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Iterative Solution of Systems of Linear Equations in Microwave Circuits Using a Block Quasi-Minimal Residual Algorithm

Rainer Schlundt[1], Georg Hebermehl[1], Friedrich-Karl Hübner[1],

Wolfgang Heinrich[2], Horst Zscheile[2]

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[1] Weierstrass-Institute
for Applied Analysis
and Stochastics
Mohrenstraße 39
D - 10117 Berlin
Germany
E-Mail: schlundt@wias-berlin.de
E-Mail: hebermehl@wias-berlin.de
E-Mail: huebner@wias-berlin.de
URL: http://www.wias-berlin.de

[2] Ferdinand-Braun-Institut
für Höchstfrequenztechnik
Albert-Einstein-Straße 11
D - 12489 Berlin
Germany
E-Mail: w.heinrich@ieee.org
E-Mail: zscheile@fbh-berlin.de
URL: http://www.fbh-berlin.de

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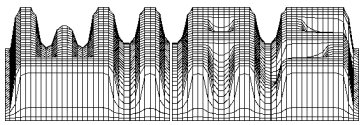

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Edited by
Weierstraß–Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail (X.400): c=de;a=d400-gw;p=WIAS-BERLIN;s=preprint
E-Mail (Internet): preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

The electrical properties of monolithic microwave integrated circuits that are connected to transmission lines are described in terms of their scattering matrix using Maxwell's equations. Using a finite-volume method the corresponding three-dimensional boundary value problem of Maxwell's equations in the frequency domain can be solved by means of a two-step procedure. An eigenvalue problem for non-symmetric matrices yields the wave modes. The eigenfunctions determine the boundary values at the ports of the transmission lines for the calculation of the fields in the three-dimensional structure. The electromagnetic fields and the scattering matrix elements are achieved by the solution of large-scale systems of linear equations with indefinite complex symmetric coefficient matrices. In many situations, these matrix problems need to be solved repeatedly for different right-hand sides, but with the same coefficient matrix. The block quasi-minimal residual algorithm is a block Krylov subspace iterative method that incorporates deflation to delete linearly and almost linearly dependent vectors in the underlying block Krylov sequences.

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1 Introduction

The design of monolithic microwave integrated circuits requires efficient CAD tools in order to avoid costly and time-consuming redesign cycles. The electromagnetic characteristics of microwave integrated circuits can be described by equivalent circuits in terms of voltages and currents. With growing frequencies the voltage and current definitions become ambiguous. Therefore, the description of the electromagnetic characteristics of microwave circuits by the scattering matrix is more appropiate. As an example, Fig. 1 illustrates the principle structure under investigation. In order to determine the scattering matrix, the circuit is inserted between trans-

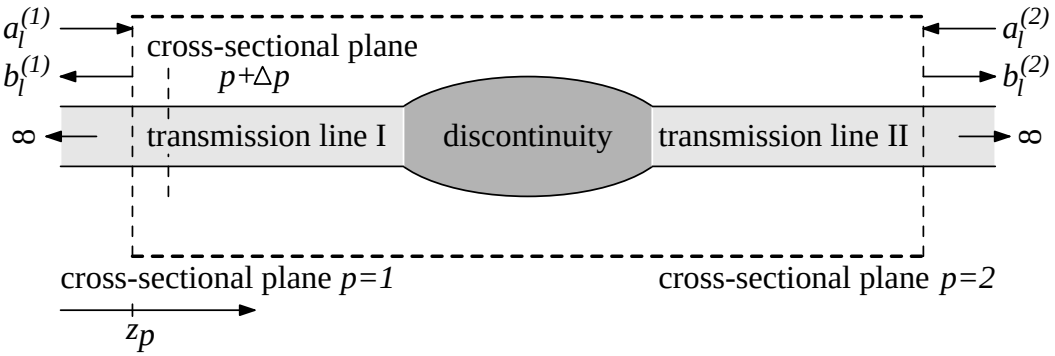

Figure 1: Structure under investigation.

mission lines. The scattering matrix describes the structure in terms of wave modes on these lines, which can be computed from the electromagnetic field. A three-dimensional boundary value problem can be formulated using Maxwell's equations in frequency domain in order to compute the electromagnetic field. Using the fimite-volume method to the three-dimensional boundary value problem for the Maxwell's

equations results in the so-called Finite-Difference method in the Frequency Domain (FDFD) (see [1], [2], and [3]). The field volume is subdivided into rectangular cells. The Maxwell's equations in integral formulation are approximated by the method of finite integration for each cell.

