies that $I_{m_2} \otimes \Lambda_1 + \kappa_2 \Lambda_2 \otimes I_{m_1}$ is nonsingular, i.e., M^{-1} exists. Hence,

$$D = I_{m_2} \otimes \Lambda_1 + \kappa_2 \Lambda_2 \otimes I_{m_1} = \mathrm{diag}(D_1, \ldots, D_{m_2}),$$

where

$$D_k = \mathrm{diag}(d_\nu),$$

$$d_\nu = 4 + 2i\kappa_1 \cos\left(\frac{j\pi}{m_1+1}\right) + \kappa_2 \lambda_{2,k}, \qquad \left\{ \begin{array}{l} \nu = (k-1)m_1 + j \\ k = 1, \ldots, m_2 \\ j = 1, \ldots, m_1 \end{array} \right. , \tag{11}$$

and the spectral decomposition of M^{-1} becomes

$$M^{-1} = (V_2 \otimes S_{m_1}) D^{-1} (V_2^{-1} \otimes S_{m_1}^H).$$

Now consider the matrix W given by

$$\begin{aligned} W &= (V_2 \otimes I_{m_1})^{-1} M^{-1} E (V_2 \otimes I_{m_1}) = \\ &= (I_{m_2} \otimes S_{m_1}) \mathrm{diag}(D_1^{-1}, \ldots, D_{m_2}^{-1})(I_{m_2} \otimes S_{m_1}^H E_1) = \\ &= \mathrm{diag}(S_{m_1} D_1^{-1} S_{m_1}^H E_1, \ldots, S_{m_1} D_{m_2}^{-1} S_{m_1}^H E_1) \equiv \mathrm{diag}(W_1, \ldots, W_{m_2}). \end{aligned}$$

As W is a similarity transformation of $M^{-1}E$ and W is block-diagonal, the eigenvalues of $M^{-1}E$ equal the eigenvalues of W_k, $k = 1, \ldots, m_2$. Due to the sparse structure of E_1, W_k only has two nonzero columns

$$W_k = \begin{pmatrix} 0 & \cdots & 0 & W_k(1, m_1 - 1) & W_k(1, m_1) \\ 0 & \cdots & 0 & W_k(2, m_1 - 1) & W_k(2, m_1) \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & W_k(m_1, m_1 - 1) & W_k(m_1, m_1) \end{pmatrix}, \tag{12}$$

where

$$
\begin{aligned}
W_k(\ell, m_1 - 1) &= -\kappa_1 \sum_{j=1}^{m_1} S_{m_1}(\ell, j) d_\nu^{-1} S_{m_1}^H(j, m_1) = \\
&= -\kappa_1 i^{\ell - m_1} \Phi_{m_1,\ell}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1), \\
W_k(\ell, m_1) &= 2\kappa_1 \sum_{j=1}^{m_1} S_{m_1}(\ell, j) d_\nu^{-1} S_{m_1}^H(j, m_1) = \\
&= 2\kappa_1 i^{\ell - m_1} \Phi_{m_1,\ell}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1), \qquad \ell = 1, \ldots, m_1,
\end{aligned}
\tag{13}
$$

where $\nu = (k-1)m_1 + j$, d_ν is defined in (11) and

$$
\Phi_{k,\ell}(\alpha, \beta) = \frac{2}{m_1 + 1} \sum_{j=1}^{m_1} F_{k,\ell}\Big(\tfrac{j\pi}{m_1+1}\Big), \tag{14}
$$

$$
F_{k,\ell}(\theta) = \frac{\sin(k\theta)\sin(\ell\theta)}{2\alpha + 2i\beta\cos(\theta)}, \quad k, \ell = 1, \ldots, m_1, \tag{15}
$$

where α is a complex number with $\Re e(\alpha) > 0$, and $\beta > 0$ is real. We now show how to evaluate the sums in (14). Using this result we can then compute the sums defined in (13).

Lemma 5.2 *$\Phi_{k,\ell}(\alpha, \beta)$ defined in (14) can be evaluated by*

$$
\Phi_{k,\ell}(\alpha, \beta) = \frac{i}{\beta} \left(\frac{z^{k+\ell} - z^{|k-\ell|}}{z - z^{-1}} + \frac{(z^k - z^{-k})(z^\ell - z^{-\ell})}{z - z^{-1}} \frac{z^{2m_1+2}}{1 - z^{2m_1+2}} \right),
$$

where

$$
z = i\left(\tfrac{\alpha}{\beta} - \sqrt{1 + \left(\tfrac{\alpha}{\beta}\right)^2} \right)
$$

and the principal branch of the square root function is employed.

Proof:
By periodicity we get

$$
\Phi_{k,\ell}(\alpha, \beta) = \frac{1}{m_1 + 1} \sum_{j=0}^{2m_1+1} F_{k,\ell}\Big(\tfrac{j\pi}{m_1+1}\Big), \quad k, \ell = 1, \ldots, m_1.
$$

$F_{k,\ell}$ is C^1 and 2π-periodic implying

$$
F_{k,\ell}(\theta) = \sum_{q=-\infty}^{\infty} c_q e^{iq\theta}, \quad c_q = \frac{1}{2\pi} \int_0^{2\pi} e^{-iq\theta} F_{k,\ell}(\theta) d\theta.
$$

The Poisson summation formula yields

$$\Phi_{k,\ell}(\alpha,\beta) = \sum_{q=-\infty}^{\infty} 2c_{q(2m_1+2)} = 2c_0 + \sum_{q=1}^{\infty} 2c_{-q(2m_1+2)} + 2c_{q(2m_1+2)}.$$

