A MINIMUM RESIDUAL INTERPOLATION METHOD FOR LINEAR EQUATIONS WITH MULTIPLE RIGHT HAND SIDES

PER LÖTSTEDT[1], MARTIN NILSSON[2] *

[1] *Department of Information Technology, Scientific Computing Uppsala University, SE-75105 Uppsala, Sweden. email: perl@tdb.uu.se*

[2] *Department of Information Technology, Scientific Computing Uppsala University, SE-75105 Uppsala, Sweden. email: martin@tdb.uu.se*

Abstract

An efficient method for solution of systems of linear equations with many right hand sides is developed. The right hand sides are assumed to depend smoothly on a parameter. The equations are solved by an iterative method and a linear least squares approximation is used as initial guess. The work spent on the iterations is bounded independently of the number of right hand sides. The method is applied to the solution of Maxwell's equations of electromagnetics in the frequency domain. The efficiency of the method is illustrated by computing the monostatic radar cross section around an aircraft model.

Keywords: system of linear equations, multiple right hand sides, iterative method, method of moments, frequency domain, Maxwell's equations

AMS subject classification (MSC2000): 65F10, 65R20, 78M05

1 Introduction

In several applications, a system of linear equations is solved for many right hand sides. Assume that the system is dense, the number of unknowns is N and the number of right hand sides is M. If the equations are solved with Gaussian elimination the solution time scales as $\mathcal{O}(N^3)$ for the factorization and $\mathcal{O}(MN^2)$ for the backsubstitution. Iterative methods based on matrix-vector multiplications

*Financial support has been obtained from Parallel and Scientific Computing Institute (PSCI), which is a competence center financed by Vinnova, The Swedish Agency for Innovation Systems, and the Swedish National Aeronautical Research Program, NFFP.

such as Krylov subspace methods [8] are appealing because their solution time scales as $\mathcal{O}(KMN^2)$, where K is the average number of iterations. If K and M are small compared to N, an iterative method is faster than Gaussian elimination. The Fast Multpole Method (FMM) [5], [9], and similar methods [4] were introduced in order to speed up the matrix-vector multiplication in an iterative method when the source of the equations is a discretization of an integral equation. An iterative method combined with such a method can reduce the solution time to $\mathcal{O}(KMN \log N)$ or in special cases to $\mathcal{O}(KMN)$. Since the constant in front of the scaling for the FMM is fairly large, Gaussian elimination is quite competitive for problems that can fit into the computer memory. The same argument is valid in favor of Gaussian elimination compared to an iterative method also for linear equations with a banded system matrix.

The presently used iterative approaches to solving problems with multiple right hand sides are either to use a block method [7], [15], or a seed method [16]. The block method utilizes the information from a block of right hand sides in a Krylov method to solve for the entire block at once. In the seed method, one right hand side is used as a seed and then the solutions of the other right hand sides are computed based on information from the seed system. Once the seed system is solved a new right hand side defines the seed system. Faster convergence is achieved with such methods and fewer expensive matrix-vector products are computed. A disadvantage with these methods is that for maximum reduction of the work per right hand side, many right hand sides must reside in memory. Gaussian elimination on the other hand only requires the right hand side currently solved for in addition to the factorization to be stored in memory. Our way of reducing the computing time is to determine an accurate initial guess.

In the Minimum Residual Interpolation (MRI) method proposed in this paper, an iterative method is combined with an accurate initial guess of the solution to solve systems of linear equations with many right hand sides. The right hand sides are assumed to depend smoothly on a parameter. The advantage is that the method can be used together with block methods or single right hand side solvers and is independent of the underlying iterative method. Furthermore, it does not need all right hand sides to be stored in memory simultaneously. It only needs the right hand side currently solved for and some additional vectors. It is also able to predict the residual of the initial guess without computation of a matrix-vector multiplication. The work for the iterative part is bounded independently of M and for large M the operations count of the whole algorithm grows as $\mathcal{O}(MN)$. The method is optimal in a certain sense.