2 Scattering Matrix

The structure under investigation (see Fig. 1) consists of infinitly long transmission lines and a discontinuity. The transmission lines are assumed to be longitudinally homogeneous. The discontinuity may have an arbitrary structure. The scattering matrix S describes the energy exchange and phase relation between all outgoing modes $b_l^{(p)}$ and all incoming modes $a_l^{(p)}$ on all ports p on the transmission lines (see [6]):

$$b_{\rho,\nu} = \sum_{\sigma=1}^{m_s} S_{\rho,\sigma} a_{\sigma,\nu}, \quad S = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1m_s} \\ S_{21} & S_{22} & \cdots & S_{2m_s} \\ \cdots & \cdots & \cdots & \cdots \\ S_{m_s1} & S_{m_s2} & \cdots & S_{m_sm_s} \end{pmatrix} = (S_{\rho,\sigma}), \tag{1}$$

$$\nu, \rho, \sigma = 1, \ldots, m_s, \; m_s = \sum_{p=1}^{\bar{p}} m^{(p)}, \; \rho = l + \sum_{q=1}^{p-1} m^{(q)}, \; l = 1, \ldots, m^{(p)}. \tag{2}$$

$\bar{p}$ is the number of ports. $m^{(p)}$ is the number of modes on the port p. The scattering matrix can be extracted from the orthogonal decomposition of the electric field at a pair of two neighboring cross-sectional planes p and $p + \Delta p$ (see Fig. 1) on each waveguide.

3 Boundary Value Problem

We use the integral form of the Maxwell's equations in the frequency domain:

$$\begin{array}{rclcrcl} \oint_{\partial\Omega} \vec{E} \cdot d\vec{s} & = & -j\omega \int_\Omega \vec{B} \cdot d\vec{\Omega}, & & \oint_\Omega \vec{B} \cdot d\vec{\Omega} & = & 0 \\ \oint_{\partial\Omega} \frac{1}{[\mu]} \vec{B} \cdot d\vec{s} & = & j\omega \int_\Omega [\epsilon] \vec{E} \cdot d\vec{\Omega}, & & \oint_\Omega [\epsilon] \vec{E} \cdot d\vec{\Omega} & = & 0 \end{array} \tag{3}$$

taking into account the constitutive relations

$$\vec{B} = [\mu]\vec{H}, \; \vec{D} = [\epsilon]\vec{E}, \; [\epsilon] = diag(\epsilon_x, \epsilon_y, \epsilon_z), \; [\mu] = diag(\mu_x, \mu_y, \mu_z). \tag{4}$$

The electric and magnetic field intensities $\vec{E}$ and $\vec{H}$ and the electric and magnetic flux densities $\vec{D}$ and $\vec{B}$ are complex functions of the spatial coordinates. The quantities $[\epsilon]$ and $[\mu]$ are diagonal tensors of dielectric permittivity and magnetic permeability, respectively. $\partial\Omega$ is the boundary of the open surface Ω.

At the port p the transverse electric field $\vec{E}_t(z_p)$ is given by superposing all transmission line modes $\vec{E}_{t,l}(z_p)$ with weighted mode-amplitude sums $w_l(z_p)$:

$$\vec{E}_t(z_p) = \sum_{l=1}^{m(p)} w_l(z_p)\vec{E}_{t,l}(z_p). \tag{5}$$

The transverse electric mode fields $\vec{E}_{t,l}(z_p)$ are computed using an eigenvalue problem for transmission lines (see [7] and [8]). The boundary conditions at all other parts of the enclosure are $\vec{E}_{tang} = 0$ and $\vec{H}_{tang} = 0$, respectively.

4 Maxwell's Grid Equations

The integrals in (3) are applied to rectangular blocks using the following relations:

$$\oint_{\partial\Omega} \vec{f} \cdot d\vec{s} \to \sum_i (\pm f_i s_i) \quad \text{and} \quad \int_{\Omega} \vec{f} \cdot d\Omega \to f_i \Omega_i, \tag{6}$$

where f_i is a center value associated with the ith cell. We use staggered grids (see [11]). Note that the discrete electric field is located at the center of an edge and the discrete magnetic flux density is normal to the center of the face. The electric field components form a primary grid and the magnetic flux density a dual grid. The discretized form of (3) results in an equation for each field component. Presenting each equation using matrices provides a compact form:

$$\begin{aligned} CD_s\vec{e} &= -j\omega D_A\vec{b}, & SD_A\vec{b} &= 0, \\ \tilde{C}D_{\tilde{s}/\tilde{\mu}}\vec{b} &= j\omega\epsilon_0\mu_0 D_{\tilde{A}\tilde{\epsilon}}\vec{e}, & \tilde{S}D_{\tilde{A}\tilde{\epsilon}}\vec{e} &= 0. \end{aligned} \tag{7}$$