Using the Euler identities in (15) gives

$$\begin{aligned} F_{k,\ell}(\theta) &= -\frac{1}{4}\frac{(e^{ik\theta}-e^{-ik\theta})(e^{i\ell\theta}-e^{-i\ell\theta})}{2\alpha+i\beta(e^{i\theta}+e^{-i\theta})} = \\ &= \frac{e^{i(k-\ell)\theta}+e^{i(\ell-k)\theta}-e^{i(k+\ell)\theta}-e^{-i(k+\ell)\theta}}{8\alpha+4i\beta(e^{i\theta}+e^{-i\theta})}. \end{aligned}$$

By making the substitution $z = e^{i\theta}$ we get

$$c_q = -\frac{i}{4\beta}\frac{1}{2\pi i}\oint_{\mathcal{C}} \frac{z^{k-\ell-q}+z^{\ell-k-q}-z^{k+\ell-q}-z^{-k-\ell-q}}{(z-z_1)(z-z_2)}dz, \tag{16}$$

where $\mathcal{C}$ is the positively oriented unit circle and

$$z_1 = i\left(\tfrac{\alpha}{\beta}-\sqrt{1+\left(\tfrac{\alpha}{\beta}\right)^2}\right), \qquad z_2 = i\left(\tfrac{\alpha}{\beta}+\sqrt{1+\left(\tfrac{\alpha}{\beta}\right)^2}\right), \tag{17}$$

where $|z_1|<1$ and $|z_2|>1$. Hence, z_1 is within $\mathcal{C}$ while z_2 is not. Note that $z_2 = z_1^{-1}$.

Two types of integrals arise, which are calculated using the residue theorem.

- $p \geq 0, \quad I_1 = \dfrac{1}{2\pi i}\displaystyle\oint_{\mathcal{C}} \frac{z^p}{(z-z_1)(z-z_2)}dz = \frac{z_1^p}{z_1-z_2} = \frac{z_1^p}{z_1-z_1^{-1}}$
- $p \geq 1, \quad I_2 = \dfrac{1}{2\pi i}\displaystyle\oint_{\mathcal{C}} \frac{z^{-p}}{(z-z_1)(z-z_2)}dz = \frac{z_1^{-p}}{z_1-z_2} + \frac{1}{(p-1)!}\varphi^{(p-1)}(0)$

  $\varphi^{(p-1)}(0)$ denotes the $(p-1)$th derivative of $\varphi(z)$ at $z=0$, where $\varphi(z)$ is defined by

  $\varphi(z) = \frac{1}{(z-z_1)(z-z_2)} = \frac{1}{z_1-z_2}\big((z-z_1)^{-1}-(z-z_2)^{-1}\big)$, yielding

  $\varphi^{(p-1)}(z) = \frac{1}{z_1-z_2}(p-1)!(-1)^{p-1}\big((z-z_1)^{-p}-(z-z_2)^{-p}\big)$, and hence

  $$I_2 = \frac{z_1^{-p}}{z_1-z_1^{-1}} + \frac{(-1)^{p-1}}{z_1-z_1^{-1}}\big((-z_1)^{-p}-(-z_2)^{-p}\big) = \frac{z_1^p}{z_1-z_1^{-1}}.$$

Using this result in (16) yields

$$\begin{cases} c_0 = \frac{i}{2\beta}\left(\frac{z_1^{k+\ell}-z_1^{|k-\ell|}}{z_1-z_1^{-1}}\right) \\ c_{-q(2m_1+2)} = \frac{i}{4\beta}\left(\frac{z_1^{k+\ell}+z_1^{-k-\ell}-z_1^{k-\ell}-z_1^{\ell-k}}{z_1-z_1^{-1}}\right)z_1^{q(2m_1+2)} \\ c_{q(2m_1+2)} = c_{-q(2m_1+2)} \end{cases}, \qquad k,\ell = 1,\ldots,m_1.$$

Since $|z_1| < 1$ we get

$$\sum_{q=1}^{\infty} (z_1^{2m_1+2})^q = \frac{z_1^{2m_1+2}}{1 - z_1^{2m_1+2}},$$

which gives

$$\sum_{q=1}^{\infty} 2c_{-q(2m_1+2)} + 2c_{q(2m_1+2)} = \frac{i}{\beta} \frac{z_1^{k+\ell} + z_1^{-k-\ell} - z_1^{k-\ell} - z_1^{\ell-k}}{z_1 - z_1^{-1}} \frac{z_1^{2m_1+2}}{1 - z_1^{2m_1+2}}.$$

Summing up we conclude that

$$\Phi_{k,\ell}(\alpha,\beta) = \frac{i}{\beta} \left(\frac{z_1^{k+\ell} - z_1^{|k-\ell|}}{z_1 - z_1^{-1}} + \frac{(z_1^k - z_1^{-k})(z_1^\ell - z_1^{-\ell})}{z_1 - z_1^{-1}} \frac{z_1^{2m_1+2}}{1 - z_1^{2m_1+2}} \right),$$

where z_1 is defined in (17), which completes the proof. $\square$

Thus, by Lemma 5.2 and using that $\Re e(4 + \kappa_2 \lambda_{2,k}) > 0$ and $\kappa_1 > 0$, we can find analytical expressions for $W_k(\ell, m_1 - 1)$ and $W_k(\ell, m_1)$ defined in (13). The characteristic equation for W_k defined in (12) is

$$\begin{aligned} 0 &= \det(\lambda I_{m_1} - W_k) = \\ &= \lambda^{m_1-2} \begin{vmatrix} \lambda - W_k(m_1-1, m_1-1) & -W_k(m_1-1, m_1) \\ -W_k(m_1, m_1-1) & \lambda - W_k(m_1, m_1) \end{vmatrix} = \\ &= \lambda^{m_1-1} \big(\lambda - i\kappa_1 \Phi_{m_1,m_1-1}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1) - 2\kappa_1 \Phi_{m_1,m_1}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1) \big). \end{aligned}$$