The method is applied to the solution of electromagnetic scattering problems in the frequency domain but other applications are possible e.g. panel methods for linearized potential flow problems and acoustic scattering. In the Method of Moments (MoM) in electromagnetics, the electromagnetic field satisfies an integral equation [12]. After discretization the result is a linear system of equations with a dense matrix. When the monostatic Radar Cross Section (RCS) is com-

puted for an object, each one of the incoming waves generates a right hand side. The right hand sides vary smoothly with angle of incidence of the waves.

The paper is organized as follows. The solution method for multiple right hand sides is described in the next section. Then the convergence is analyzed in the third section. The integral equation and its discretization are presented in the following section. Finally, the performance of the method is demonstrated in numerical experiments. The norm in the paper is the Euclidean vector norm and its subordinate spectral matrix norm. Vectors and matrices are typeset with a bold font.

2 Minimum Residual Interpolation

The method for solution of a system of linear equations with many right hand sides is discussed and an iterative algorithm is presented. By assuming that the right hand sides depend smoothly on a parameter an accurate initialization of the iterations can be computed.

The systems of linear equations to be solved are

$$\mathbf{A}\mathbf{x}_i = \mathbf{b}_i,\ i = 1 \dots M,\ \mathbf{A} \in \mathbb{C}^{N \times N},\ \mathbf{x}_i, \mathbf{b}_i \in \mathbb{C}^N. \tag{1}$$

The system matrix is constant and the residual is

$$\mathbf{r}_i = \mathbf{b}_i - \mathbf{A}\mathbf{x}_i.$$

The equations are solved with an iterative method such that $\mathbf{r}_i$ satisfies a convergence criterion $\|\mathbf{r}_i\| \leq \varepsilon$ for some given ε.

Assume that the solutions to $m < M$ right hand sides are known to some precision given by the residual and that the solutions are linearly independent. The initial guess $\mathbf{x}_{m+1}^{(0)}$ for an iterative method applied to the solution of

$$\mathbf{A}\mathbf{x}_{m+1} = \mathbf{b}_{m+1} \tag{2}$$

is generated based on the observation: if $\mathbf{b}_{m+1} \approx \sum_{i=1}^{m} y_i \mathbf{b}_i$ then setting $\mathbf{x}_{m+1} = \sum_{i=1}^{m} y_i \mathbf{x}_i$ implies that $\mathbf{A}\mathbf{x}_{m+1} \approx \sum_{i=1}^{m} y_i \mathbf{b}_i$ if we assume that $\|\mathbf{r}_i\| \ll \|\mathbf{b}_i\|$. A linear least squares problem determines y_i.

Let $\mathbf{s}_i$, $\mathbf{S}_m$, and $\mathbf{X}_m$ be defined by

$$\mathbf{A}\mathbf{x}_i = \mathbf{b}_i - \mathbf{r}_i \equiv \mathbf{s}_i,\ i = 1 \dots m,\ \mathbf{X}_m = \left[\mathbf{x}_1\, \mathbf{x}_2\, \dots\, \mathbf{x}_m\right],\ \mathbf{S}_m = \left[\mathbf{s}_1\, \mathbf{s}_2\, \dots\, \mathbf{s}_m\right]. \tag{3}$$

Using Gram-Schmidt or Householder transformations [2] one can compute the $\mathbf{QR}$-decomposition of $\mathbf{S}_m$

$$\mathbf{A}\mathbf{X}_m = \mathbf{S}_m = \mathbf{Q}_{\mathbf{S}_m}\mathbf{R}_{\mathbf{S}_m}. \tag{4}$$

A linear combination of $\mathbf{s}_i$ is chosen to minimize

$$\begin{aligned}\|\mathbf{r}_{m+1}\| &= \|\mathbf{b}_{m+1} - \mathbf{A}\mathbf{x}_{m+1}\| = \|\mathbf{b}_{m+1} - \mathbf{A}\mathbf{X}_m\mathbf{y}_m\| \\ &= \|\mathbf{b}_{m+1} - \mathbf{S}_m\mathbf{y}_m\| = \|\mathbf{b}_{m+1} - \mathbf{Q}_{\mathbf{S}_m}\mathbf{R}_{\mathbf{S}_m}\mathbf{y}_m\|.\end{aligned} \tag{5}$$