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 [10]):

$$SC = 0, \quad \tilde{S}\tilde{C} = 0, \quad C = \tilde{C}^T. \tag{8}$$

5 System of Linear Algebraic Equations

Using (8), eliminating the components of the magnetic flux density $(\vec{b})$ in (7), and multiplying by $D_s^{1/2}$ yields a symmetric form of linear algebraic equations:

$$\bar{A}_E(D_s^{1/2}\vec{e}) = 0, \quad \bar{A}_E = D_s^{1/2}C^T D_{\tilde{s}/\tilde{\mu}} D_A^{-1} C D_s^{1/2} - k_0^2 D_{\tilde{A}\tilde{\epsilon}}, \tag{9}$$

where $k_0 = \omega\sqrt{\epsilon_0\mu_0}$. The gradient of the electric-field divergence

$$[\epsilon]\nabla([\epsilon]^{-2}\nabla \cdot [\epsilon]\vec{E}) = 0 \tag{10}$$

is equivalent to the matrix equation (symmetric form by multiplying by $D_s^{1/2}$)

$$\bar{B}_D(D_s^{1/2}\vec{e}) = 0, \quad \bar{B}_D = D_s^{-1/2} D_{\tilde{A}\tilde{\epsilon}} \tilde{S}^T D_{\tilde{V}\tilde{\epsilon}\tilde{\epsilon}}^{-1} \tilde{S} D_{\tilde{A}\tilde{\epsilon}} D_s^{-1/2} . \tag{11}$$

The diagonal matrix $D_{\tilde{V}\tilde{\epsilon}\tilde{\epsilon}}$ is a volume matrix for the 8 partial volumes of the dual elementary cell.
Taking into account the boundary conditions the two equations (9) and (11) are transformed in

$$\bar{A}_E x = 0 \quad \longrightarrow \quad A_E x = b, \tag{12}$$

$$\bar{B}_D x = 0 \quad \longrightarrow \quad B_D x = 0, \tag{13}$$

where $x = D_s^{1/2}\vec{e}$.
The effect of the addition of the two equations (12) and (13) can be interpreted as preconditioning with the preconditioner $(I + B_D A_E^{-1})^{-1}$ for the system (12):

$$(I + B_D A_E^{-1}) A_E x = (I + B_D A_E^{-1}) b \quad \rightarrow \quad Ax = (A_E + B_D)x = b, \tag{14}$$

where A is symmetric, indefinite, and complex. Fig. 2 shows the typical structure of the system matrix A. Due to the structure of the matrices C, $\tilde{C}$, $\tilde{S}$, and $\tilde{S}^T$

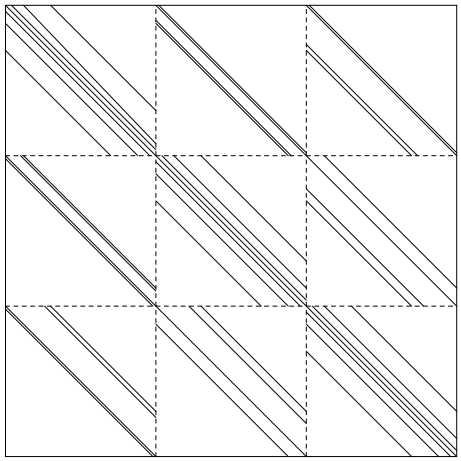

Figure 2: Structure of the system matrix A.

the diagonal entries of A are nonzero and sufficiently large compared with the off-diagonal entries.