Hence, W_k only has one nonzero eigenvalue λ_k given by

$$\begin{aligned} \lambda_k &= i\kappa_1 \Phi_{m_1,m_1-1}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1) + 2\kappa_1 \Phi_{m_1,m_1}(\tfrac{4+\kappa_2\lambda_{2,k}}{2}, \kappa_1) = \\ &= -z_k^2 \frac{1 - z_k^{2m_1-2}}{1 - z_k^{2m_1+2}} + 2iz_k \frac{1 - z_k^{2m_1}}{1 - z_k^{2m_1+2}}, \end{aligned}$$

where

$$z_k = i \left(\tfrac{4+\kappa_2\lambda_{2,k}}{2\kappa_1} - \sqrt{1 + \left(\tfrac{4+\kappa_2\lambda_{2,k}}{2\kappa_1} \right)^2} \right). \tag{18}$$

We summarize this result in a theorem.

Theorem 5.3 *The matrix $M^{-1}A$, where M is defined in (7) and A in (3), has $(m_1 - 1)m_2$ eigenvalues that are identically one. The remaining m_2 eigenvalues μ_k are given by*

$$\mu_k = 1 - z_k^2 \frac{1 - z_k^{2m_1-2}}{1 - z_k^{2m_1+2}} + 2iz_k \frac{1 - z_k^{2m_1}}{1 - z_k^{2m_1+2}}, \quad k = 1, \ldots, m_2, \tag{19}$$

where z_k is defined in (18).

As the dimension of the nullspace of E is $(m_1 - 1)m_2$, it is clear that the eigenvalue zero to $M^{-1}E$ has $(m_1 - 1)m_2$ linearly independent eigenvectors. Hence, we know that a minimal residual iteration will converge in at most $m_2 + 1$ iterations. We now derive the eigenvectors of $M^{-1}A$.

Theorem 5.4 *Assume that the nontrivial eigenvalues λ_k, $k = 1, \ldots, m_2$, defined in (18) are nonzero. Then the matrix $M^{-1}A$ has a nonsingular eigenvector matrix*

$$W_{M^{-1}A} = (V_2 \otimes I_{m_1})\mathrm{diag}(U_1, \ldots, U_{m_2}).$$

V_2 is the eigenvector matrix of A_2 and U_k is given by

$$U_k = \left[e_1, \ldots, e_{m_1-2}, (2e_{m_1-1} + e_{m_1})/\sqrt{5}, u^{(k)}/\|u^{(k)}\|_2\right], \quad k = 1, \ldots, m_2,$$

where e_j denotes the jth canonical column vector and

$$u_\ell^{(k)} = i^\ell(z_k^\ell - z_k^{-\ell}), \quad \ell = 1, \ldots, m_1,$$

where z_k is defined in (18).

Proof:
In the proof of Theorem 5.3 we derived

$$(V_2 \otimes I_{m_1})^{-1}M^{-1}E(V_2 \otimes I_{m_1}) = \mathrm{diag}(W_1, \ldots, W_{m_2}),$$

where the eigenvalues of W_k are λ_k and zero with multiplicity $m_1 - 1$. The first $m_1 - 2$ columns of W_k are identically zero, and combining (13) and Lemma 5.2 yields

$$\left.\begin{array}{rcl} W_k(\ell, m_1 - 1) & = & \dfrac{i^{-m_1+1}z_k^{m_1+1}}{1 - z_k^{2m_1+2}} i^\ell(z_k^\ell - z_k^{-\ell}) \\ W_k(\ell, m_1) & = & -2W_k(\ell, m_1 - 1) \end{array}\right., \quad \ell = 1, \ldots, m_1.$$

We now investigate the eigenvector matrix U_k of W_k. Due to the structure of W_k we conclude that $\left\{\{e_j\}_{j=1}^{m_1-2}, (2e_{m_1-1} + e_{m_1})/\sqrt{5}\right\} \in \mathrm{null}(W_k)$. Consequently those $m_1 - 1$ orthonormal vectors are eigenvectors of W_k corresponding to the eigenvalue zero. The assumption $\lambda_k \neq 0$ implies that the corresponding eigenvector $u^{(k)} \notin \mathrm{null}(W_k)$. Thus, W_k has m_1 linearly independent eigenvectors. From $0 < |z_k| < 1$ it follows that column $m_1 - 1$ of W_k is nonzero. Furthermore, the structure of W_k implies that column $m_1 - 1$ is an eigenvector corresponding to λ_k. By rescaling the column we can choose

$$u_\ell^{(k)} = i^\ell(z_k^\ell - z_k^{-\ell}), \quad \ell = 1, \ldots, m_1,$$

as the nontrivial eigenvector to W_k. We then obtain

$$U_k^{-1}W_kU_k = \Lambda_k = \mathrm{diag}(0, \ldots, 0, \lambda_k), \quad k = 1, \ldots, m_2.$$

Now the matrix $W_{M^{-1}A} \equiv (V_2 \otimes I_{m_1})\mathrm{diag}(U_1, \ldots, U_{m_2})$ is nonsingular and

$$W_{M^{-1}A}^{-1} M^{-1} A W_{M^{-1}A} =$$

$$= I + \left(\mathrm{diag}(U_1, \ldots, U_{m_2})\right)^{-1} (V_2 \otimes I_{m_1})^{-1} M^{-1} E (V_2 \otimes I_{m_1}) \mathrm{diag}(U_1, \ldots, U_{m_2}) =$$

$$= I + \mathrm{diag}(U_1^{-1}, \ldots, U_{m_2}^{-1}) \mathrm{diag}(W_1, \ldots, W_{m_2}) \mathrm{diag}(U_1, \ldots, U_{m_2}) =$$