Thus, $\mathbf{y}_m = \mathbf{R}_{\mathbf{S}_m}^{-1}\mathbf{Q}_{\mathbf{S}_m}^H\mathbf{b}_{m+1}$ and the initial guess is

$$\mathbf{x}_{m+1}^{(0)} = \mathbf{X}_m\mathbf{R}_{\mathbf{S}_m}^{-1}\mathbf{Q}_{\mathbf{S}_m}^H\mathbf{b}_{m+1}. \tag{6}$$

If $\|\mathbf{r}_{m+1}\| \leq \varepsilon$ in (5), then a satisfactory solution $\mathbf{x}_{m+1}^{(0)}$ is obtained without any iterations. If $m = N$ the exact solution is obtained already by the initial guess.

The residual for the initial guess $\mathbf{x}_{m+1}^{(0)}$ in (6) is

$$\mathbf{r}_{m+1}^{(0)} = \mathbf{b}_{m+1} - \mathbf{A}\mathbf{X}_m\mathbf{y}_m = \mathbf{b}_{m+1} - \mathbf{S}_m\mathbf{R}_{\mathbf{S}_m}^{-1}\mathbf{Q}_{\mathbf{S}_m}^H\mathbf{b}_{m+1} = (\mathbf{I} - \mathbf{Q}_{\mathbf{S}_m}\mathbf{Q}_{\mathbf{S}_m}^H)\mathbf{b}_{m+1}. \tag{7}$$

This is an expression for $\mathbf{r}_{m+1}^{(0)}$ which is cheap to evaluate since $m \ll N$ and $\mathbf{Q}_{\mathbf{S}_m}^H\mathbf{b}_{m+1}$ is already computed in (6). The residual is small if $\mathbf{b}_{m+1}$ is almost spanned by the previous $\mathbf{s}_i$. This is the case if $\mathbf{b}_i$ depends in a smooth way on a parameter ϕ_i so that $\mathbf{b}_i = \mathbf{b}(\phi_i)$ and the difference $\Delta\phi = \phi_{i+1} - \phi_i$ is small. This is the starting point for the analysis in the next section.

If $\|\mathbf{r}_{m+1}^{(0)}\| > \varepsilon$ then $\mathbf{x}_{m+1}$ has to be improved by the iterative method. Let the k:th iteration of $\mathbf{x}_{m+1}$ be $\mathbf{x}_{m+1}^{(k)}$ with its residual $\mathbf{r}_{m+1}^{(k)}$. Then

$$\mathbf{s}_{m+1}^{(k)} = \mathbf{b}_{m+1} - \mathbf{r}_{m+1}^{(k)} = \mathbf{S}_m\mathbf{y}_m + \mathbf{r}_{m+1}^{(0)} - \mathbf{r}_{m+1}^{(k)}.$$

If $\|\mathbf{r}_{m+1}^{(k)}\| \leq \varepsilon_I$ for an $\varepsilon_I \leq \varepsilon$ then the iterations are interrupted and $\mathbf{s}_{m+1}^{(k)}$ is included in the basis $\mathbf{S}_m$ if

$$\|(\mathbf{I} - \mathbf{Q}_{\mathbf{S}_m}\mathbf{Q}_{\mathbf{S}_m}^H)\mathbf{s}_{m+1}^{(k)}\| = \|(\mathbf{I} - \mathbf{Q}_{\mathbf{S}_m}\mathbf{Q}_{\mathbf{S}_m}^H)(\mathbf{r}_{m+1}^{(0)} - \mathbf{r}_{m+1}^{(k)})\| > \varepsilon_s, \tag{8}$$

where $\varepsilon_s > \varepsilon + \varepsilon_I$. How to choose ε_I in relation to ε is treated in the next section. Otherwise, $\mathbf{s}_{m+1}^{(k)}$ is almost linearly dependent of the columns of $\mathbf{S}_m$ and $\mathbf{R}_{\mathbf{S}_{m+1}}$ would be ill-conditioned. This is particularly the case when $\mathbf{x}_{m+1} = \mathbf{x}_{m+1}^{(0)}$ and no iterations are necessary.