5.1 Independent Set Ordering

A commonly used approach for solving large sparse linear systems (14) is to find sets of unknowns which are independent (see [9]). A set of such unknowns is called an independent set. Independent set orderings are permutations P_i to transform the matrix A_i with $A_0 = A$ (14) in the form

$$A_i \quad \longrightarrow \quad P_i A_i P_i^T = \begin{pmatrix} D_i & E_i^T \\ E_i & H_i \end{pmatrix}, \tag{15}$$

where D_i is a diagonal, E_i, and H_i are sparse matrices. The unknows of the independent set D_i are eliminated to get the next reduced matrix

$$A_{i+1} = H_i - E_i D_i^{-1} E_i^T. \tag{16}$$

We get a system of linear equations

$$P_i A_i P_i^T P_i x_i = P_i b_i \tag{17}$$

with $y_i = P_i x_i = (y_{i,1}, y_{i,2})^T$ and $c_i = P_i b_i = (c_{i,1}, c_{i,2})^T$ and have to solve the reduced system of linear equations

$$A_{i+1} x_{i+1} = b_{i+1}, \quad x_{i+1} = y_{i,2}, \quad b_{i+1} = c_{i,2} - E_i D_i^{-1} c_{i,1} \tag{18}$$

for $y_{i,2}$, and then we get

$$y_{i,1} = D_i^{-1}(c_{i,1} - E_i^T y_{i,2}). \tag{19}$$

Then we have to permute the solution vector y_i back to the vector x_i.

5.2 Preconditioning

Let D_A the diagonal matrix of A, where $A \equiv A_{i+1}$. Using $x \equiv x_{i+1}$ and $b \equiv b_{i+1}$ then we set $M_1 = M_2 = D_A^{1/2}$ and apply the Jacobi preconditioning

$$Ax = b \quad \longrightarrow \quad \hat{A}\hat{x} = D_A^{-1/2} A D_A^{-1/2} D_A^{1/2} x = D_A^{-1/2} b = \hat{b}\,. \tag{20}$$

The SSOR preconditioner matrices for the matrix $\hat{A}$ parametrized by ω are defined as

$$\hat{A} = L + I + L^T \quad \longrightarrow \quad \hat{M}_1 = (I + \omega L),\ \hat{M}_2 = \hat{M}_1^T,\ 0 < \omega < 2, \tag{21}$$

where L is the strictly lower triangular part of $\hat{A}$. The optimal value of the ω parameter reduces the number of iterations to a lower order (Table 3). The matrix vector products $r = (\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1})v$ can be computed very efficiently by using Eisenstat's trick (see [4]) for any vector v:

$$\begin{aligned} r &= (\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1})v \\ &= \tfrac{1}{\omega}[(I + \omega L^T)^{-1}v + (I + \omega L)^{-1}(v - (2-\omega)(I + \omega L^T)^{-1}v)]. \end{aligned} \tag{22}$$

The result $r = (\hat{M}_1^{-1}\hat{A}\hat{M}_2^{-1})v$ can be obtained as follows:

1. Solve $(I + \omega L^T)t = v$ for t.
2. Set $\tilde{t} = v - (2-\omega)t$.
3. Solve $(I + \omega L)\hat{t} = \tilde{t}$ for $\hat{t}$.
4. Set $r = \frac{1}{\omega}(t + \hat{t})$.

5.3 Block Quasi-Minimal Residual Algorithm

We first describe the general block Krylov subspace method. Then, we describe a J-symmetric variant of the block Krylov method, which includes the complex symmetric form as a special case.
The system of linear equations (14) is solved repeatedly with the same coefficient matrix A, but m_s different right-hand sides, i.e., we have linear systems

$$Ax^{(j)} = b^{(j)},\ j = 1, 2, \ldots, m = m_s \quad \longrightarrow \quad AX = B, \tag{23}$$

where $A \in \mathbb{C}^{n\times n}$, $B \in \mathbb{C}^{n\times m}$, and $X \in \mathbb{C}^{n\times m}$. An iterative scheme for solving (23) is said to be a block Krylov subspace method if it generates block iterates $X_l \in \mathbb{C}^{n\times m}, l = 1, 2, \ldots$, with $x_l^{(j)} \in x_0^{(j)} + \mathcal{K}_l^{\mathrm{dl}}(A, R),\ j = 1, 2, \ldots, m$. The block Krylov subspace $\mathcal{K}_l^{\mathrm{dl}}(A, R)$ is spanned by the first l linearly independent vectors in the block Krylov sequence

$$R, AR, A^2R, \ldots, A^{k-1}R, \ldots,\ R = B - AX_0\ . \tag{24}$$

All linearly dependent or almost linearly dependent vectors on previous vectors are deleted by scanning the block Krylov sequence from left to right. We obtain the deflated block Krylov sequence

$$R^{(1)}, AR^{(2)}, A^2R^{(3)}, \ldots, A^{k-1}R^{(k)}, \ldots,\ R^{(0)} = R, \tag{25}$$