$$= I + \mathrm{diag}(\Lambda_1, \ldots, \Lambda_{m_2}),$$

i.e., $W_{M^{-1}A}$ is the eigenvector matrix of $M^{-1}A$. □

From Theorem 5.6 it is easy to establish that the assumption in Theorem 5.4 is valid, when m_1 and m_2 are sufficiently large. To compare the condition of the eigenvectors for A and $M^{-1}A$, we define the *condition number reduction*

$$\psi \equiv \mathrm{cond}_2(W_{M^{-1}A}) \big/ \mathrm{cond}_2(W_A), \tag{20}$$

where W_A is the eigenvector matrix of A. Following the technique in [9] ψ can be estimated. Under the same assumption as in Theorem 5.4 we obtain

$$\psi \le \psi_0 = \max_{1 \le k \le m_2} \|U_k\|_2 \cdot \max_{1 \le k \le m_2} \|U_k^{-1}\|_2 \big/ \mathrm{cond}_2(V_1), \tag{21}$$

where V_1 is the eigenvector matrix of A_1 defined in (4). Therefore we determine $\|U_k\|_2$ and $\|U_k^{-1}\|_2$.

Theorem 5.5 *Under the same assumption as in Theorem 5.4,*

$$\begin{array}{rcl} \|U_k\|_2 & = & \left(1 + \sqrt{1 - a_k}\right)^{1/2} \\ \|U_k^{-1}\|_2 & = & \left(1 - \sqrt{1 - a_k}\right)^{-1/2} \end{array}, \quad k = 1, \ldots, m_2,$$

where

$$a_k = \frac{\frac{1}{5}|z_k^{m_1-1} - z_k^{-m_1+1}|^2 + \frac{4}{5}|z_k^{m_1} - z_k^{-m_1}|^2 - \frac{4}{5}\Im m\left((z_k^{m_1-1} - z_k^{-m_1+1})(\bar{z}_k^{m_1} - \bar{z}_k^{-m_1})\right)}{\dfrac{|z_k|^2 - |z_k|^{2m_1+2}}{1 - |z_k|^2} + \dfrac{|z_k|^{-2} - |z_k|^{-2m_1-2}}{1 - |z_k|^{-2}} - 2\Re e\left(\dfrac{z_k \bar{z}_k^{-1} - (z_k \bar{z}_k^{-1})^{m_1+1}}{1 - z_k \bar{z}_k^{-1}}\right)}.$$

Proof:
To derive the results we examine the eigenvalues of $U_k^H U_k$. Using the notation in Theorem 5.4, we define the auxiliary vectors $w^{(k)}$, $k = 1, \ldots, m_2$;

$$\begin{array}{rcl} w_\ell^{(k)} & = & u_\ell^{(k)} / \|u^{(k)}\|_2, \quad \ell = 1, \ldots, m_1 - 2, \\ w_{m_1-1}^{(k)} & = & \left(\frac{2}{\sqrt{5}} u_{m_1-1}^{(k)} + \frac{1}{\sqrt{5}} u_{m_1}^{(k)}\right) / \|u^{(k)}\|_2. \end{array}$$

Exploiting the orthonormality of the first $m_1 - 1$ columns of U_k yields

$$U_k^H U_k = \begin{pmatrix} I_{m_1-1} & w^{(k)} \\ (w^{(k)})^H & 1 \end{pmatrix}.$$

The characteristic polynomial $P_k(\lambda)$ of $U_k^H U_k$ satisfies

$$\begin{aligned}
(1-\lambda)P_k(\lambda) &= (1-\lambda)\det(U_k^H U_k - \lambda I_{m_1}) = \\
&= \begin{vmatrix} I_{m_1-1} & 0 \\ -(w^{(k)})^H & 1-\lambda \end{vmatrix} \begin{vmatrix} (1-\lambda)I_{m_1-1} & w^{(k)} \\ (w^{(k)})^H & 1-\lambda \end{vmatrix} = \\
&= \begin{vmatrix} (1-\lambda)I_{m_1-1} & w^{(k)} \\ 0 & (1-\lambda)^2 - (w^{(k)})^H w^{(k)} \end{vmatrix} = \\
&= (1-\lambda)^{m_1-1}\big((1-\lambda)^2 - \|w^{(k)}\|_2^2\big).
\end{aligned}$$

Thus,

$$P_k(\lambda) = (1-\lambda)^{m_1-2}\big((1-\lambda)^2 - \|w^{(k)}\|_2^2\big).$$

Consequently the eigenvalues of $U_k^H U_k$ are one with multiplicity $m_1 - 2$ and

$$\begin{aligned}
\lambda_{k,1} &= 1 + \|w^{(k)}\|_2, \\
\lambda_{k,2} &= 1 - \|w^{(k)}\|_2.
\end{aligned}$$

We obtain

$$\left.\begin{aligned}
\|U_k\|_2 &= \big(\max(1, \lambda_{k,1}, \lambda_{k,2})\big)^{1/2} = (1 + \|w^{(k)}\|_2)^{1/2} \\
\|U_k^{-1}\|_2 &= \big(\max(1, \lambda_{k,1}^{-1}, \lambda_{k,2}^{-1})\big)^{1/2} = (1 - \|w^{(k)}\|_2)^{-1/2}
\end{aligned}\right., \qquad k = 1, \ldots, m_2.$$