Once the solution is found and (8) is satisfied we can construct $\mathbf{X}_{m+1} = [\mathbf{X}_m\,\mathbf{x}_{m+1}]$ and $\mathbf{S}_{m+1} = [\mathbf{S}_m\,\mathbf{s}_{m+1}]$. A problem with this approach is that the memory requirements increase linearly with each new solution added. This is also a drawback with the GMRES method [14]. The solution in GMRES is to let the dimension of the Krylov space reach a maximum and then restart the iteration. In our case, one of the columns in $\mathbf{S}_m$ and $\mathbf{R}_{\mathbf{S}_m}$ is dropped when a new one is introduced.

The $\mathbf{QR}$-decomposition of $\mathbf{S}_m$ is updated after solution of (2) when a column is appended to and deleted from $\mathbf{S}_m$ following [2]. This procedure can cause a loss of orthogonality in $\mathbf{Q}$ because of round-off errors. If necessary, this is corrected

by computing a new **QR**-decomposition of **Q** and multiplying the new **R** matrix with the old one.

The Arnoldi process in the block version of the GMRES algorithm [14], [15], adapted for multiple right hand sides as in [7] generates an orthonormal basis $\mathbf{V}_q \in \mathbb{C}^{N\times q}$ for $\mathbf{X}_m$ such that

$$\mathbf{A}\mathbf{V}_q = \mathbf{V}_{q+1}\mathbf{H}_{q+1\times q},\ \mathbf{X}_m = \mathbf{V}_q\mathbf{Z}_m, \tag{9}$$

where $\mathbf{H}_{q+1\times q} \in \mathbb{C}^{q+1\times q}$ is an upper Hessenberg matrix, $\mathbf{V}_{q+1} \in \mathbb{C}^{N\times q+1}$ is another orthonormal matrix, and $\mathbf{Z}_m \in \mathbb{C}^{q\times m}$, $q > m$. This basis can be utilized to determine an initial guess in the following way. Let

$$\mathbf{x}_{m+1}^{(0)} = \mathbf{X}_m\mathbf{y}_m = \mathbf{V}_q\mathbf{Z}_m\mathbf{y}_m = \mathbf{V}_q\mathbf{z}_m.$$

Then the residual is

$$\mathbf{r}_{m+1} = \mathbf{b}_{m+1} - \mathbf{A}\mathbf{X}_m\mathbf{y}_m = \mathbf{b}_{m+1} - \mathbf{A}\mathbf{V}_q\mathbf{Z}_m\mathbf{y}_m = \mathbf{b}_{m+1} - \mathbf{V}_{q+1}\mathbf{H}_{q+1\times q}\mathbf{z}_m. \tag{10}$$

The squared norm of $\mathbf{r}_{m+1}$ is (cf. (5))

$$\begin{aligned} \|\mathbf{r}_{m+1}\|^2 &= \|\mathbf{b}_{m+1} - \mathbf{V}_{q+1}\mathbf{H}_{q+1\times q}\mathbf{z}_m\|^2 \\ &= \|(\mathbf{I} - \mathbf{V}_{q+1}\mathbf{V}_{q+1}^H)\mathbf{b}_{m+1}\|^2 + \|\mathbf{V}_{q+1}^H\mathbf{b}_{m+1} - \mathbf{H}_{q+1\times q}\mathbf{z}_m\|^2. \end{aligned} \tag{11}$$

