Weierstraß-Institut

für Angewandte Analysis und Stochastik

Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 0946 – 8633

Shifted linear systems in electromagnetics. Part II: Systems with multiple right-hand sides.

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submitted: September 30, 2011

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No. 1646

Berlin 2011

2010 *Mathematics Subject Classification.* 35Q60, 65F10, 65F15, 65N22, 78M25.

Key words and phrases. Microwave device, Maxwell's equations, Scattering matrix, Boundary value problem, PML boundary condition, Eigenvalue problem, Linear algebraic equations, Multiple shifts, Multiple right-hand sides, Krylov subspace method, Polynomial preconditioning, Initial guesses.

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Abstract

We consider the solution of multiply shifted linear systems for multiple right-hand sides. The coefficient matrix is symmetric, complex, and indefinite. The matrix is shifted by different multiples of the identity. Such problems arise in a number of applications, including the electromagnetic simulation in the development of microwave and mm-wave circuits and modules.

The properties of microwave circuits can be described in terms of their scattering matrix which is extracted from the orthogonal decomposition of the electric field. We discretize the Maxwell's equations with orthogonal grids using the Finite Integration Technique (FIT). Some Krylov subspace methods have been used to solve systems with multiple right-hand sides. We use both the block-QMR method and a symmetric band Lanczos process based on coupled recurrences with polynomial preconditioning.

We present a method for providing initial guesses to a linear solver both for systems with multiple shifts and for systems with multiple right-hand sides each with a different shift.

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1 Introduction

Today, electromagnetic simulation forms an indispensable tool in the development of microwave circuits. The description of the boundary of the computational domain has always been a key issue in bringing up efficiency of electromagnetic simulation. The Perfectly Matched Layer (PML) concept provides an excellent solution to this issue. However, the benefits of PML do not come for free. In the frequency-domain case, the material tensors worsen the numerical properties of the system of equations to be solved, which results in increased CPU time [20].
The subject under investigation are three-dimensional structures of arbitrary geometry which are connected to the remaining circuit by transmission lines. Ports are defined at the outer terminations of the transmission lines (see Fig. 1).

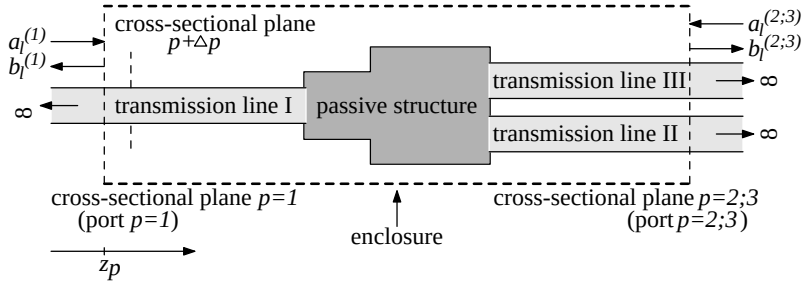

Figure 1: The basic structure under investigation

Calculating the excitations at the ports, one obtains eigenvalue problems and then large-scale systems of linear algebraic equations. In general, the computation of the eigenvalue problem and of the system of linear algebraic equations have to be done for several frequencies. Moreover, these linear equation problems have to be solved repeatedly for different right-hand sides. The number of right-hand sides depends on the number of ports and modes.

2 Scattering Matrix

The scattering matrix describes the structure in terms of the wave modes on the transmission line sections at the ports. We consider all exciting modes with amplitudes a_l towards the discontinuity and all amplitudes b_l outwards from the discontinuity (see Fig. 1). As example for the waves at the left port of Fig. 1 the transverse mode field at a cross-sectional plane z is given by

$$\vec{E}_t(z) = \sum_{l=1}^{m^{(p)}} a_l \vec{E}_{t,l} e^{-\jmath k_{z_l} z} + \sum_{l=1}^{m^{(p)}} b_l \vec{E}_{t,l} e^{+\jmath k_{z_l} z} = \sum_{l=1}^{m^{(p)}} w_l(z) \vec{E}_{t,l} \tag{1}$$

with

$$w_l(z) = a_l e^{-\jmath k_{z_l} z} + b_l e^{+\jmath k_{z_l} z} = \tilde{a}_l(z) + \tilde{b}_l(z), \tag{2}$$

where k_{z_l} is the propagation constant. We consider the application of (1) with (2) at a pair of neighboring cross-sectional planes z_p and $z_{p+\Delta p}$. $m^{(p)}$ denotes the number of modes which have to be taken into account at the port p.
We get $\vec{E}_{t,l}(z_p)$ solving eigenvalue problems for the transmission lines. The scattering matrix S (see [10]) is defined by

$$\vec{\tilde{b}}_\nu = S \vec{\tilde{a}}_\nu, \quad \nu = 1(1) m_s \ . \tag{3}$$

The dimension m_s of this matrix is determined by the total number of modes at all ports. That means, we have to solve m_s boundary value problems (see [9, 10]).

3 Boundary Value Problem

A three-dimensional boundary value problem can be formulated using the integral form of Maxwell's equations in the frequency domain [2] in order to compute the electromagnetic field:

$$\begin{aligned} \oint_{\partial\Omega} \vec{H} \cdot d\vec{s} &= \jmath\omega \int_\Omega [\epsilon] \vec{E} \cdot d\vec{\Omega} \quad , \quad \oint_\Omega [\epsilon] \vec{E} \cdot d\vec{\Omega} = 0 \ , \\ \oint_{\partial\Omega} \vec{E} \cdot d\vec{s} &= -\jmath\omega \int_\Omega [\mu] \vec{H} \cdot d\vec{\Omega} \quad , \quad \oint_\Omega [\mu] \vec{H} \cdot d\vec{\Omega} = 0 \ , \end{aligned} \tag{4}$$

$$\vec{D} = [\epsilon]\vec{E}, \ \ \vec{B} = [\mu]\vec{H}. \tag{5}$$

The electric and magnetic flux densities $\vec{D}$ and $\vec{B}$ are complex functions of the spatial coordinates. $\omega = 2\pi f$ is the angular frequency of the sinusoidal excitation. f denotes the frequency.

At the ports p the transverse electric field $\vec{E}_t(z_p)$ is given by superposing weighted transmission line modes $\vec{E}_{t,l}(z_p)$ (see (1)):

$$\vec{E}_t(z_p) = \sum_{l=1}^{m^{(p)}} w_l(z_p)\vec{E}_{t,l}(z_p)\,. \tag{6}$$

All other parts of the surface of the computation domain are assumed to be an electric or a magnetic wall:

$$\vec{E} \times \vec{n} = 0\,, \quad \vec{H} \times \vec{n} = 0\,. \tag{7}$$

We introduce a complex permittivity $[\epsilon]$ and a complex permeability $[\mu]$ diagonal tensor to obtain a reflection-free interface between the computational area and the lossy PML region:

$$[\epsilon] = (\epsilon)[\Lambda^{(\epsilon)}]\,, \quad [\mu] = (\mu)[\Lambda^{(\mu)}] \tag{8}$$

with

$$(\epsilon) = \mathrm{diag}(\epsilon_x, \epsilon_y, \epsilon_z)\,, \quad (\mu) = \mathrm{diag}(\mu_x, \mu_y, \mu_z)\,. \tag{9}$$

$[\Lambda^{(\epsilon)}]$ and $[\Lambda^{(\mu)}]$ are defined for a PML in x-, y-, or z-direction as follows ($\nu \in \{\epsilon, \mu\}$):

$$[\Lambda^{(\nu)}] = \left\{ \begin{array}{l} [\Lambda^{(\nu)}]_x = \mathrm{diag}(\frac{1}{\lambda_\nu}, \lambda_\nu, \lambda_\nu) \\ [\Lambda^{(\nu)}]_y = \mathrm{diag}(\lambda_\nu, \frac{1}{\lambda_\nu}, \lambda_\nu) \\ [\Lambda^{(\nu)}]_z = \mathrm{diag}(\lambda_\nu, \lambda_\nu, \frac{1}{\lambda_\nu}) \end{array} \right\} \quad \text{with} \tag{10}$$

$$\lambda_\nu = 1 - \jmath\frac{\kappa_\nu}{\nu_0\omega} \quad \text{and} \quad \frac{\kappa_\epsilon}{\epsilon_0} = \frac{\kappa_\mu}{\mu_0}\,. \tag{11}$$

In case of overlapping at edges and corners the resulting PML tensor is the product of the PML tensors of the individual PML walls that form the edges and corners, respectively.

4 Maxwellian Grid Equations

Maxwellian grid equations are formulated for staggered nonequidistant rectangular grids (see Fig. 2) using the Finite Integration Technique with lowest order integration formulae [2, 14, 21]:

$$\oint_{\partial\Omega} \vec{f}\cdot d\vec{s} \to \sum(\pm f_i s_i)\,, \quad \int_{\Omega} \vec{f}\cdot d\vec{\Omega} \to f\Omega\,, \quad \oint_{\Omega} \vec{f}\cdot d\vec{\Omega} \to \sum(\pm f_i \Omega_i)\,. \tag{12}$$

The discretized form of (4) results in an equation for each field component. Presenting each equation using matrices provides a compact form:

$$\begin{array}{rclcrcl} \tilde{C}D_{\tilde{s}/\tilde{\mu}}\vec{b} & = & \jmath\omega\epsilon_0\mu_0 D_{\tilde{A}\tilde{\epsilon}}\vec{e} & , & \tilde{S}D_{\tilde{A}\tilde{\epsilon}}\vec{e} & = & 0\,, \\ CD_s\vec{e} & = & -\jmath\omega D_A\vec{b} & , & SD_A\vec{b} & = & 0\,. \end{array} \tag{13}$$