It now remains to derive a formula for $\|w^{(k)}\|_2$. From the definition of $w^{(k)}$ and Theorem 5.4 it follows that

$$\begin{aligned}
\|w^{(k)}\|_2^2 &= \sum_{\ell=1}^{m_1-1} |w_\ell^{(k)}|^2 = \|u^{(k)}\|_2^{-2}\big(\tfrac{1}{5}|2u_{m_1-1}^{(k)} + u_{m_1}^{(k)}|^2 + \sum_{\ell=1}^{m_1-2} |u_\ell^{(k)}|^2\big) = \\
&= 1 - \|u^{(k)}\|_2^{-2}\big(\tfrac{1}{5}|u_{m_1-1}^{(k)}|^2 + \tfrac{4}{5}|u_{m_1}^{(k)}|^2 - \tfrac{4}{5}\Re e(u_{m_1-1}^{(k)}\bar{u}_{m_1}^{(k)})\big) = \\
&= 1 - \|u^{(k)}\|_2^{-2}\Big(\tfrac{1}{5}|z_k^{m_1-1} - z_k^{-m_1+1}|^2 + \tfrac{4}{5}|z_k^{m_1} - z_k^{-m_1}|^2 - \\
&\qquad \tfrac{4}{5}\Im m\big((z_k^{m_1-1} - z_k^{-m_1+1})(\bar{z}_k^{m_1} - \bar{z}_k^{-m_1})\big)\Big).
\end{aligned}$$

By contradiction one can derive that $z_k \neq \bar{z}_k$. This and $|z_k| \neq 1$ makes $\|u^{(k)}\|_2^2$ computable from geometric series

$$\|u^{(k)}\|_2^2 = \sum_{\ell=1}^{m_1} |u_\ell^{(k)}|^2 = \sum_{\ell=1}^{m_1} (\bar{z}_k^\ell - \bar{z}_k^{-\ell})(z_k^\ell - z_k^{-\ell}) =$$

$$= \sum_{\ell=1}^{m_1} |z_k^2|^\ell + |z_k^{-2}|^\ell - (z_k \bar{z}_k^{-1})^\ell - (\bar{z}_k z_k^{-1})^\ell =$$

$$= \frac{|z_k|^2 - |z_k|^{2m_1+2}}{1-|z_k|^2} + \frac{|z_k|^{-2} - |z_k|^{-2m_1-2}}{1-|z_k|^{-2}} - 2\Re e\Big(\frac{z_k \bar{z}_k^{-1} - (z_k \bar{z}_k^{-1})^{m_1+1}}{1 - z_k \bar{z}_k^{-1}}\Big),$$

which completes the proof. □

From Theorem 5.3 we derive the following asymptotic result.

Theorem 5.6 *Assume that*

$$\Delta t = c h_1^\alpha, \quad 0 < \alpha < 1, \quad c > 0, \tag{22}$$

and

$$m_1 = \left\lceil \frac{m_2(1 + 2m_2^{-\frac{3}{2}})}{\phi} \right\rceil, \quad 0 < \phi < 1, \tag{23}$$

where $\lceil \frac{a}{b} \rceil$ *denotes the closest integer greater than* $\frac{a}{b}$. *In the limit* $m_1 \to \infty$, *the* m_2 *eigenvalues of* $M^{-1}A$ *that are different from one all reside on a curve-segment* $\mu(\gamma)$

$$\mu(\gamma) = 2 - 2\gamma^2 + 2\sqrt{1-\gamma^2} - 2i\gamma\big(1 + \sqrt{1-\gamma^2}\big), \quad -\phi \leq \gamma \leq \phi. \tag{24}$$

Proof:
Define ζ_k as

$$\zeta_k \equiv \tfrac{4 + \kappa_2 \lambda_{2,k}}{2\kappa_1}, \qquad k = 1, \ldots, m_2.$$

By (22) we get

$$\zeta_k = \frac{2h_1}{c h_1^\alpha} + \frac{h_1}{2h_2}\lambda_{2,k} = 2c^{-1} m_1^{\alpha-1} + w_k,$$

where

$$w_k = \tfrac{m_2}{2m_1}\lambda_{2,k}. \tag{25}$$

Lemma 5.1 together with (25) yields

$$w_k \in \mathcal{E}^+\big(2\tfrac{m_2^{\frac{1}{4}}}{m_1}, \tfrac{m_2}{m_1}(1 + 2m_2^{-\frac{3}{2}})\big), \qquad k = 1, \ldots, m_2.$$

By (23) $m_2 < m_1$ and $\frac{m_2}{m_1}(1 + 2m_2^{-\frac{3}{2}}) \leq \phi$ yielding

$$w_k \in \mathcal{E}^+(2\frac{m_2^{\frac{1}{4}}}{m_1}, \phi) \in \mathcal{E}^+(2m_1^{-\frac{3}{4}}, \phi).$$

Now define

$$\epsilon = c^{-1}m_1^{\alpha-1} + \delta_k m_1^{-\frac{3}{4}}, \quad 0 \leq \delta_k \leq 1,$$

which gives

$$\zeta_k = 2\epsilon + i\gamma_k, \quad -\phi \leq \gamma_k \leq \phi. \tag{26}$$

For $m_1 \gg 1$ we have $0 < \epsilon \ll 1$, and (26) combined with (18) and a Taylor expansion yields

$$z_k = i\big(\zeta_k - \sqrt{1+\zeta_k^2}\big) = 2i\epsilon - \gamma_k - i\sqrt{1-\gamma_k^2} + \frac{2\epsilon\gamma_k}{\sqrt{1-\gamma_k^2}} + \mathcal{O}(\epsilon^2).$$

We obtain

$$z_{k,\infty} \equiv \lim_{m_1\to\infty} z_k = -\gamma_k - i\sqrt{1-\gamma_k^2}, \quad -\phi \leq \gamma_k \leq \phi. \tag{27}$$

For m_1 sufficiently large there is a positive constant c_k such that

$$|z_k|^2 = 1 - \frac{4\epsilon}{\sqrt{1-\gamma_k^2}} + \mathcal{O}(\epsilon^2) < 1 - c_k m_1^{\alpha-1}.$$

Thus, we get $|z_k|^{2m_1} \to 0$, which together with equation (19) gives

$$\lim_{m_1\to\infty} \mu_k = 1 - z_{k,\infty}^2 + 2iz_{k,\infty}, \quad k = 1, \ldots, m_2. \tag{28}$$