Solve the linear least squares problem

$$\min_z \|\mathbf{V}_{q+1}^H\mathbf{b}_{m+1} - \mathbf{H}_{q+1\times q}\mathbf{z}_m\|$$

for $\mathbf{z}_m$. The **QR**-decomposition of $\mathbf{H}_{q+1\times q}$ is available from the GMRES iteration. Then take

$$\mathbf{x}_{m+1}^{(0)} = \mathbf{V}_q\mathbf{z}_m.$$

If $\mathbf{r}_{m+1}^{(0)}$ determined by (5) is smaller or greater than in (11) depends on how well $\mathbf{b}_{m+1}$ is represented by the columns of $\mathbf{Q}_{\mathbf{S}_m}$ and $\mathbf{V}_{q+1}$. We note that this method is similar to the seed method in [16] without Richardson iteration. This method is competitive with our method if one obtains an improved convergence rate with the same m.

Sometimes the purpose of the computation is not the solution $\mathbf{x}_i$ of (1) but rather the calculation of S linear functionals

$$\mathbf{\Phi}(\mathbf{x}_i) = \mathbf{C}^T\mathbf{x}_i, \tag{12}$$

with $\mathbf{C} = [\mathbf{c}_1\mathbf{c}_2\ldots\mathbf{c}_S]$. Let $\mathbf{D}$ be the solution of the adjoint or dual problem

$$\mathbf{A}^T\mathbf{D} = \mathbf{C}. \tag{13}$$

Then $\mathbf{\Phi}$ in (12) can be written

$$\mathbf{\Phi}(\mathbf{x}_i) = \mathbf{C}^T\mathbf{A}^{-1}(\mathbf{b}_i - \mathbf{r}_i) = \mathbf{D}^T(\mathbf{b}_i - \mathbf{r}_i). \tag{14}$$

If $\mathbf{C}$ is constant for more than S right hand sides $\mathbf{b}_i$, then (14) saves computing time since only S systems of linear equations have to be solved instead of M. In addition, the effect $\delta\mathbf{\Phi}$ on $\mathbf{\Phi}$ of the termination criterion on $\mathbf{r}$ is derived from (14)

$$\|\delta\mathbf{\Phi}\| \leq \|\mathbf{D}\|\varepsilon.$$

If the system matrix $\mathbf{A}$ also is smoothly varying such that $\mathbf{A}_i = \mathbf{A}(\phi_i)$

$$\mathbf{A}_i\mathbf{x}_i = \mathbf{b}_i,\ i = 1 \ldots M, \tag{15}$$

then the initial guess $\mathbf{x}_{m+1}^{(0)}$ for the $(m+1)$:th linear system can be interpolated in a similar manner. Let

$$\mathbf{s}_i = \mathbf{A}_{m+1}\mathbf{x}_i = \mathbf{b}_i - \mathbf{r}_i + (\mathbf{A}_{m+1} - \mathbf{A}_i)\,\mathbf{x}_i,\ i = 1 \ldots m,$$

and define $\mathbf{X}_m$ and $\mathbf{S}_m$ as before. The linear combination of $\mathbf{x}_i$ is chosen to minimize the initial residual

$$\mathbf{r}_{m+1}^{(0)} = \mathbf{b}_{m+1} - \mathbf{A}_{m+1}\mathbf{X}_m\mathbf{y}_m = \mathbf{b}_{m+1} - \mathbf{S}_m\mathbf{y}_m$$

as in (5). Note that in certain cases $\mathbf{A}_{m+1} - \mathbf{A}_i$ is easily obtained, for instance if $\mathbf{A}_i = \mathbf{A} + \phi_i\mathbf{I}$.

In order to implement an algorithm based on the above observations we need an iterative method for solution of (2). For simplicity we assume that the iterative method returns the residual $\mathbf{r}$. This will give us a method that can compute an initial guess without any expensive matrix-vector multiplications. In an iterative method the residual is often used in the termination criterion and can be computed by a simple update formula instead of computing it explicitly [1]. Then the number of expensive matrix-vector multiplications is reduced.