The diagonal matrices $D_{\tilde{s}/\tilde{\mu}}$, $D_{\tilde{A}\tilde{\epsilon}}$, D_s, and D_A represent all cell quantities. The so-called curl ($C, \tilde{C}$) and source matrices ($S, \tilde{S}$) describe the topology of the two grids with the following properties (see [22]):

$$SC = 0\,, \quad \tilde{S}\tilde{C} = 0\,, \quad C = \tilde{C}^T\,. \tag{14}$$

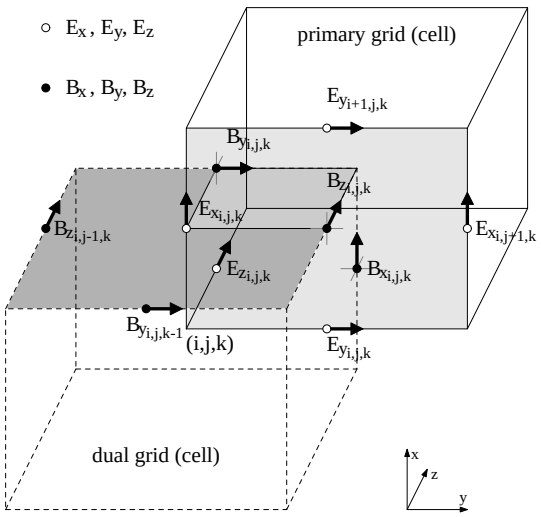

Figure 2: Primary and dual grid

4.1 System of Linear Algebraic Equations

Using (14), eliminating the components of the magnetic flux density ($\vec{b}$) in (13), and multiplying by $D_s^{1/2}$ yields a symmetric form of linear algebraic equations:

$$(D_s^{1/2} C^T D_{\tilde{s}/\tilde{\mu}} D_A^{-1} C D_s^{1/2} - k_0^2 D_{\tilde{A}\tilde{\epsilon}}) D_s^{1/2} \vec{e} = 0 \,, \tag{15}$$

where $k_0 = \omega\sqrt{\epsilon_0 \mu_0}$ denotes the wavenumber in vacuum. Moreover, the gradient of the electric field divergence

$$[\epsilon]\nabla([\epsilon]^{-2}\nabla \cdot [\epsilon]\vec{E}) = 0 \tag{16}$$

is equivalent to the matrix equation

$$(D_s^{-1/2} D_{\tilde{A}\tilde{\epsilon}} \tilde{S}^T D_{\tilde{V}\tilde{\epsilon}\tilde{\epsilon}}^{-1} \tilde{S} D_{\tilde{A}\tilde{\epsilon}} D_s^{-1/2}) D_s^{1/2} \vec{e} = 0 \,. \tag{17}$$

The diagonal matrix $D_{\tilde{V}\tilde{\epsilon}\tilde{\epsilon}}$ is a volume matrix for the 8 partial volumes of the dual elementary cell.

The addition of Eqs. (15) and (17) yields the form

$$(B^{(G)} - k_0^2 D^{(G)}) y^{(G)} = 0 \,. \tag{18}$$

Taking into account the constitutive relations (5), the boundary conditions (7), and the transmission line modes $\vec{E}_{t,l}(z_p)$ (see (1)) we transform Eq. (18) into an inhomogeneous linear system of equations where its right-hand side depends on (6). For it, we use the notations given in Table 1. Thus, we get from Eq. (18):

$$\begin{pmatrix} 0 \\ B^{(G)} - k_0^2 D^{(G)} \end{pmatrix} \begin{pmatrix} y_E^{(G)} \\ y_I^{(G)} \end{pmatrix} = \begin{pmatrix} I_E - I_E & 0 \\ B_E^{(G)} & B_I^{(G)} - k_0^2 D_I^{(G)} \end{pmatrix} \begin{pmatrix} y_E^{(G)} \\ y_I^{(G)} \end{pmatrix} = 0 \,,$$

Table 1: Notations

$y^{(G)} = (y_E^{(G)}, y_I^{(G)})^T$, vector of the unknown electric flux densities			
$y_E^{(G)} = (y_{2d}^{(G)}, y_{3d}^{(G)})^T$, given components of the solution vector $y^{(G)}$			
$y_E^{(G)}$	external points, dim($y_E^{(G)}$) = n_E	$y_{2d}^{(G)}$	solution of the $2d$ eigenvalue problem
$y_I^{(G)}$	internal points, dim($y_I^{(G)}$) = $n_I, N = n_E + n_I$	$y_{3d}^{(G)}$	given boundary points of the $3d$ problem
$B^{(G)}$	$= (B_E^{(G)}, 0) + (0, B_I^{(G)})$	dim($B^{(G)}$) = (n_I, N) , dim($B_E^{(G)}$) = (n_I, n_E) , dim($B_I^{(G)}$) = (n_I, n_I)	
$D^{(G)}$	$= (0, D_I^{(G)})$	dim($D^{(G)}$) = (n_I, N) , dim($D_I^{(G)}$) = (n_I, n_I)	
I_E	identity	dim(I_E) = (n_E, n_E)	

$$\begin{pmatrix} I_E & 0 \\ 0 & B_I^{(G)} - k_0^2 D_I^{(G)} \end{pmatrix} \begin{pmatrix} y_E^{(G)} \\ y_I^{(G)} \end{pmatrix} + \begin{pmatrix} -I_E & 0 \\ B_E^{(G)} & 0 \end{pmatrix} \begin{pmatrix} y_E^{(G)} \\ y_I^{(G)} \end{pmatrix} = 0\,,$$

$$\begin{pmatrix} I_E & 0 \\ 0 & B_I^{(G)} - k_0^2 D_I^{(G)} \end{pmatrix} \begin{pmatrix} y_E^{(G)} \\ y_I^{(G)} \end{pmatrix} = \begin{pmatrix} y_E^{(G)} \\ -B_E^{(G)} y_E^{(G)} \end{pmatrix} = \begin{pmatrix} y_E^{(G)} \\ c_I^{(G)} \end{pmatrix} = c^{(G)}\,. \quad (19)$$

Therefore, the systems of linear algebraic equations

$$(B_I^{(G)} - k_0^2 D_I^{(G)}) y_I^{(G)} = c_I^{(G)} \quad (20)$$

are to be solved. The number of such systems (20) is m_s (see Section 2).

4.2 Eigenvalue Problem

The vector $y_{2d}^{(G)}$ is the solution of the $2d$ eigenvalue problem. In the following, we consider a longitudinally homogeneous transmission line. Thus, any field can be expanded into a sum of so-called modal fields which vary exponentially in the longitudinal direction:

$$\vec{E}(x, y, z \pm 2h) = \vec{E}(x, y, z) e^{\mp \jmath k_z 2h}\,, \quad (21)$$

where k_z is the propagation constant, and $2h$ is the length of an elementary cell in z-direction (see Fig. 3). Thus, we get a two-dimensional eigenvalue problem for the transverse electric fields $\vec{y} = \vec{E}_{t,l}(z_p),\ l = 1(1)m^{(p)}$, (see (6)) on the transmission line region:

$$A\vec{y} = \gamma\vec{y},\ \gamma = e^{-\jmath k_z 2h} + e^{+\jmath k_z 2h} - 2 = -4\sin^2(hk_z). \quad (22)$$

A detailed derivation of the eigenvalue problem can be found in [11, 12, 13, 15].

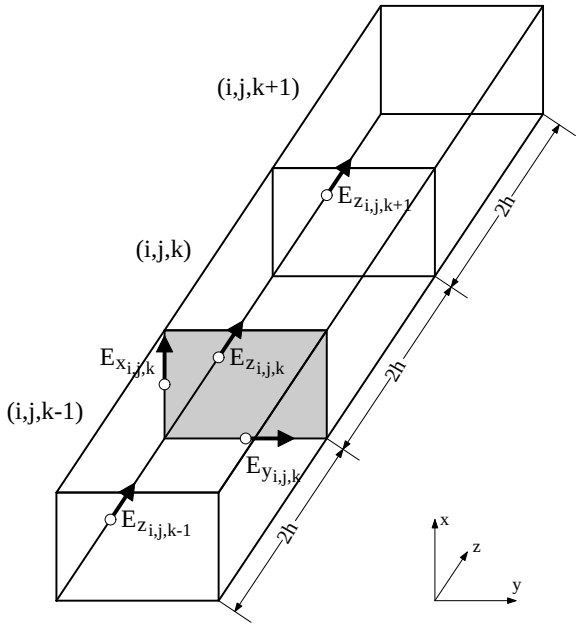

Figure 3: Transmission line

5 Symmetric Band Lanczos Process

We consider the iterative solution of large systems of linear algebraic equations which not only have multiple right-hand sides, but also have multiple shifts for each right-hand side. The generalized form of Eq. (20) is the problem

$$(\alpha_j B + \beta_j D) y^{(j,k)} = c^{(k)} \ , \quad \alpha_j, \beta_j \in \mathbb{C} \ , \tag{23}$$

with $j = 1, \ldots, n_s$ and $k = 1, \ldots, n_b$. Let n_b be the number of right-hand sides and n_s be the number of shifts. The Matrix B is complex, symmetric, and indefinite. A standard way to solve systems with multiple right-hand sides is to use a block approach [18, 8, 3].

Eq. (23) can be transformed into

$$(D^{-1/2} B D^{-1/2} + \alpha_j^{-1} \beta_j I)(\alpha_j D^{1/2} y^{(j,k)}) = D^{-1/2} c^{(k)} \ . \tag{24}$$

Thus, we get then the common equation

$$A^{(j)} x^{(j,k)} = (A + \sigma_j I) x^{(j,k)} = b^{(k)} \ , \quad \sigma_j \in \mathbb{C} \, , \tag{25}$$

i.e.,

$$\begin{pmatrix} A^{(1)} & & & \\ & \ddots & & 0 \\ & & A^{(j)} & \\ & 0 & & \ddots \\ & & & & A^{(n_s)} \end{pmatrix} \begin{pmatrix} x^{(1,1)} & \ldots & x^{(1,k)} & \ldots & x^{(1,n_b)} \\ \vdots & & \vdots & & \vdots \\ x^{(j,1)} & \ldots & x^{(j,k)} & \ldots & x^{(j,n_b)} \\ \vdots & & \vdots & & \vdots \\ x^{(n_s,1)} & \ldots & x^{(n_s,k)} & \ldots & x^{(n_s,n_b)} \end{pmatrix} =$$

$$\begin{pmatrix} b^{(1)} & \dots & b^{(k)} & \dots & b^{(n_b)} \\ \vdots & & \vdots & & \vdots \\ b^{(1)} & \dots & b^{(k)} & \dots & b^{(n_b)} \\ \vdots & & \vdots & & \vdots \\ b^{(1)} & \dots & b^{(k)} & \dots & b^{(n_b)} \end{pmatrix} \begin{matrix} \\ 1 \\ \\ j \\ \\ n_s \end{matrix}$$

with

$$A = D^{-1/2} B D^{-1/2},\ x^{(j,k)} = \alpha_j D^{1/2} y^{(j,k)},\ b^{(k)} = D^{-1/2} c^{(k)},\ \text{and}\ \sigma_j = \alpha_j^{-1} \beta_j\ .$$

For the special case that all right-hand sides in (25) are identical, i.e.,

$$x^{(j)} = x^{(j,k)}\ ,\ b^{(k)} = b \quad \text{for all} \quad k = 1, \dots, n_b\,, \tag{26}$$

it is straightforward to exploit the shift structure when solving the n_s systems by Krylov subspace methods. We use the initial guess $x_0^{(j)} = 0$ for all j. In this case, the Krylov subspaces for all n_s systems are identical:

$$\mathcal{K}_m(A + \sigma_j I, b) = \mathcal{K}_m(A, b) \quad \text{for all} \quad j = 1, \dots, n_s \quad \text{and} \quad m \geq 1\,. \tag{27}$$

This means that the computation of suitable basis vectors for the underlying Krylov subspaces has to be performed only once. A lot of Krylov subspace methods have been developed for shifted matrix problems. A detailed derivation of a shifted coupled two-term algorithm without look-ahead for

$$A^{(j)} x^{(j)} = (A + \sigma_j I) x^{(j)} = b\ , \quad \sigma_j \in \mathbb{C}\ , \quad j = 1, \dots, n_s\ , \tag{28}$$

can be found in [19].