where $R^{(k)}$ is a submatrix of $R^{(k-1)}$. The Lanczos-type algorithm described in [5] generates a sequence of basis vectors $v_1, v_2, \ldots$ for the block Krylov subspaces $\mathcal{K}_j^{\mathrm{dl}}(A, R)$ and a sequence of basis vectors $w_1, w_2, \ldots$ for the block Krylov subspaces $\mathcal{K}_j^{\mathrm{dl}}(A^T, L)$ with $L \in \mathbb{C}^{n\times m}$. The vectors in the v and w sequences are constructed to be biorthogonal, i.e., $w_i^T v_k = \delta_{ik}$. Thus, all block iterates X_l can be represented in the form

$$X_l = X_0 + V^{(l)}Z, \quad V^{(l)} = [v_1, v_2, \ldots, v_l], \quad Z \in \mathbb{C}^{l\times m}. \tag{26}$$

The recursions for constructing the first ν basis vectors $v_1, v_2, \ldots, v_\nu$ can be summarized in matrix formulation as follows:

$$AV^{(l)} = V^{(\nu)}T^{(l)} + V_{\mathrm{dl}}^{(l)}\ , \quad l = \nu - m_{\mathrm{cr}} > 0, \tag{27}$$

where m_{cr} denotes the reduced size of the current block in the block Krylov sequence. The matrix $T^{(l)} \in \mathbb{C}^{\nu\times l}$ contains coefficients of the recursions in the Lanczos-type algorithm and the matrix $V_{\mathrm{dl}}^{(l)} \in \mathbb{C}^{n\times l}$ consists of mostly zero column vectors and at most $m - m_{\mathrm{cr}}$ nonzero column vectors corresponding to the deflated v vectors. The recurrences for the initial block of Lanczos vectors $v_1, v_2, \ldots, v_{m_1}$ can be stated as

$$V^{(m_1)}T^{(0)} + V_{\mathrm{dl}}^{(0)} = R_0, \tag{28}$$

where $T^{(0)} \in \mathbb{C}^{m_1\times m}$ and $V_{\mathrm{dl}}^{(0)} \in \mathbb{C}^{n\times m}$. After each deflation in the v sequence, the size of the current block $R^{(k)}$ in the corresponding deflated block Krylov sequence

(25) decreases by one. Let $X_l^{\rm cr} \in \mathbb{C}^{n \times m_{\rm cr}}$ denote the current block iterate after each deflation, then we can rewrite (26) for $X_l^{\rm cr}$ as

$$X_l^{\rm cr} = X_0^{\rm cr} + V^{(l)} Z^{\rm cr},\ Z^{\rm cr} \in \mathbb{C}^{l \times m_{\rm cr}},\ m_{\rm cr} < m,\ \text{and}\ AX^{\rm cr} = B^{\rm cr} \tag{29}$$

is the subset of linear systems in (23) that correspond to the current active block iterate $X_l^{\rm cr}$. Using (27), (28), and (29), the residual block $R_l^{\rm cr}$ corresponding to $X_l^{\rm cr}$ satisfies:

$$\begin{aligned} R_l^{\rm cr} &= B^{\rm cr} - AX_l^{\rm cr} \\ &= B^{\rm cr} - A(X_0^{\rm cr} + V^{(l)} Z^{\rm cr}) \\ &= R_0^{\rm cr} - AV^{(l)} Z^{\rm cr} \\ &= R_0^{\rm cr} - V^{(\nu)} T^{(l)} Z^{\rm cr} - V_{\rm dl}^{(l)} Z^{\rm cr} \\ &= V^{(m_1)} T^{(0)} + V_{\rm dl}^{(0)} - V^{(\nu)} T^{(l)} Z^{\rm cr} - V_{\rm dl}^{(l)} Z^{\rm cr} \\ &= V^{(\nu)} \left[\begin{pmatrix} T^{(0)} \\ 0 \end{pmatrix} - T^{(l)} Z^{\rm cr} \right] - V_{\rm dl}^{(l)} Z^{\rm cr}. \end{aligned} \tag{30}$$

We would like to choose the free parameter matrix $Z^{\rm cr}$ in (30) such that $\|R_l^{\rm cr}\|$ is minimal. In general, $V^{(\nu)}$ is not unitary and $V_{\rm dl}^{(l)}$ has some nonzero columns. Thus, we will minimize the Euclidean norm of the bracketed term in (30). Therefore, the block iterates X_l are characterized by a quasi-minimization of the residuals. For further implementation details of the block-QMR method see [5].