Algorithm 1 proceeds by solving for k right hand sides using an iterative method. The method could be a block method, a seed method, a single right hand side solver or another type of method. The **QR**-decomposition is then updated. With the **QR**-decomposition, initial guesses for k new right hand sides are computed. If there are initial guesses that do not fulfill the tolerance requirement the solution is determined by the iterative method. The process continues until the solutions to all M right hand sides are computed. The algorithm is slightly more general than in (6) and (7) by computing the solution $\mathbf{x}_i$ as a sum of an initial basis vector $(\mathbf{x}_i)_0$ given by e.g. a different method and a correction to it. The residual corresponding to $(\mathbf{x}_i)_0$ is $(\mathbf{r}_i)_0$. The right hand sides for which interpolation is not sufficiently accurate are collected in the set $\mathcal{I}$.

Algorithm 1 The Minimum Residual Interpolation algorithm for computing solutions to systems of linear equations with multiple right hand sides.

Require: An iterative method, residual tolerances ε_I for the iterative method and ε for the interpolation method, $\mathbf{b}_1 \dots \mathbf{b}_M$, $\mathbf{X}_0$.
Ensure: $\mathbf{X}$ where $\|\mathbf{b}_i - \mathbf{A}\mathbf{x}_i\| \leq \varepsilon$
  Solve $\mathbf{A}\mathbf{x}_i = \mathbf{b}_i$ such that $\|\mathbf{r}_i\| \leq \varepsilon_I$ for $i = 1 : k$ with the initial guess $\mathbf{X}_0$.
  Compute $\mathbf{s}_i = \mathbf{b}_i - \mathbf{r}_i$ for $i = 1 : k$.
  Compute $\mathbf{S}_k = \mathbf{Q}_{\mathbf{S}_k}\mathbf{R}_{\mathbf{S}_k}$.
  for $j = k + 1 : M$ stepsize k **do**
    Set $\mathcal{I} = \varnothing$.
    for $i = j : j + k - 1$ **do**
      $\mathbf{x}_i^{(0)} = (\mathbf{x}_i)_0 + \mathbf{X}_{j-1}\mathbf{R}_{\mathbf{S}_{j-1}}^{-1}\mathbf{Q}_{\mathbf{S}_{j-1}}^H (\mathbf{r}_i)_0$.
      $\mathbf{r}_i^{(0)} = \left(\mathbf{I} - \mathbf{Q}_{\mathbf{S}_{j-1}}\mathbf{Q}_{\mathbf{S}_{j-1}}^H\right)(\mathbf{r}_i)_0$.
      if $|\mathbf{r}_i^{(0)}| > \varepsilon$ **then**
        Set $\mathcal{I} = \mathcal{I} \cup i$.
      end if
    end for
    Solve $\mathbf{A}\mathbf{x}_\mathcal{I} = \mathbf{b}_\mathcal{I}$ such that $\|\mathbf{r}_\mathcal{I}\| \leq \varepsilon_I$.
    for $i = j : j + k - 1$ **do**
      if $i \in \mathcal{I}$ and (8) is fulfilled **then**
        Compute $\mathbf{s}_i = \mathbf{b}_i - \mathbf{r}_i$.
        Update $\mathbf{X}_i = (\mathbf{X}_{i-1}, \mathbf{x}_i)$ and $\mathbf{S}_i = \mathbf{Q}_{\mathbf{S}_i}\mathbf{R}_{\mathbf{S}_i}$.
      else
        $\mathbf{X}_i = \mathbf{X}_{i-1}$ and $\mathbf{S}_i = \mathbf{Q}_{\mathbf{S}_{i-1}}\mathbf{R}_{\mathbf{S}_{i-1}}$.
      end if
    end for
  end for

The work to solve the linear least squares problem for $\mathbf{x}_i^{(0)}$ and to update the residual $\mathbf{r}_i^{(0)}$ is proportional to N in the algorithm. The **QR**-decomposition is updated in $\mathcal{O}(N)$ operations. The solution of the system of equations depends on the number of iterations K and the cost of one matrix-vector multiplication. With a standard matrix-vector multiplication for a dense matrix the number of operations is of $\mathcal{O}(KN^2)$ and for FMM of $\mathcal{O}(KN \log N)$. For a sparse matrix with $\mathcal{O}(N)$ nonzero elements the cost of the iterative solution is proportional to $\mathcal{O}(KN)$.