5.1 Symmetric Block-QMR Method

We first describe the general form of block Krylov subspace iterative methods for the simultaneous solution of linear systems with multiple right-hand sides (see [8, 16]). Solving the n_b systems

$$A x^{(j)} = b^{(j)}\ ,\ j = 1, \dots, n_b\ , \tag{29}$$

where $A \in \mathbb{C}^{N \times N}$, $x^{(j)} \in \mathbb{C}^N$, and $b^{(j)} \in \mathbb{C}^N$ is equivalent to solving the block system of linear equations

$$A\, X = B\ , \tag{30}$$

where $B = [b^{(1)}\ b^{(2)}\ \dots\ b^{(n_b)}] \in \mathbb{C}^{N \times n_b}$ and $X = [x^{(1)}\ x^{(2)}\ \dots\ x^{(n_b)}] \in \mathbb{C}^{N \times n_b}$.

The block Krylov method generates a sequence of block iterates

$$X_\mu = [x_\mu^{(1)}\ x_\mu^{(2)}\ \dots\ x_\mu^{(n_b)}]\ ,\ \mu = 1, 2, \dots\ , \tag{31}$$

where $x_\mu^{(j)} \in x_0^{(j)} + \mathcal{K}_\mu(A, R)$ for each $j = 1, \dots, n_b$ and $R \in \mathbb{C}^{N \times n_b}$.
Here, $R = R_0 = B - A X_0$ is the block of initial residual vectors and $\mathcal{K}_\mu(A, R)$ denotes the

μ-th block Krylov subspace generated by A and R, i.e., the first μ linearly independent vectors in the block Krylov sequence

$$R, AR, \ldots, A^{k-1}R, \ldots \tag{32}$$

span the subspace $\mathcal{K}_\mu(A, R)$.
By scanning the vectors in (32) from left to right and deleting each vector that is either linearly dependent or almost linearly dependent on previous vectors, we obtain the so-called deflated block Krylov sequence

$$R_1, AR_2, \ldots, A^{k-1}R_k, \ldots \ . \tag{33}$$

For $k = 1$, we set $R = R_0$.

In addition to the matrices A and R, the Lanczos-type process requires a second sequence of vectors that span the block Krylov subspace $\mathcal{K}_\mu(A^T, L)$ generated by A^T and L, i.e., the Lanczos-type process has produced right and left Lanczos vectors

$$\{v_1, \ \ldots \ , v_\mu\} \quad \text{and} \quad \{w_1, \ \ldots \ , w_\mu\} \ , \tag{34}$$

respectively, with

$$\mathcal{K}_\mu(A, R) = span\{v_1, \ \ldots \ , v_\mu\}$$

and

$$\mathcal{K}_\mu(A^T, L) = span\{w_1, \ \ldots \ , w_\mu\}.$$

The vectors (34) are constructed to be biorthogonal, i.e.,

$$w_i^T v_j = \begin{cases} \delta_j \neq 0 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases} \qquad \text{for all} \quad i, j = 1, \ldots, \mu \ .$$

An important feature of the Lanczos-type process is that the vectors (34) are generated by means $(2n_b + 1)$-term recurrences. These recurrences can be summarized in compact form as follows:

$$AV_\mu = V_n T_\mu + V_\mu^{df} \ , \ \mu = n - m_{cr} \geq 1 \ . \tag{35}$$

Here, m_{cr} denotes the reduced size of the current block in the deflated block Krylov sequence (33) and n is the iteration index. $V_n = [v_1 \ v_2 \ \ldots \ v_n] \in \mathbb{C}^{N \times n}$ contains the first n basis vectors, $T_\mu \in \mathbb{C}^{n \times \mu}$ is a banded matrix with lower and upper band width $n_b + 1$ containing the recurrence coefficients, and the matrix $V_\mu^{df} \in \mathbb{C}^{N \times \mu}$ consists of mostly zero column vectors and a few nonzero columns with very small entries.
Each deflation step in the block Krylov sequence (33) reduces the lower band width of T_μ by one. Additionally, the recurrences (35) are complemented by recurrences for the initial block R, i.e.,

$$V_{m_1} \Theta + V_0^{df} = R \ , \quad V_{m_1} \in \mathbb{C}^{N \times m_1} \ , \quad m_1 \leq rank(R) \leq n_b \ . \tag{36}$$

The matrix $\Theta \in \mathbb{C}^{m_1 \times n_b}$ contains recurrence coefficients up to iteration when $\mu = 0$. The matrix $V_0^{df} \in \mathbb{C}^{N \times n_b}$ consists of zero vectors and deflated vectors.
Notice that (35) only holds for $\mu \geq 1$, or equivalent for $n > m_1$, where m_1 is the size of the first block in the sequence (33), i.e., $m_1 = rank(R_1)$.

The left Lanczos vectors in (34) are generated by means of recurrences similar to (35) and (36). All possible block iterates (31) can be represented in the form

$$X_\mu = X_0 + V_\mu Z_\mu \ , \quad Z_\mu \in \mathbb{C}^{\mu \times n_b} \ . \tag{37}$$

After each deflation in the v sequence, the size of the current block in the corresponding deflated block Krylov sequence (33) decrease by one. Additionally, one of the linear system of (30) can be dropped from subsequent block QMR iteration (see [8]). The solution of all such deflated systems can be recovered from the solution of the converged remaining linear systems. Therefore, one of the columns from the matrices X_μ, X_0, and Z_μ in (37) can be dropped and only the remaining iterates need to be updated. Then, for the current block iterate X_μ^{cr}, we can rewrite (37) as

$$X_\mu^{cr} = X_0^{cr} + V_\mu Z_\mu \ , \quad Z_\mu \in \mathbb{C}^{\mu \times m_{cr}} \ , \ m_{cr} \leq n_n. \tag{38}$$

The residual block R_μ^{cr} corresponding to X_μ^{cr} is given by

$$\begin{aligned} R_\mu^{cr} &= B^{cr} - A X_\mu^{cr} \\ &= R_0^{cr} - V_n T_\mu Z_\mu - V_\mu^{df} Z_\mu \\ &= V_n \left(\begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} - T_\mu Z_\mu \right) - V_\mu^{df} Z_\mu \ . \end{aligned} \tag{39}$$

The matrix $\Theta^{cr} \in \mathbb{C}^{m_1 \times m_{cr}}$ consists of those columns of Θ in (36) that correspond to columns of X_μ retained in X_μ^{cr}.
The free parameter matrix Z_μ in (38) is determined as the solution of the matrix least-squares problem

$$\left\| \begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} - T_\mu Z_\mu \right\| = \min_{Z \in \mathbb{C}^{\mu \times m_{cr}}} \left\| \begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} - T_\mu Z \right\| \tag{40}$$

in the Euclidean norm. The matrix least-squares problem (40) is solved by means standard techniques based on QR factorization of T_μ. This allows to obtain the solution Z_μ by updating the solution $Z_{\mu-1}$ from the previous step. Implementation details are described in [8].
The banded matrix T_μ is factorized into a unitary matrix $(Q_\mu)^H$and a nonsingular upper triangular matrix U_μ:

$$T_\mu = (Q_\mu)^H \begin{bmatrix} U_\mu \\ 0 \end{bmatrix} \ , \quad Q_\mu \in \mathbb{C}^{n \times n} \ , \quad U_\mu \in \mathbb{C}^{\mu \times \mu} \ .$$

The lower bandwidth of the matrix T_μ is at most $n_b + 1$. Its QR factorization can be updated using n_b Givens rotations at each iteration of the block QMR method. The update of the block QMR iterates can be performed by means the following quantities:

$$\begin{bmatrix} t_\mu^{cr} \\ \tau_\mu^{cr} \end{bmatrix} = Q_\mu \begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} \ , \quad t_\mu^{cr} \in \mathbb{C}^{\mu \times m_{cr}} \ , \quad \tau_\mu^{cr} \in \mathbb{C}^{m_{cr} \times m_{cr}} \ ,$$

$$t_\mu^{cr} = \begin{bmatrix} t_{\mu-1}^{cr} \\ y_\mu^T \end{bmatrix} \ , \quad y_\mu^T \in \mathbb{C}^{1 \times m_{cr}} \ .$$

The solution Z_μ of (40) is given by

$$Z_\mu = U_\mu^{-1} t_\mu^{cr} \ .$$

We also define a sequence of direction vectors $p_1, p_2, \ldots, p_\mu,\ \mu = 1, 2, \ldots$, with

$$P_\mu = [p_1\ p_2\ \ldots\ p_\mu] = V_\mu U_\mu^{-1}.$$

Finally, the block QMR iterates can be updated by means

$$\begin{aligned} X_\mu^{cr} &= X_0^{cr} + V_\mu U_\mu^{-1} t_\mu^{cr} \\ &= X_{\mu-1}^{cr} + p_\mu y_\mu^T \,. \end{aligned}$$

It is well known that the classical Lanczos process for general matrices A simplifies when applied to complex symmetric matrices. The resulting Lanczos process only involves one sequence of Lanczos vectors. The resulting simplified block QMR method does not require matrix-vector multiplications with A^T.