By inserting (27) in (28) and exploiting that $-\phi \leq \gamma_k \leq \phi$, we conclude that the eigenvalues of $M^{-1}A$ that are different from one all reside upon the curve-segment $\mu(\gamma)$ defined by (24). □

From Theorem 5.6 we see that when Δt is defined by (22), the eigenvalues stay bounded and are well separated from the origin when the problem-size increases. If time-accuracy is not required, as in steady-state computations, it is preferable to choose the time-step almost independently of the space-step, i.e., $\alpha \approx 0$. For time accurate computations, the time-step should be almost proportional to the space-step, i.e., $\alpha \approx 1$. In Figures 1 and 2 we show how well the asymptotic formula (24) agrees with the eigenvalues for large problems.
Numerical experiments show that $\mathrm{cond}_2(W_{M^{-1}A})$ grows rapidly with m_2. However, in Figures 3 and 4 we note that the upper bound ψ_0 of the condition number reduction is favorable. For all values of α and ϕ examined, ψ_0 is less than 0.1 and decreases when the problem-size increases. The conclusion is that the semi-Toeplitz preconditioner improves the condition of the eigenvectors to the iteration matrix.

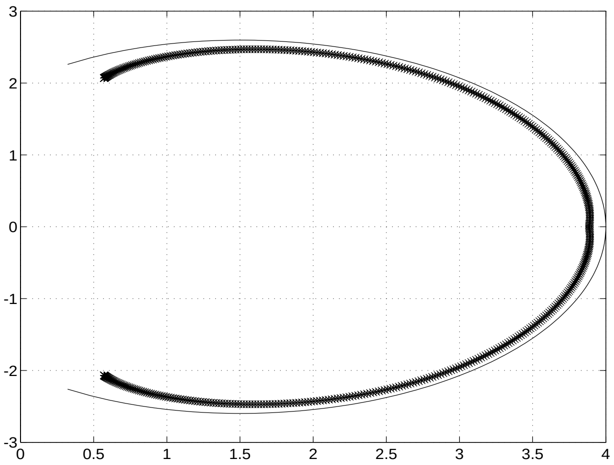

Figure 1: Asymptotic spectrum solid line and eigenvalues marked with stars for $\alpha = 0.99$, $c = 100$, $\phi = 0.99$, and $m_2 = 505$.

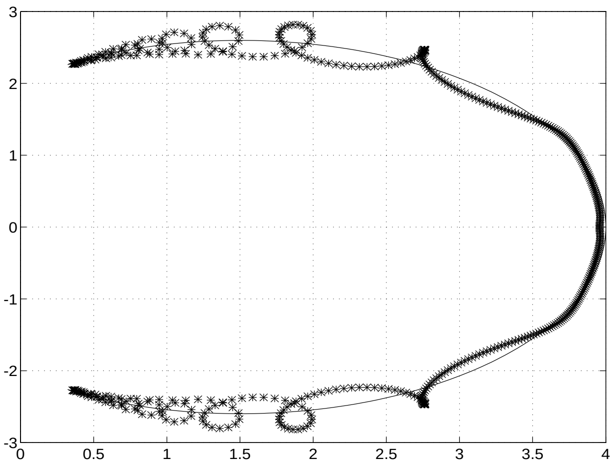

Figure 2: Asymptotic spectrum solid line and eigenvalues marked with stars for $\alpha = 0.1$, $c = 10$, $\phi = 0.99$, and $m_2 = 505$.

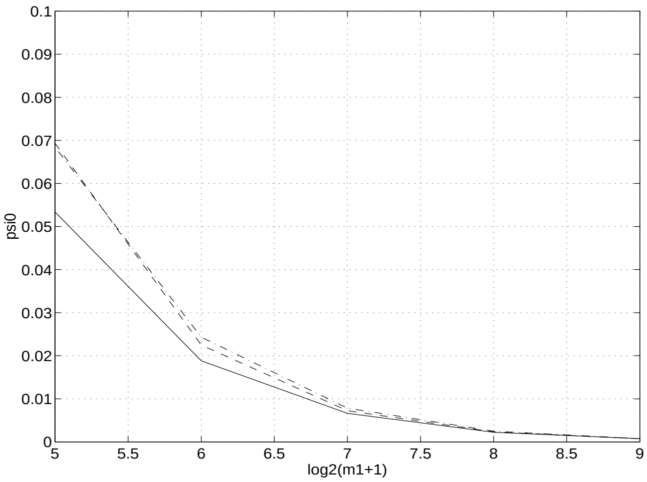

Figure 3: ψ_0 for $\alpha = 0.99$ and $c = 100$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

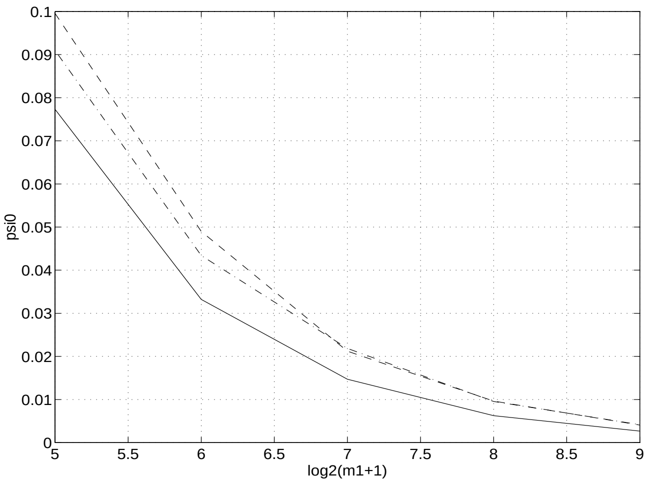

Figure 4: ψ_0 for $\alpha = 0.1$ and $c = 10$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

6 Convergence properties

In this section we determine the *asymptotic convergence factor* ρ defined by

$$\rho \equiv \lim_{i\to\infty} \varepsilon_i^{1/i}, \tag{29}$$

where ε_i is defined in (5). We enclose the asymptotic spectrum μ, defined in (24), in a circle $\mathcal{C}(4,R)$ and use the general result from [10]. Here $\mathcal{C}(c,R)$ denotes the circle with center c and radius R.