5.3.1 Symmetric Systems

The classical Lanczos process can be simplified when A is a J-symmetric matrix by choosing appropriate left starting vectors, i.e.,

$$A^T J = JA,\ L = JR \ \longrightarrow\ w_l = \eta_l J v_l,\ \eta_l \in \mathbb{C}, \eta_l \neq 0,\ l = 1, 2, \ldots\ . \tag{31}$$

We consider the solution of the complex symmetric block system (23), where A itself is complex symmetric, i.e., $A = A^T$. We want to use the matrix $M \in \mathbb{C}^{n \times n}$ with

$$M = M_1 M_2 = M_2^T M_1^T = M^T \tag{32}$$

as a preconditioner for the system (23). The two-sided preconditioned block system

$$\hat{A}\hat{X} = \hat{B},\quad \hat{A} = M_1^{-1} A M_2^{-1},\quad \hat{X} = M_2 X,\quad \hat{B} = M_1^{-1} B \tag{33}$$

is J-symmetric using $J = M_1^T M_2^{-1}$.

6 Numerical Results

The reduction of the iteration number is demonstrated calculating the systems of linear algebraic equations of a structure under investigation (two coupled rectangular waveguides with different diameters).

The order of the system of linear algebraic equations is 86 016. The number of stored nonzeros amounts to 593 141. We apply an independent set ordering to obtain the reduced matrix. In general, for a linear system arising in the design of monolithic microwave integrated circuits one reduction is more efficient than no, two, or more reductions. In addition the preprocessing cost for independent set ordering with one level of reduction is modest. The order of the reduced system of linear equations is 62 542, the number of stored nonzeros amounts to 1 017 395. The stopping criterion was a reduction of the norm of the residual for the preconditioned system by 10^{-8}, i.e., $\|r_l^{(j)}\| \leq 10^{-8} \cdot \|r_0^{(j)}\|$ for $j = 1, 2, \ldots, m_{\mathrm{cr}}$. In Table 1, we compare cumulative iteration counts required to individually solve each of the m linear systems using QMR with the number of block-QMR iterations required to solve all the m systems simultaneously. Table 2 shows the corresponding cumulative

Table 1: Comparison of block-QMR with individual solution of each right-hand side using QMR with $\omega = 1.66$.

Number of RHS (m)	1	2	3	4	5
Cumulative QMR iterations	176	351	525	699	874
Block-QMR iterations	176	261	318	381	441
Block-QMR iter./RHS	176	131	106	96	89
Number of RHS (m)	6	7	8	9	10
Cumulative QMR iterations	1052	1232	1412	1595	1776
Block-QMR iterations	511	610	671	693	709
Block-QMR iter./RHS	86	88	84	77	71

execution times using QMR and the execution times of block-QMR. Furthermore,

Table 2: Comparison of execution times of block-QMR with individual solution of each right-hand side using QMR with $\omega = 1.66$.

Number of RHS (m)	1	2	3	4	5
Cumulative QMR iter. time (s)	98	196	293	389	487
Block-QMR iter. time (s)	109	172	219	278	331
Block-QMR iter. time/RHS (s)	109	86	73	70	66
Number of RHS (m)	6	7	8	9	10
Cumulative QMR iter. time (s)	587	687	787	889	990
Block-QMR iter. time (s)	396	491	557	608	630
Block-QMR iter. time/RHS (s)	66	70	70	68	63

Table 3 shows the number of block-QMR iterations for different values of ω for one right-hand side. The choice of ω affects the performance of preconditioner for the class of problems considered here.

Table 3: Number of block-QMR iterations for different values of ω.

ω	0.1	0.3	0.5	0.7	0.9	1.0	1.1	1.3
Iterations	733	600	485	391	313	279	249	201
ω	1.4	1.5	1.57	1.6	1.66	1.7	1.8	1.9
Iterations	186	182	178	179	176	177	193	250

Concluding Remarks. We have considered the iterative solution of systems of linear equations with multiple right-hand sides. We used a J-symmetric variant of the block-QMR method. The block-QMR method constructs basis vectors for block Krylov subspaces. The block iterates are characterized by a quasi-minimal residual property. The choice of ω affects the performance of the SSOR preconditioner. Furthermore, Eisenstat's trick reduces the time for the iteration algorithm.

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