Now, we consider an adaption of block QMR to shifted systems, i.e., systems of the type

$$(A + \sigma_j I)x^{(j)} = b^{(j)} \,, \quad \sigma_j \in \mathbb{C} \,, \quad j = 1, \ldots, n_b \,. \tag{41}$$

We sketch the general case (41) or the case (28) if non zero initial guesses, $x_0^{(j)} \neq 0$, are chosen. Then, the Krylov subspaces depend on j. We use the Lanczos process to still exploit the shift structure of (41). Using the right initial block

$$R = R_0 = [r_0^{(1)}\ r_0^{(2)}\ \ldots\ r_0^{(n_b)}] \,, \quad r_0^{(j)} = b^{(j)} - (A + \sigma_j I)x_0^{(j)} \,, \tag{42}$$

we generate basis vectors $\{v_1\ v_2\ \ldots\ v_\mu\}$ for th μ-th Krylov subspace $\mathcal{K}_\mu(A, R)$. The μ-th iterate $x_\mu^{(j)}$ for the j-th system in (41) is then defined by

$$x_\mu^{(j)} = x_0^{(j)} + V_\mu z_\mu^{(j)} \,, \tag{43}$$

where $z_\mu^{(j)} \in \mathbb{C}^\mu$ is the solution of the least-squares problem

$$\left\| \begin{bmatrix} \Theta_j^{cr} \\ 0 \end{bmatrix} - T_\mu^{(j)} z_\mu^{(j)} \right\| = \min_{z \in \mathbb{C}^\mu} \left\| \begin{bmatrix} \Theta_j^{cr} \\ 0 \end{bmatrix} - T_\mu^{(j)} z \right\| \,. \tag{44}$$

Using (35) and $A^{(j)} = A + \sigma_j I$, we get

$$A^{(j)} V_\mu = V_n T_\mu^{(j)} + V_\mu^{df} \,. \tag{45}$$

Furthermore,

$$\begin{aligned} (A + \sigma_j I)V_\mu &= AV_\mu + \sigma_j V_\mu \\ &= V_n T_\mu + \sigma_j V_\mu + V_\mu^{df} \\ &= V_n \left(T_\mu + \sigma_j \begin{bmatrix} I_\mu \\ 0 \end{bmatrix} \right) + V_\mu^{df} \,. \end{aligned}$$

With $T_\mu^{(j)} = T_\mu + \sigma_j \begin{bmatrix} I_\mu \\ 0 \end{bmatrix}$ we get from (44) the least-squares problem

$$z_\mu^{(j)} = \arg\min_{z \in \mathbb{C}^\mu} \left\| \begin{bmatrix} \Theta_j^{cr} \\ 0 \end{bmatrix} - \left((T_\mu + \sigma_j \begin{bmatrix} I_\mu \\ 0 \end{bmatrix}) z \right\| \,. \tag{46}$$

In (46), T_μ is the matrix of Lanczos recurrence coefficients given by (35). The vector Θ_j^{cr} is defined as the j-th column of the matrix Θ^{cr} (see (36) and (39)).

5.2 Symmetric Band Lanczos Method

The symmetric band Lanczos process is an extension of the classical Lanczos algorithm for symmetric matrices and single starting vectors to multiple starting vectors (see [1, 4]). First, we consider the n_b linear systems (29), where A is a complex symmetric matrix and $R = [r^{(1)}\ r^{(2)}\ \ldots\ r^{(n_b)}]$ is a block of n_b right starting vectors. The symmetric band Lanczos process generates orthogonal basis vectors for the subspaces spanned by leading columns of the block Krylov matrix (see (32)):

$$\mathcal{K}(A, R) = [R\ AR\ \ldots\ A^{N-1}R]\,. \tag{47}$$

The columns of the matrix $\mathcal{K}(A, R)$ in (47) are all vectors of length N, and thus at most N of them are linearly independent. One needs to perform so-called deflation of linearly dependent or in some sence almost linearly dependent vectors.

After n iterations, the algorithm has generated the first n Lanczos vectors

$$v_1, v_2,\ \ldots\ , v_n \in \mathbb{C}^N\,. \tag{48}$$

It will be convenient to introduce the notation

$$V_n = [v_1\ v_2\ \ldots\ v_n]\,, \quad V_n^T V_n = I_n\,, \tag{49}$$

for the matrices whose columns are just the right Lanczos vectors (48). In addition to (48), the algorithm has constructed the $m_{cr} = m_{cr}(n)$ vectors

$$\hat{v}_{n+1}, \hat{v}_{n+2},\ \ldots\ , \hat{v}_{n+m_{cr}} \in \mathbb{C}^N\,, \tag{50}$$

that are candidates for the next m_{cr} Lanczos vectors, $v_{n+1}, v_{n+2},\ \ldots\ , v_{n+m_{cr}}$. Here m_{cr} is the current block size. At the initialization phase, i.e., $n = 0$, we have

$$m_{cr} = n_b \quad \text{and} \quad \hat{v}_j = r^{(j)}\,,\ 1 \le j \le n_b\,.$$

Within the algorithm, m_{cr} is reduced by one every time a deflation occurs. The vectors (50) are constructed so that they satisfy the orthogonality relations

$$V_n^T \hat{v}_{n+j} = 0 \quad \text{for all} \quad j = 1, \ldots, m_{cr}\,. \tag{51}$$

The recurrences can be summarized compactly as follows:

$$AV_n = V_n T_n + [\underbrace{0\ \ldots\ 0}_{n-m_{cr}}\ \underbrace{\hat{v}_{n+1}\ \hat{v}_{n+2}\ \ldots\ \hat{v}_{n+m_{cr}}}_{m_{cr}}] + \hat{V}_n^{df}\,. \tag{52}$$

The entries of the matrix T_n, $T_n \in \mathbb{C}^{n\times n}$, are chosen so that the orthogonality conditions (49) and (51) are satisfied. The matrix $\hat{V}_n^{df}$ contains mostly zero columns together with the $\hat{v}_j$ vectors that have been deflated during the first n iterations. We remark that $n_b - m_{cr}$ is the number of deflated $\hat{v}_j$ vectors. It turns out that orthogonality only has to be explicitly enforced among $2m_{cr}+1$ consecutive Lanczos vectors and, once deflation has occurred, against $n_b - m_{cr}$ fixed earlier right Lanczos vectors. Thus, the matrix T_n is essentially banded. More precisely, T_n has

lower as well as upper bandwidth $m_{cr}+1$. Additionally, the recurrences (52) are complemented by recurrences for the initial block R, i.e.,

$$R = R_0 = V_{m_1}\Theta + \hat{V}_0^{df} \ , \quad V_{m_1} \in \mathbb{C}^{N\times m_1} \ , \quad m_1 \leq rank(R) \leq n_b \, . \tag{53}$$

Here, $m_1 \leq n_b$ denotes the number of columns of the block R that have not been deflated. The matrix $\hat{V}_0^{df} \in \mathbb{C}^{N\times n_b}$ contains the $n_b - m_1$ deflated starting vectors and m_1 zero vectors as columns, and $\Theta \in \mathbb{C}^{m_1\times n_b}$ is an upper triangular matrix whose entries are chosen such that the columns of V_{m_1} are orthonormal.
If no deflation has occured or if only exact deflation is performed,i.e.,

$$\hat{V}_0^{df} = 0 \quad \text{and} \quad \hat{V}_n^{df} = 0 \, ,$$

then

$$V_n^T A V_n = V_n^T V_n T_n = T_n \, . \tag{54}$$

Furthermore, the so-called n-th Lanczos matrix T_n is symmetric:

$$T_n^T = (V_n^T A V_n)^T = V_n^T A V_n = T_n \, . \tag{55}$$

In the case $\hat{V}_n^{df} \neq 0$, we get

$$\tilde{T}_n = V_n^T A V_n + V_n^T \hat{V}_n^{df} = T_n + V_n^T \hat{V}_n^{df} \ , \quad \tilde{T}_n \in \mathbb{C}^{n\times n} \, .$$

The matrix $\tilde{T}_n$ consists of a symmetric banded part, T_n, with decreasing bandwidth and a spiked part with potentially nonzero elements only in rows and columns with index $i \in \mathcal{I}$ and outside of the banded part. The index set $\mathcal{I}$ records the positions of the potentially nonzero columns of $\hat{V}_n^{df}$ due to deflation.
The matrix T_n is decomposed in $T_n = L_n U_n$, where $L_n \in \mathbb{C}^{n\times n}$ and $U_n \in \mathbb{C}^{n\times n}$ are lower and upper triangular matrices,respectively. The unit upper triangular U_n consists of a banded part with bandwidth decreasing from $n_b + 1$ to $m_{cr} + 1$. Analogous, the lower triangular L_n consists of a banded part with bandwidth decreasing from $n_b + 1$ to $m_{cr} + 1$:

$$L_n = \begin{pmatrix} l_{11} & & 0 \\ \vdots & \ddots & \\ l_{1n} & \cdots & l_{nn} \end{pmatrix} \quad , \quad U_n = \begin{pmatrix} 1 & \cdots & u_{1n} \\ & \ddots & \vdots \\ 0 & & 1 \end{pmatrix} \, , \tag{56}$$

where $l_{ij} = u_{ji} = 0$ for $j + m_{cr} < i \leq n$, $j = 1, \ldots, n - m_{cr}$, and $n > m_{cr}$.

We generate a second set of vectors

$$p_1, p_2, \ \ldots \ , p_n \in \mathbb{C}^N \ , \quad P_n = [p_1 \ p_2 \ \ldots \ p_n] \, , \tag{57}$$

that span the same subspaces as V_n, i.e.,

$$span\{v_1, v_2, \ \ldots \ , v_j\} = span\{p_1, p_2, \ \ldots \ , p_j\} \quad \text{for all} \quad 1 \leq j \leq n \, .$$

Then we set

$$V_n = P_n U_n \, . \tag{58}$$

All block iterates can be represented in the form

$$X_n = X_0 + V_n Z_n \ , \quad Z_n \in \mathbb{C}^{n \times n_b} \, . \tag{59}$$

After each deflation, for the current block iterate X_n^{cr}, we can rewrite (59) as

$$\begin{aligned} X_n^{cr} &= X_0^{cr} + V_n Z_n \ , \quad Z_n \in \mathbb{C}^{n \times m_{cr}} \ , \\ &= X_0^{cr} + P_n U_n Z_n \\ &= X_0^{cr} + P_n Y_n \ , \quad Y_n = U_n Z_n \in \mathbb{C}^{n \times m_{cr}} \ , \\ &= X_{n-1}^{cr} + p_n (e_n^T Y_n) \, . \end{aligned} \tag{60}$$

Using (52), (53), (58) – (60), and $\hat{V}_n^{cr} = [0 \ \ldots \ 0 \ \hat{v}_{n+1} \ \ldots \ \hat{v}_{n+m_{cr}}]$ the residual block R_n^{cr} corresponding to X_n^{cr} can be represented as follows:

$$\begin{aligned} R_n^{cr} &= B^{cr} - A X_n^{cr} \\ &= B^{cr} - A X_0^{cr} - A V_n Z_n \\ &= R_0^{cr} - V_n T_n Z_n - \hat{V}_n^{cr} Z_n - \hat{V}_n^{df} Z_n \\ &= V_{m_{cr}} \Theta^{cr} - V_n L_n Y_n - \hat{V}_n^{cr} Z_n - \hat{V}_n^{df} Z_n \\ &= V_n \left(\begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} - L_n Y_n \right) - \hat{V}_n^{cr} Z_n - \hat{V}_n^{df} Z_n \, . \end{aligned} \tag{61}$$