Lemma 6.1 *The circle $\mathcal{C}(4,R)$, where R is defined as*

$$R = |\mu(\pm\phi) - 4| = \sqrt{8 + 12\phi^2 - 8\sqrt{1-\phi^2}},$$

encloses the asymptotic spectrum μ defined in (24).

Proof:
Define $r(\gamma)$ as the distance between 4 and $\mu(\gamma)$. Then

$$\begin{aligned} r^2 &= \left(-2 - 2\gamma^2 + 2\sqrt{1-\gamma^2}\right)^2 + \left(2\gamma(1+\sqrt{1-\gamma^2})\right)^2 = \\ &= 8 + 12\gamma^2 - 8\sqrt{1-\gamma^2} \end{aligned}$$

and

$$\frac{d^2r^2}{d\gamma^2} = 24 + \frac{8}{(1-\gamma^2)^{3/2}} > 0.$$

Hence, r^2 obtains its maximum value at the endpoints yielding $r(\gamma) \le R$, which proves the lemma. □

Theorem 6.2 *For $0 < \phi < \frac{\sqrt{8}}{3}$ the asymptotic convergence factor ρ fulfills*

$$\rho \le \frac{\sqrt{2 + 3\phi^2 - 2\sqrt{1-\phi^2}}}{2} < 1.$$

Proof:
For $0 < \phi < \frac{\sqrt{8}}{3}$ we obtain $8 + 12\phi^2 < 8 + 12\cdot\frac{8}{9} = 8\sqrt{1-\frac{8}{9}} + 16 < 8\sqrt{1-\phi^2} + 16$, and consequently $\sqrt{8 + 12\phi^2 - 8\sqrt{1-\phi^2}} < 4$. Using Lemma 6.1 and the general result in [10] yields

$$\rho \le \frac{R}{4} = \frac{\sqrt{2 + 3\phi^2 - 2\sqrt{1-\phi^2}}}{2} < 1.$$

□

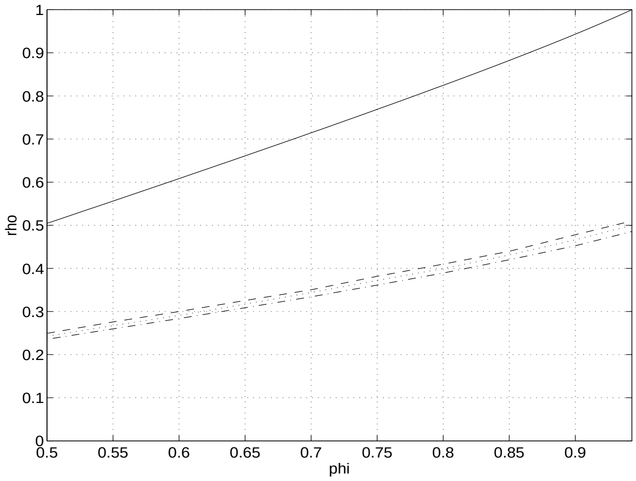

Figure 5: The solid line represents the asymptotic convergence factor for $\alpha = 0.99$ and $c = 100$. The residual reduction is plotted for $m_1 = 127$ dashed line, $m_1 = 255$ dotted line, and $m_1 = 511$ dashed-dotted line.

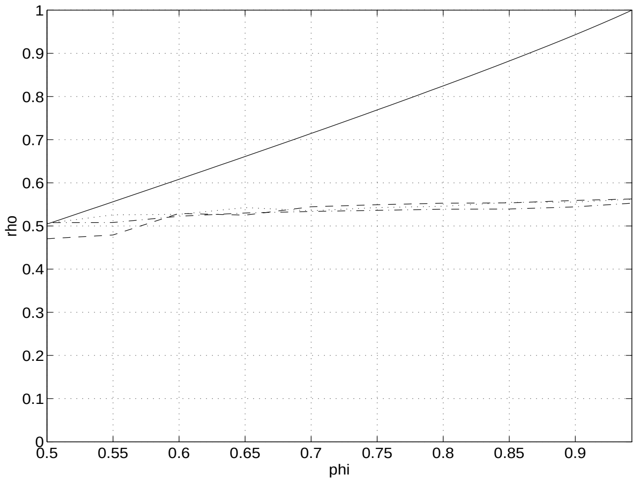

Figure 6: The solid line represents the asymptotic convergence factor for $\alpha = 0.1$ and $c = 10$. The residual reduction is plotted for $m_1 = 127$ dashed line, $m_1 = 255$ dotted line, and $m_1 = 511$ dashed-dotted line.

In Figures 5 and 6 we display the asymptotic convergence factor as a function of ϕ. In the same figures we present the residual reduction $\tilde{\rho}$ defined by

$$\tilde{\rho} \equiv \left(\frac{\|r^{(i)}\|_2}{\|r^{(0)}\|_2} \right)^{1/i}, \tag{30}$$

for different problem-sizes using GMRES [11] with $i = 20$.

Figures 7 and 8 show the actual number of iterations obtained from restarted GMRES(20) for different problem-sizes. The iteration has converged when $\|r^{(i)}\|_2/\|M^{-1}b\|_2 < 10^{-6}$.