Using (61), Y_n is the unique solution of the least-squares problem

$$Y_n = \arg \min_{Y \in \mathbb{C}^{n \times m_{cr}}} \left\| \begin{bmatrix} \Theta^{cr} \\ 0 \end{bmatrix} - L_n Y \right\| \, . \tag{62}$$

We describe now the basic steps of the QMR approach. We first consider the solution of the least-squares problem (62) for the case when no deflation occurs at iteration n, while generating v_n:

$$V_n = [V_{n-1} \ v_n] \, .$$

Using (56), we consider the decomposition of the n-th Lanczos matrix T_n:

$$T_n = \left(\begin{array}{ccc|c} & T_{n-1} & & \begin{matrix} t_{1n} \\ \vdots \\ t_{n-1n} \end{matrix} \\ \hline t_{n1} & \cdots & t_{nn-1} & t_{nn} \end{array} \right) \ , \quad t_{ij} = t_{ji} \ , \quad 1 \le i, j \le n \ ,$$

$$T_n = L_n U_n = \left(\begin{array}{ccc|c} & L_{n-1} & & 0 \\ \hline l_{n1} & \cdots & l_{nn-1} & l_{nn} \end{array} \right) \left(\begin{array}{ccc|c} & & & u_{1n} \\ & U_{n-1} & & \vdots \\ & & & u_{n-1n} \\ \hline 0 & & & 1 \end{array} \right) \, .$$

Due to the fact that the lower and upper triangular L_n and U_n, respectively, consist of a banded

part with bandwidth $m_{cr}+1$ we get the following terms:

$$\begin{aligned} l_{ni} &= t_{ni} - \sum_{j=j^*}^{i-1} l_{nj}u_{ji}\ , \quad u_{ii}=1\ , \\ u_{in} &= \frac{1}{l_{ii}}\left(t_{in} - \sum_{j=j^*}^{i-1} l_{ij}u_{jn}\right)\ , \\ u_{nn} &= 1\ , \\ l_{nn} &= t_{nn} - \sum_{i=i^*}^{n-1} l_{ni}u_{in}\ , \end{aligned}$$

for $i^* = \max(1, n-m_{cr})$, $j^* = \max(1, n-m_{cr})$, and $i = i^*, \ldots, n-1$. For the solution of the least-squares problem (62) we get

$$L_n Y_n = S_n\ , \quad L_n \in \mathbb{C}^{n\times n}\ , \quad Y_n \in \mathbb{C}^{n\times m_{cr}}\ , \quad S_n \in \mathbb{C}^{n\times m_{cr}}\ , \text{i.e.,}$$

$$\left(\begin{array}{ccc|c} & L_{n-1} & & 0 \\ \hline l_{nj^*} & \cdots & l_{nn-1} & l_{nn} \end{array}\right)\left(\begin{array}{ccc} & Y_{n-1} & \\ \hline y_{n1} & \cdots & y_{nm_{cr}} \end{array}\right) = \left(\begin{array}{ccc} & S_{n-1} & \\ \hline s_{n1} & \cdots & s_{nm_{cr}} \end{array}\right)\ ,$$

and

$$\begin{aligned} L_{n-1}Y_{n-1} &= S_{n-1} \\ y_{ni} &= \frac{1}{l_{nn}}\left(s_{ni} - (l_{nj^*}\ \cdots\ l_{nn-1})Y_{n-1}^{(i)}\right)\ , \quad i=1,\ldots,m_{cr}\,, \end{aligned} \tag{63}$$

where $Y_{n-1}^{(i)}$ is the i-th column of the matrix Y_{n-1}. We set $S_n = \Theta^{cr}$ for $n = m_{cr}$ and $s_{ni} = 0$ for $i = 1, \ldots, m_{cr}$ and $n > m_{cr}$.

Next, we describe the effect of deflation in the Lanczos-type algorithm for updating the block iterates X_n^{cr}. In this case, we set $v_n = 0$, which implies that

$$V_n = [V_{n-1}\ 0]\,.$$

V_n now only has column rank $n-1$.

$$T_n = V_n^T A V_n = \left[\begin{array}{c} V_{n-1}^T \\ 0 \end{array}\right] A[V_{n-1}\ 0] = \left(\begin{array}{c|c} T_{n-1} & 0 \\ \hline 0 & 0 \end{array}\right)$$

$$T_n = L_n U_n = \left(\begin{array}{c|c} L_{n-1}U_{n-1} & 0 \\ \hline 0 & 0 \end{array}\right) = \left(\begin{array}{c|c} L_{n-1} & 0 \\ \hline 0 & 0 \end{array}\right)\left(\begin{array}{c|c} U_{n-1} & 0 \\ \hline 0 & 1 \end{array}\right)$$

For the case when no deflation occurs we get

$$L_n Y_n = \left[\begin{array}{c} t_n^{cr} \\ \tau_n^{cr} \end{array}\right]\ , \quad t_n^{cr} \in \mathbb{C}^{(n-m_{cr})\times m_{cr}}\ , \quad \tau_n^{cr} \in \mathbb{C}^{m_{cr}\times m_{cr}}\ .$$

In the other case we get

$$L_n Y_n = \left[\begin{array}{c} t_n^{cr} \\ \tilde{\tau}_n^{cr} \\ 0 \end{array}\right] = \left[\begin{array}{c} t_{n-1}^{cr} \\ \tau_{n-1}^{cr} \\ 0 \end{array}\right] = \left[\begin{array}{c} L_{n-1}Y_{n-1} \\ 0 \end{array}\right] \quad \text{with} \quad \tilde{\tau}_n^{cr} \in \mathbb{C}^{(m_{cr}-1)\times m_{cr}}\ .$$

At a deflation step, the residual block R_n^{cr} corresponding to the block iterate X_n^{cr} in (60) is given by

$$R_n^{cr} = V_{n-1} \begin{bmatrix} 0 \\ \tilde{\tau}_n^{cr} \end{bmatrix} . \tag{64}$$

The matrices $\hat{V}_n^{cr}$ and $\hat{V}_n^{df}$ consist only of zero column vectors. Since $\tilde{\tau}_n^{cr}$ is a rectangular matrix, there exist a vector γ with $\tilde{\tau}_n^{cr}\gamma = 0$. Multiplying (64) from the right by γ gives

$$R_n^{cr}\gamma = V_{n-1} \begin{bmatrix} 0 \\ \tilde{\tau}_n^{cr} \end{bmatrix} \gamma = 0 . \tag{65}$$

In practice, the vector γ is computed by means of the last m_{cr} columns and the last $m_{cr} - 1$ rows of the matrix L_{n-1}.
Using (65), we can express the approximate solution of the single linear system $Ax_\gamma = B^{cr}\gamma$ in terms of a linear combination of columns of X_n^{cr} by setting

$$x_\gamma = X_n^{cr}\gamma . \tag{66}$$

Consequently, it is possible to delete one of the linear systems from block iterations, e.g., one can delete the j-th system. The solution vector corresponding to the j-th system can be constructed when all vectors in the updated block iterate X_n^{cr} have converged after n_{max} iterations. Using (66), we get

$$x_{n_{max}}^{(i_j)} = \frac{1}{\gamma_j} \left(x_\gamma - \sum_{\substack{k=1 \\ k \neq j}}^{m_{cr}} x_{n_{max}}^{(i_k)} \gamma_k \right) . \tag{67}$$

Now, we consider shifted systems of the type (41) with (42). Using

$$V_n = P_n^{(j)} U_n^{(j)} \quad \text{for all} \quad 1 \leq j \leq n ,$$

then the n-th iterate $x_n^{(j)}$ for the j-th system is defined by

$$\begin{aligned} x_n^{(j)} &= x_0^{(j)} + V_n z_n^{(j)} , \quad z_n^{(j)} \in \mathbb{C}^n , \\ &= x_0^{(j)} + P_n^{(j)} U_n^{(j)} z_n^{(j)} \\ &= x_0^{(j)} + P_n^{(j)} y_n^{(j)} , \quad y_n^{(j)} = U_n^{(j)} z_n^{(j)} \in \mathbb{C}^n , \\ &= x_{n-1}^{(j)} + p_n^{(j)} (e_n^T y_n^{(j)}) . \end{aligned} \tag{68}$$

Using (54) and $A^{(j)} = A + \sigma_j I$, we get

$$T_n^{(j)} = V_n^T A^{(j)} V_n = V_n^T (A + \sigma_j I) V_n = T_n + \sigma_j I . \tag{69}$$

Using the decomposition $T_n^{(j)} = L_n^{(j)} U_n^{(j)}$, $y_n^{(j)}$ is the unique solution of the least-squares problem

$$y_n^{(j)} = \arg\min_{y \in \mathbb{C}^n} \left\| \begin{bmatrix} \Theta_j^{cr} \\ 0 \end{bmatrix} - L_n^{(j)} y \right\| . \tag{70}$$

5.3 Preconditioned System of Linear Algebraic Equations

Unfortunately, standard preconditioning techniques with a preconditioner

$$M = M_1 M_2 = (M_1 M_2)^T = M^T, \tag{71}$$

such as SSOR preconditioning, destroy the special structure when they are applied to shifted linear systems. The only technique we are aware of that allows to preserve the shifted structure is polynomial preconditioning (see [7]).

Using standard preconditioning techniques, we apply the symmetric band Lanczos method to the shifted linear systems (41)

$$\tilde{A}^{(j)} \tilde{x}^{(j)} = \tilde{b}^{(j)} \ , \quad j = 1, \ldots, n_b \ , \tag{72}$$

with

$$\begin{aligned} \tilde{A}^{(j)} &= M_1^{-1}(A + \sigma_j M_1 M_2) M_2^{-1} = M_1^{-1} A M_2^{-1} + \sigma_j I \ , \\ \tilde{b}^{(j)} &= M_1^{-1} b^{(j)} \quad \text{and} \quad \tilde{x}^{(j)} = M_2 x^{(j)} \, . \end{aligned} \tag{73}$$

It is easy to see that the linear systems (41) and (72) with (73) are not equivalent. Only, for $M = I$ the systems (41) and (72) are equivalent.

It is common when implementing algorithms which involve a two-sided preconditioner to avoid the use of the $\tilde{x}^{(j)}$ variable. It is possible to write the resulting algorithm in terms of quantities corresponding to the system (41). We have the following analogies:

$v_n \ \rightarrow \ \tilde{v}_n = M_1^{-1} v_n \ ,$	$p_n \ \rightarrow \ \tilde{p}_n = M_2 p_n \ ,$
$\tilde{v}_n^T \tilde{v}_n = v_n^T M^{-1} v_n \ ,$	$\tilde{p}_n^T \tilde{p}_n = p_n^T M p_n \ ,$
$\tilde{v}_n^T \tilde{A} \tilde{v}_n = v_n^T M^{-1} A M^{-1} v_n \ ,$	$\tilde{p}_n^T \tilde{A} \tilde{p}_n = p_n^T A p_n \, .$

5.4 Algorithm

We summarize the basic structure of the symmetric band Lanczos QMR method with deflation, but without look-ahead (see [8, 4]).

0. **Input**: $A = A^T$, $B = [b^{(1)} \, b^{(2)} \, \ldots \, b^{(n_b)}]$, $\{\sigma_1, \ldots, \sigma_{n_b}\}$.
   A deflation tolerance $dtol$.
   Choose X_0 and set $R = [r^{(1)} \, r^{(2)} \, \ldots \, r^{(n_b)}] = R_0 = B - A X_0$.
   For $j = 1, \ldots, n_b$, set $\hat{v}_j = r^{(j)}$. Set $m_{cr} = n_b$ and index set $\mathcal{I} = \emptyset$.

For $n = 1, 2, \ldots,$ **do**:

1. Compute $\beta = \|M_1^{-1} \hat{v}_n\|$. Set $\mu = n - m_{cr}$.
   Decide if $\hat{v}_n$ should be deflated. If yes, i.e., $\beta < dtol$, do the following:

   1.1 If $\mu \leq 0$, then delete one column vector from X_0^{cr}, R_0^{cr}, and Θ^{cr}.

1.2 If $\mu > 0$ and the deflated vector $\hat{v}_n$ is nonzero, then set $\mathcal{I} = \mathcal{I} \cup \{\mu\}$. Delete one column vector from X_n^{cr} and R_n^{cr}.

1.3 Set $m_{cr} = m_{cr} - 1$. If $m_{cr} = 0$, set $n = n - 1$ and stop.
For $j = n, n+1, \ldots, n + m_{cr} - 1$, set $\hat{v}_j = \hat{v}_{j+1}$.
Return to Step 1.

2. Update V and preconditioned V sequences.

2.1 Normalize $\hat{v}_n$ to become the n-th Lanczos vector: $v_n = \dfrac{\hat{v}_n}{\beta}$.

2.2 If $\mu \leq 0$, then set $\theta_{n,n}^{cr} = \beta$.

2.3 If $\mu > 0$, then set $t_{n,\mu} = \beta$.

2.4 Compute $\delta_n = v_n^T M^{-1} v_n$. If $\delta_n = 0$ stop.

2.5 Advance the right Krylov subspace: $\hat{v}_{n+m_{cr}} = A(M^{-1} v_n)$.

2.6 Set $k = \max\{1, \mu\}$. Orthogonalize the vector $\hat{v}_{n+m_{cr}}$ against vectors v_j, $j \in \mathcal{I} \cup \{k, \ldots, n-1\}$:

$$t_{j,n} = \frac{v_j^T M^{-1} \hat{v}_{n+m_{cr}}}{\delta_j} \quad \text{and} \quad \hat{v}_{n+m_{cr}} = \hat{v}_{n+m_{cr}} - v_j t_{j,n} \, .$$

2.7 Orthogonalize the vectors $\hat{v}_{n+j}, j = 1, \ldots, m_{cr}$, against vector v_n:
If $\mu + j \leq 0$, then

$$\theta_{n,n+j}^{cr} = \frac{v_n^T M^{-1} \hat{v}_{n+j}}{\delta_n} \quad \text{and} \quad \hat{v}_{n+j} = \hat{v}_{n+j} - v_n \theta_{n,n+j}^{cr} \, .$$

If $\mu + j > 0$, then

$$t_{n,\mu+j} = \frac{v_n^T M^{-1} \hat{v}_{n+j}}{\delta_n} \quad \text{and} \quad \hat{v}_{n+j} = \hat{v}_{n+j} - v_n t_{n,\mu+j} \, .$$

For all $j = 1, \ldots, n_b$ for which $x_n^{(j)}$ has not converged yet:

3. Compute the decomposition of the matrix $T_n^{(j)}$:

$$T_n^{(j)} = T_n + \sigma_j I = L_n^{(j)} U_n^{(j)} \, .$$

4. Compute the vector $p_n^{(j)}$:

$$P_n^{(j)} = [p_1^{(j)} \; p_2^{(j)} \; \ldots \; p_n^{(j)}] = V_n (U_n^{(j)})^{-1} \, , \quad p_n^{(j)} = M^{-1} v_n - \sum_{i=\max\{1,\mu\}}^{n-1} p_i^{(j)} u_{i,n}^{(j)} \, .$$

5. Compute the solution $y_n^{(j)}$ of the least-squares problem (70).

6. Compute the n-th iterate $x_n^{(j)}$ (see (68)).

End for (j).

7. Check if all solution vectors $x_n^{(j)}$ have converged. If yes, then recover solution vectors (see (67)) and stop.

End for (n).

6 Polynomial Preconditioning

We consider the shifted linear system

$$A^{(\sigma)}x = (A + \sigma I)x = b\,. \tag{74}$$

We use polynomial preconditioning to speed up the convergence of the iterative methods for the solution of (74), i.e.,

$$\mathcal{P}_m^{(\sigma)}(A^{(\sigma)})A^{(\sigma)}x = \mathcal{P}_m^{(\sigma)}(A^{(\sigma)})b \tag{75}$$

for left preconditioning and

$$A^{(\sigma)}\mathcal{P}_m^{(\sigma)}(A^{(\sigma)})y = \mathcal{P}_m^{(\sigma)}(A^{(\sigma)})A^{(\sigma)}y = b\,, \quad x = \mathcal{P}_m^{(\sigma)}(A^{(\sigma)})y\,, \tag{76}$$

for right preconditioning, respectively. Here, $\mathcal{P}_m^{(\sigma)}$ is a suitable chosen polynomial in $A^{(\sigma)}$ of a small degree, i.e., with degree no more than m. Both linear systems (75) and (76) are equivalent. We seek a polynomial $\mathcal{P}_m^{(\sigma)}$ with the following two properties [6, 5]:

- The coefficient matrix $\mathcal{P}_m^{(\sigma)}(A^{(\sigma)})A^{(\sigma)}$ is again a shifted matrix.
- $\mathcal{P}_m^{(\sigma)}(A^{(\sigma)})$ is an optimal polynomial preconditioner, i.e., the convergence of the iterative method, applied to the preconditioned system, is speed up optimally.

First, for any polynomial, we can represent $A^{(\sigma)}\mathcal{P}_m^{(\sigma)}(A^{(\sigma)})$ in the form

$$A^{(\sigma)}\mathcal{P}_m^{(\sigma)}(A^{(\sigma)}) = (A + \sigma I)\mathcal{P}_m^{(\sigma)}(A + \sigma I) = A\mathcal{P}_m(A) + \tau I \tag{77}$$

with $\tau \in \mathbb{C}$. Note that $\mathcal{P}_m^{(\sigma)}$, $\mathcal{P}_m$, and τ are related by

$$(z + \sigma)\mathcal{P}_m^{(\sigma)}(z + \sigma) = z\mathcal{P}_m(z) + \tau \quad \text{and} \quad \tau = \sigma\mathcal{P}_m(-\sigma)\,. \tag{78}$$

We note that the coefficient matrix $A\mathcal{P}_m(A)$ of the preconditioned system (77) is Hermitian if, and only if, $\mathcal{P}_m$ is a real polynomial. In order to guarantee that $A\mathcal{P}_m(A)$ is nonsingular, we require that $\mathcal{P}_m(z) \neq 0$ for all $z \in S$ with

$$\varrho(A) \subseteq S = [a, b] \cup [c, d]\,, \quad c < d < 0 < a < b\,,$$

where $\varrho(A)$ is the spectrum of A.

Next, we turn to the question of optimal choice of polynomial $\mathcal{P}_m$. We have two different cases:

- $z\mathcal{P}_m(z) > 0 \quad \forall z \in S$
- $z\mathcal{P}_m(z) > 0 \quad \forall z \in [a, b] \quad \text{and} \quad z\mathcal{P}_m(z) < 0 \quad \forall z \in [c, d]\,.$

If the last case holds, then the preconditioned system remains indefinite. We can now state the main result in the following form [6]:

Let $S = [a, b] \cup [c, d]$ be the union of a positive and negative interval with $c < d < 0 < a < b$ and $\Gamma = \{(\gamma, \delta) \in \mathbb{R} \times \mathbb{R} \, : \, \delta > 0\}$ a parameter set. The optimal polynomial $\mathcal{P}_m^*(z)$ of

$$\begin{aligned} w(\gamma, \delta) &= \min_{\mathcal{P}_m} \|f - z\mathcal{P}_m\|_g \, , \\ \|f - z\mathcal{P}_m\|_g &= \max_{z \in S} |g(z)(f(z) - z\mathcal{P}_m(z))| \, , \end{aligned} \tag{79}$$

where

$$g(z) = \begin{cases} 1 & \text{if} \quad z > 0 \\ \delta & \text{if} \quad z < 0 \end{cases} \quad , \quad f(z) = \begin{cases} 1 & \text{if} \quad z > 0 \\ \gamma & \text{if} \quad z < 0 \end{cases}$$

is an indefinite polynomial preconditioner with

$$\gamma = \frac{\bar{d} + \bar{c}}{\bar{b} + \bar{a}} \quad \text{and} \quad \delta = \frac{\bar{b} - \bar{a}}{\bar{d} - \bar{c}} \, .$$

The numbers $\bar{a}$, $\bar{b}$, $\bar{c}$, and $\bar{d}$ are defined by

$$\begin{aligned} \bar{a} &= \min_{z \in [a,b]} z\mathcal{P}_m(z) \, , \quad \bar{b} = \max_{z \in [a,b]} z\mathcal{P}_m(z) \, , \\ \bar{c} &= \min_{z \in [c,d]} z\mathcal{P}_m(z) \, , \quad \bar{d} = \max_{z \in [c,d]} z\mathcal{P}_m(z) \, . \end{aligned}$$

Moreover, there exist parameters γ_0 and δ_0, $(\gamma_0, \delta_0) \in \Gamma$, such that $\mathcal{P}_m^*(z, \gamma_0, \delta_0)$ is an optimal indefinite polynomial preconditioner.

(79) is a linear Chebyshev approximation problem depending on the two parameters $(\gamma, \delta) \in \Gamma$. We seek to approximate $f(z)$ by polynomials of the form $z\mathcal{P}_m(z)$ in the weighted uniform norm $\|.\|_g$. The standard tool for the numerical solution of such general real Chebyshev approximation problems is the method of Remez. The Remez type procedure is based on the equioscillation property [6]. Implementation details are described in [19].