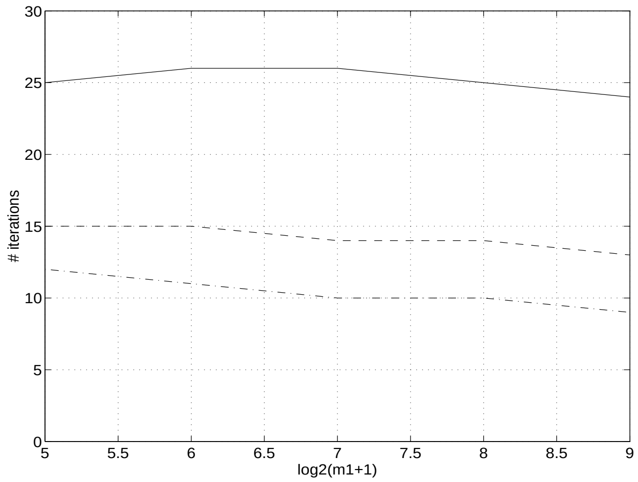

Figure 7: Number of iterations for $\alpha = 0.99$ and $c = 100$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

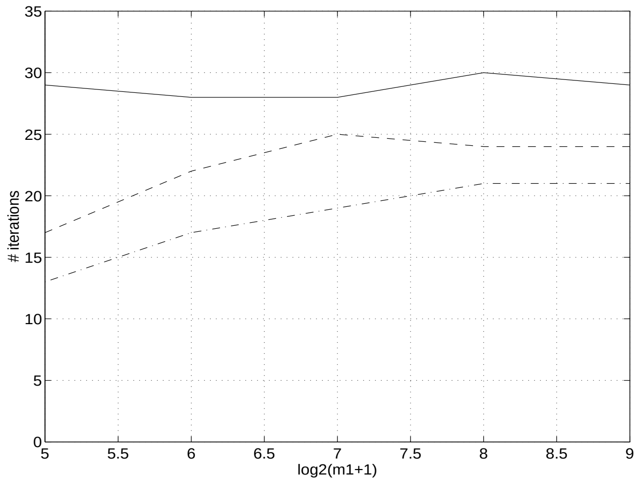

Figure 8: Number of iterations for $\alpha = 0.1$ and $c = 10$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

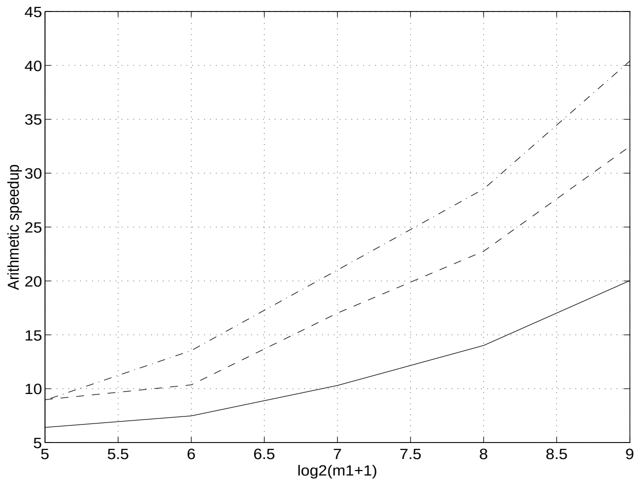

Figure 9: Arithmetic speedup for $\alpha = 0.99$ and $c = 100$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

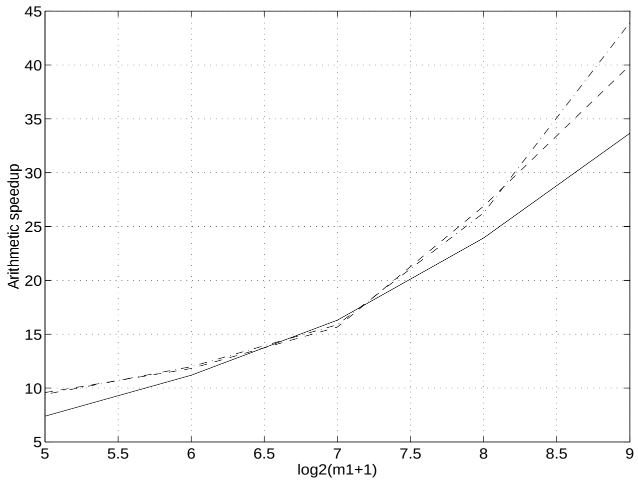

Figure 10: Arithmetic speedup for $\alpha = 0.1$ and $c = 10$. Solid line represents $\phi = 0.99$, dashed line $\phi = 0.75$, and dashed-dotted line $\phi = 0.5$.

From Figures 5, 6, 7, and 8 we observe that the convergence seems to depend only on the quotient between the number of grid-points in the different space-directions and not on the number of unknowns. Finally in Figures 9 and 10 we present the arithmetic speedup using GMRES(20) and the semi-Toeplitz preconditioner compared to the unpreconditioned system (3). Clearly the speedup is large for large problems, and it is greater than one also for small problems. Notice that lowering ϕ yields a gain in speedup. We conclude that the semi-Toeplitz preconditioner results in a significant improvement.

7 Conclusions

We have studied semi-Toeplitz preconditioners and minimal residual iterations to solve block-tridiagonal systems of equations. Analytical formulas for the eigenvalues and the eigenvectors of the preconditioned system are derived. It is numerically verified that the eigenvector matrix to the preconditioned system is better conditioned than its unpreconditioned counterpart. We have also shown that in the limit $m_d \to \infty$, the eigenvalues of the preconditioned system all lie on a curve-segment. The eigenvalues stay bounded and are well separated from the origin independently of the problem-size. From this eigenvalue distribution we derive upper bounds of the asymptotic convergence factor. These bounds have been corroborated numerically. Finally we show empirically that the number of iterations does not grow when we increase the number of unknowns. This leads to a substantial arithmetic speedup compared to the unpreconditioned system.

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