7 Initial Guesses

The use of initial guesses for systems with multiple shifts is not as simple. The problem of initial guesses is related to the more general problem of solving systems with multiple shifts each with a different right-hand side (see [17]).

7.1 Multiple Shifts with Identical Right-Hand Sides

We consider the systems (41) with the same right-hand sides (see (28)). Using the initial guesses, $x_0^{(j)}$, we get the residuals

$$r_0^{(j)} = b - (A + \sigma_j I)x_0^{(j)} \, , \quad j = 1, \ldots, n_b \, , \tag{80}$$

and then solve

$$\begin{aligned} b - (A+\sigma_j I)x_0^{(j)} &= r_0^{(j)} \\ (A+\sigma_j I)x^{(j)} - (A+\sigma_j I)x_0^{(j)} &= r_0^{(j)} \\ (A+\sigma_j I)(x^{(j)} - x_0^{(j)}) &= r_0^{(j)} \\ (A+\sigma_j I)z^{(j)} &= r_0^{(j)} \ , \quad j = 1, \ldots, n_b \, . \end{aligned} \tag{81}$$

Then, the solutions are given by $x^{(j)} = x_0^{(j)} + z^{(j)}$ for all $j = 1, \ldots, n_b$. In general, the new right-hand sides, $r_0^{(j)}$, are not collinear. Therefore, the Krylov subspaces, $\mathcal{K}_n(A + \sigma_j I, r_0^{(j)})$, are not the same. Take

$$x_0^{(j)} = \left\{ \prod_{\substack{i=1 \\ i \neq j}}^{n_b} (A + \sigma_i I) \right\} w \tag{82}$$

for any vector w, then the new right-hand sides are all equal to

$$r_0^{(j)} = b - (A+\sigma_j I) \left\{ \prod_{\substack{i=1 \\ i \neq j}}^{n_b} (A + \sigma_i I) \right\} w = b - \left\{ \prod_{i=1}^{n_b} (A + \sigma_i I) \right\} w \, . \tag{83}$$

The n_b systems (81) with (82) and (83) can be solved with standard multi-shift Krylov methods [19]. The problem is to find the best vector w for (82).

Given approximate solutions

$$\tilde{x}^{(j)} \approx (A+\sigma_j I)^{-1} b \ , \quad j = 1, \ldots, n_b \, . \tag{84}$$

Using (83), we get

$$b \approx \left\{ \prod_{i=1}^{n_b} (A + \sigma_i I) \right\} w \, .$$

Next, from the above expression, we derive the vector w:

$$\begin{aligned} \tilde{x}^{(j)} \approx (A+\sigma_j I)^{-1} b &\approx \left\{ \prod_{\substack{i=1 \\ i \neq j}}^{n_b} (A + \sigma_i I) \right\} w \\ &\approx (A+\sigma_k I) \left\{ \prod_{\substack{i=1 \\ i \neq j,k}}^{n_b} (A + \sigma_i I) \right\} w \ , \quad 1 \leq j \leq n_b \ , \end{aligned}$$

$$
\begin{aligned}
\tilde{x}^{(k)} \approx (A+\sigma_k I)^{-1} b &\approx \left\{ \prod_{\substack{i=1 \\ i\neq k}}^{n_b} (A+\sigma_i I) \right\} w \\
&\approx (A+\sigma_j I) \left\{ \prod_{\substack{i=1 \\ i\neq j,k}}^{n_b} (A+\sigma_i I) \right\} w \ , \quad 1 \le k \le n_b \ , \\
\tilde{x}^{(l)} \approx (A+\sigma_l I)^{-1} b &\approx (A+\sigma_j I) \left\{ \prod_{\substack{i=1 \\ i\neq j,l}}^{n_b} (A+\sigma_i I) \right\} w \ , \quad 1 \le l \le n_b \ , \\
&\Downarrow \\
\frac{\tilde{x}^{(j)} - \tilde{x}^{(k)}}{\sigma_k - \sigma_j} &\approx \left\{ \prod_{\substack{i=1 \\ i\neq j,k}}^{n_b} (A+\sigma_i I) \right\} w \\
&\approx (A+\sigma_l I) \left\{ \prod_{\substack{i=1 \\ i\neq j,k,l}}^{n_b} (A+\sigma_i I) \right\} w \ , \quad 1 \le j,k \le n_b \ , \\
\frac{\tilde{x}^{(j)} - \tilde{x}^{(l)}}{\sigma_l - \sigma_j} &\approx \left\{ \prod_{\substack{i=1 \\ i\neq j,l}}^{n_b} (A+\sigma_i I) \right\} w \\
&\approx (A+\sigma_k I) \left\{ \prod_{\substack{i=1 \\ i\neq j,k,l}}^{n_b} (A+\sigma_i I) \right\} w \ , \quad 1 \le j,l \le n_b \ , \\
&\Downarrow \\
\frac{\tilde{x}^{(j)}}{(\sigma_k - \sigma_j)(\sigma_l - \sigma_j)} &+ \\
\frac{\tilde{x}^{(k)}}{(\sigma_j - \sigma_k)(\sigma_l - \sigma_k)} &+ \\
\frac{\tilde{x}^{(l)}}{(\sigma_j - \sigma_l)(\sigma_k - \sigma_l)} &\approx \left\{ \prod_{\substack{i=1 \\ i\neq j,k,l}}^{n_b} (A+\sigma_i I) \right\} w \ , \quad 1 \le j,k,l \le n_b \ .
\end{aligned}
$$

This process can be continued up to $\prod_i^{n_b}(A+\sigma_i I) \equiv 1$. Using (84), we get

$$w = \sum_{j=1}^{n_b} c_j \tilde{x}^{(j)} \quad \text{with} \quad c_j = \prod_{\substack{i=1 \\ i\neq j}}^{n_b} \frac{1}{\sigma_i - \sigma_j} \,. \tag{85}$$

Note that the coefficients c_j can be become very large if the shifts σ_j with smaller differences increase.

7.2 Multiple Shifts with Multiple Sources

Next, we are interested in solving the systems (41) with multiple sources. We need to find a set of initial values, $x_0^{(j)}, j = 1, \ldots, n_b$, that give a common residul r_0:

$$r_0 = r_0^{(j)} = b^{(j)} - (A+\sigma_j I)x_0^{(j)} \;, \quad j = 1, \ldots, n_b \,.$$

This can be solved by setting

$$x_0^{(j)} = \sum_{k=0}^{n_b-2} A^k z^{(j,k)} \,.$$

Then we get

$$\begin{aligned} r_0 &= b^{(j)} - (A+\sigma_j I)x_0^{(j)} \\ &= b^{(j)} - (A+\sigma_j I)\left\{\sum_{k=0}^{n_b-2} A^k z^{(j,k)}\right\} \\ &= b^{(j)} - \left\{\sum_{k=0}^{n_b-2} A^{k+1} z^{(j,k)} + \sigma_j \sum_{k=0}^{n_b-2} A^k z^{(j,k)}\right\} \;, \; j = 1, \ldots, n_b \,. \end{aligned}$$

Equating powers of A and solve for $z^{(j,k)}$ in terms of $b's$ gives the following equations for $i, j = 1, \ldots, n_b$:

$$\begin{aligned} z^{(j,n_b-2)} &= z^{(i,n_b-2)} \,, \\ z^{(j,k-1)} + \sigma_j z^{(j,k)} &= z^{(i,k-1)} + \sigma_i z^{(i,k)} \;, \quad k = n_b-2, \ldots, 1 \,, \\ b^{(j)} - \sigma_j z^{(j,0)} &= b^{(i)} - \sigma_i z^{(i,0)} \,. \end{aligned}$$

One can also solve this by considering the polynomials

$$q_j(A) = (A+\sigma_j I)p_j(A) \quad \text{with} \quad x_0^{(j)} = \sum_{k=0}^{n_b-2} A^k z^{(j,k)} \equiv p_j(A)$$

at the special cases $A = -\sigma_l I \,, 1 \leq l \leq n_b$:

$$r_0^{\sigma_l} = b^{(l)} - q_l(-\sigma_l I) = b^{(l)} - (-\sigma_l I + \sigma_l I)x_0^{(l)} = b^{(l)} \,.$$

This gives the n_b equations for fixed j

$$q_j(-\sigma_l I) = b^{(j)} - r_0^{\sigma_l} = b^{(j)} - b^{(l)}\,, 1 \le l \le n_b\,.$$

Since $q_j(A)$ is a polynomial of order $n_b - 1$ in A the system is uniquely determined. The polynomial

$$q_j(A) = \sum_{k=1}^{n_b} \left\{ \prod_{\substack{i=1 \\ i\neq k}}^{n_b} \frac{A+\sigma_i I}{\sigma_i - \sigma_k} \right\} (b^{(j)} - b^{(k)}) \tag{86}$$

satisfies these equations. Using $x_0^{(j)} = p_j(A) = (A+\sigma_j I)^{-1} q_j(A)$ we get

$$x_0^{(j)} = \sum_{\substack{k=1 \\ k\neq j}}^{n_b} \left\{ \prod_{\substack{i=1 \\ i\neq j,k}}^{n_b} \frac{A+\sigma_i I}{\sigma_i - \sigma_k} \right\} \left(\frac{b^{(j)} - b^{(k)}}{\sigma_j - \sigma_k} \right)\,. \tag{87}$$

8 Numerical Results

A nonequidistant mesh of 57 664 elementary cells including graded PML regions is used for the discretization of (4), that means the order of the system of linear algebraic equations is 172 992 (see (19)). The number of internal points $y_I^{(G)}$ (see Table 1 and Eq. (20)) is 152 608. We use three different matrices D (see (23)):

(I) $D = diag(A)$, (II) $D = \frac{1}{10} \cdot diag(A)$, (III) $D = 10 \cdot diag(A)$.

We analyze the following systems of linear equations:

	Linear system		I	II	III
0	$Ax^{(j)} = b^{(j)}$	$(\alpha_j = 1, \beta_j = 0)$	I_0		
1	$(\alpha_j A + \beta_j D)x^{(j)} = b^{(j)}$	(see Sec. 5.2)	I_1	II_1	III_1
2	$(\alpha_j A + \beta_j D)x^{(j)} = b^{(j)}$	(see Sec. 5.2)	I_2	II_2	III_2
3	$(\alpha_j A + \beta_j D)x^{(j)} = b^{(j)}$	(see Sec. 7.2)	I_3	II_3	III_3

The systems of linear equations in row 2 (I_2, II_2, III_2) are computed separately. The systems of linear equations in row 3 (I_3, II_3, III_3) are computed with new initial guesses (see (87)) and a common new right-hand side (see Sec. 7.2). This method does not work very good for more and/or smaller shifts. The initial residuals may be large. Thus, we use a fixed number of right-hand sides, nbm, to get new initial guesses and a new right-hand side:

$$I_3: \ nbm = 6, \quad II_3: \ nbm = 3, \quad III_3: \ nbm = 10.$$

The right-hand sides $b^{(j)}, j = 1, \ldots, n_b$, are generated by an uniformly distributed random number generator. The stopping criterion was a reduction of the norm of the residual for the preconditioned system (41–43) by 10^{-8}.

Based on the family of approximation problems (79), we have computed indefinite polynomial preconditioners. For this purpose, the Remez algorithm in [19, Sec. 6.1] was used. Using the

Nelder-Mead method (see [19, Sec. 6.2]), optimal indefinite polynomial preconditioners were computed by solving the constrained optimization problem numerically. The experiments were conducted on a workstation with Intel Xeon CPU W3520 (2,67 GHz, 8 cores) running 64-bit Linux system.

We compare the iteration counts required to solve the $n_b \in \{1, 3, 5, 10\}$ linear systems (see (29) and (41)) using the symmetric band Lanczos method without polynomial preconditioning with the number of iterations required to solve with polynomial preconditioning. The choice of the parameters $(\gamma, \delta) \in \Gamma$ and the computation of the 'optimal' parameters (γ_0, δ_0) is described in [19].
In Table 2 are denoted the estimated boundaries for the sets S, the parameters $(\gamma, \delta) \in \Gamma$ for the examples considered here, and also the computed 'optimal' parameters $(\gamma_0, \delta_0) \in \Gamma$. The degree of the Lagrange polynomial $L_j(z)$ is $l = 8$ and $l = 9$, respectively [19, Eq. (51)].

Table 2: The boundaries for S

I	a	b	c	d
	$2.24 \cdot 10^{-6}$	2.00	-0.45	$-5.20 \cdot 10^{-7}$
	$\gamma \approx -0.2241\ , \quad \delta \approx 4.4610$			
	$l = 9\ : \quad \gamma_0 \approx -0.7339\ , \quad \delta_0 \approx 4.3407$			

II	a	b	c	d
	$1.27 \cdot 10^{-4}$	20.00	-3.66	$-5.19 \cdot 10^{-6}$
	$\gamma \approx -0.1825\ , \quad \delta \approx 5.4782$			
	$l = 8\ : \quad \gamma_0 \approx -0.5635\ , \quad \delta_0 \approx 5.5894$			

III	a	b	c	d
	$9.48 \cdot 10^{-7}$	0.20	$-6.48 \cdot 10^{-2}$	$-5.19 \cdot 10^{-8}$
	$\gamma \approx -0.3240\ , \quad \delta \approx 3.0864$			
	$l = 9\ : \quad \gamma_0 \approx -0.5066\ , \quad \delta_0 \approx 3.2273$			

We choose for the preconditioner $\mathcal{P}_m(A)$ (see (77)) the linear case. This choice decreases the numerical effort and is more stable. The Tables 3 – 6 shows the numbers of iterations for shifted and unshifted linear system, respectively. A convergence history of the three examples (see Tables 4–6) can be found graphically in the Figs. 4–6.

Table 3: Number of iterations for unshifted matrices, I_0

I_0	Number of unshifted linear systems, n_b	1	3	5	10
	No preconditioning	1 128	2 712	4 355	8 844
	Preconditioning: (γ_0, δ_0)	569	1 219	1 965	4 385

Table 4: Number of iterations for shifted matrices, I_1–III_1

I_1	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	119	10 722	18 064	36 212
	Preconditioning: (γ_0, δ_0)	58	5 374	9 225	18 784

II_1	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	369	13 329	14 209	76 780
	Preconditioning: (γ_0, δ_0)	195	4 726	5 657	34 868

III_1	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	41	3 642	6 103	12 581
	Preconditioning: (γ_0, δ_0)	20	1 716	2 953	6 084

9 Conclusions

We have analyzed the solution of linear systems of equations with multiple right-hand sides each with a different shift. We have presented a variant of the symmetric band Lanczos process with multiple starting vectors. The symmetric band Lanczos process is based on coupled recurrences. Polynomial preconditioners for indefinite linear systems leads to indefinite preconditioned coefficient matrices. Such polynomials can be obtained via the solution of linear Chebyshev approximation problems.

We have presented a method that produce initial guesses with a common right-hand side. It could be very useful. The main difficulty then is keeping the initial residual under control.

Another problem is to find suitable informations on the location of the eigenvalues of A, i.e., the bounds of the two intervals $[a, b]$ and $[c, d]$.

Table 5: Number of iterations for shifted matrices, I_2–III_2

I_2	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	119	4 883	5 683	13 975
	Preconditioning: (γ_0, δ_0)	58	2 433	2 823	6 975

II_2	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	369	6 549	8 826	33 506
	Preconditioning: (γ_0, δ_0)	195	3 364	4 569	18 246

III_2	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	41	2 480	2 746	3 921
	Preconditioning: (γ_0, δ_0)	20	1 221	1 343	2 081

Table 6: Number of iterations for shifted matrices, I_3–III_3

I_3	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	115	3 381	2 970	5 360
	Preconditioning: (γ_0, δ_0)	56	1 647	1 575	2 720

II_3	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	364	4 803	6 551	22 341
	Preconditioning: (γ_0, δ_0)	178	2 425	3 318	11 036

III_3	Number of shifted linear systems, n_b	1	3	5	10
	No preconditioning	37	1 100	1 135	1 175
	Preconditioning: (γ_0, δ_0)	20	581	594	637

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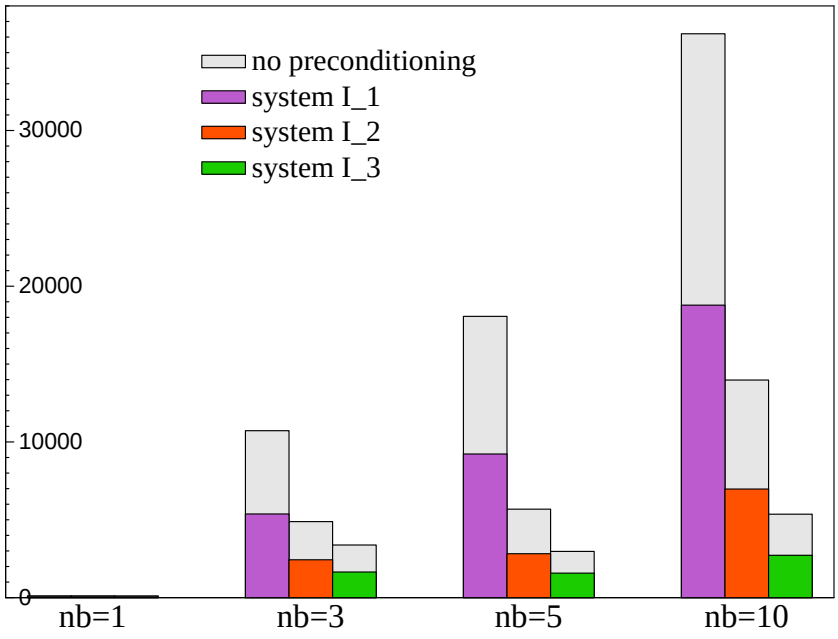

Figure 4: Number of iterations for (I)

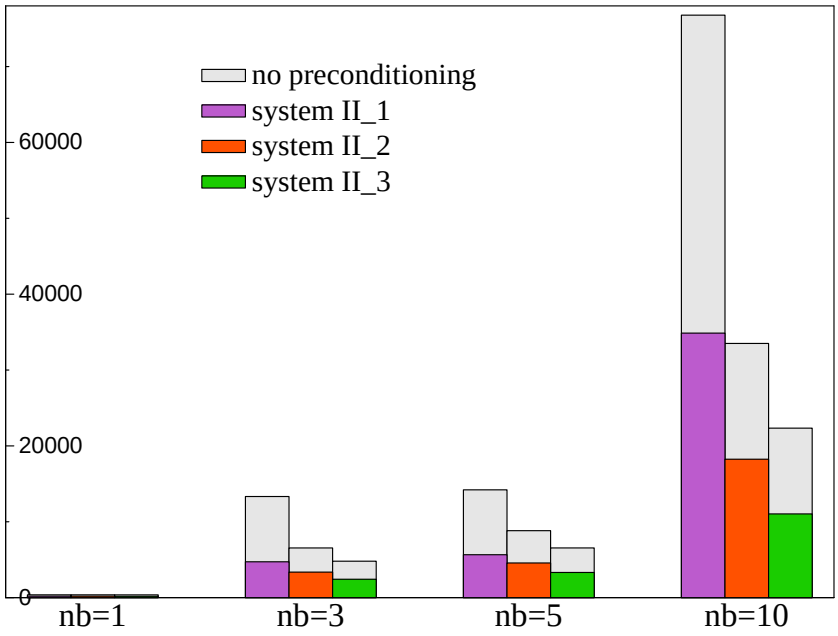

Figure 5: Number of iterations for (II)

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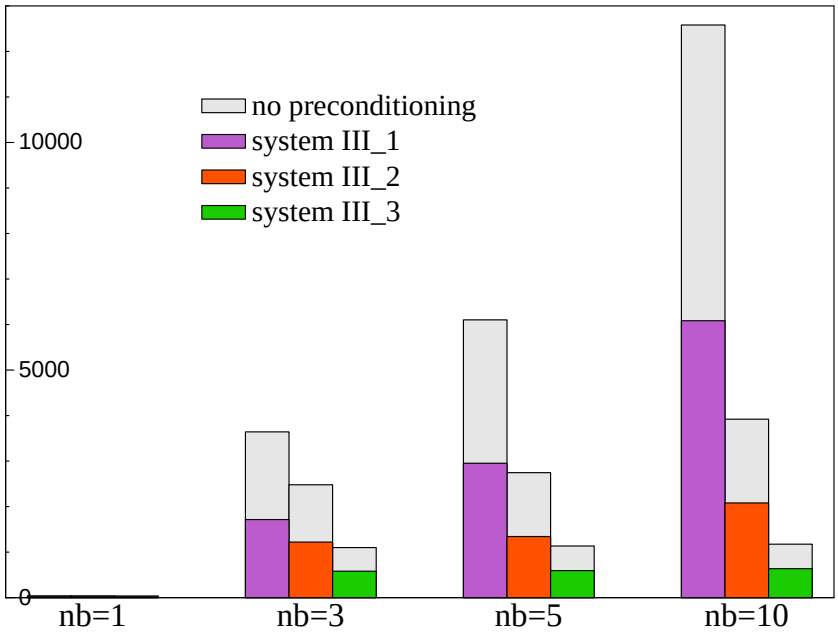

Figure 6: Number of iterations for (III)

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