The order of processing of the vectors is not specified in Algorithm 1. Assume that the right hand sides in (1) depend smoothly on an angle ϕ in an interval $[\phi_1, \phi_M]$ of length ϕ_I so that $\mathbf{b}_i = \mathbf{b}(\phi_i)$, $i = 1 \dots M$ and that $\phi_{i+1} = \phi_i + \Delta\phi$. Partition the set of right hand sides $\mathcal{B}$ into $L + 1$ subsets or levels $\mathcal{B}_l$, $l = 0 \dots L$, so that $\mathcal{B}_L = \mathcal{B}$ and $\mathcal{B}_{l-1} \subset \mathcal{B}_l$. Let the number of vectors in $\mathcal{B}_l$ be m_l and

$m_L = M$. At level l, the vectors are chosen so that the separation $\Delta\phi_l$ between the angles is $\gamma^{L-l}\Delta\phi$ for some integer $\gamma > 1$. At level 0 with m_0 vectors, $\mathbf{b}_1, \mathbf{b}_M$, and $m_0 - 2$ more vectors are included in $\mathcal{B}_0$ and

$$(m_0 - 1)\Delta\phi_0 = (m_0 - 1)\gamma^L\Delta\phi \geq \phi_I = (M - 1)\Delta\phi.$$

A simple method to generate the sequence of right hand sides with $\gamma = 2$ is first to solve for $\mathbf{b}_1$, $\mathbf{b}_M$, and $\mathbf{b}_{2^k}$ with a k such that $2^{k+1} \geq M$. The process is continued by solving for $\mathbf{b}_j$, $j = 2^{k-1}$, and stepping with the increment 2^k until $j \geq M$. Then k is reduced by one again and the process is repeated until all right hand sides are solved. The right hand sides are thus picked level by level from a binary tree.

In the numerical experiments in the last section and in Fig. 1, we let $\gamma = 2$ and the right hand sides are partitioned into the sets $\mathcal{B}_l$. In the figure, $L = 3$ and $M = m_3 = 16$. The solutions at angles marked by `X` in the figure are computed by an interpolated initial guess and possibly iteration. Those marked by `O` are already known from the previous level. The solutions at `I` at level 0 are computed by iteration from an initial guess provided by the user.

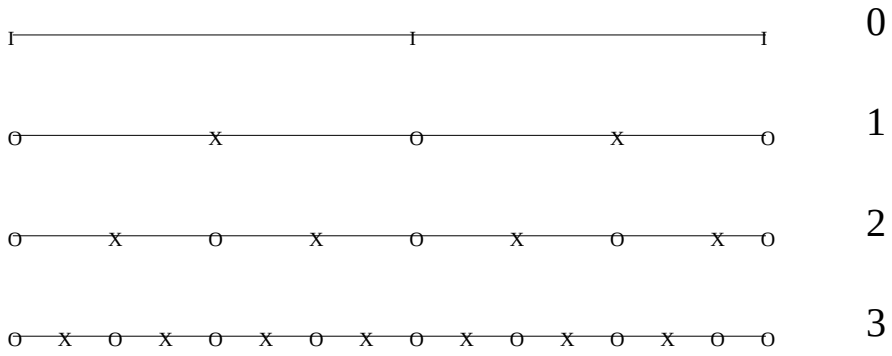

Figure 1: The right hand sides have been partitioned into four levels.

By initializing the iterative solution of linear systems accurately, the number of iterations to convergence is reduced and may not be needed at all. Hence, expensive matrix-vector multiplications for dense matrices are avoided in Krylov subspace methods.

3 Convergence properties

In this section we study the convergence of the interpolated initialization for the iterations. An upper bound on the computational work spent in the iterative method is derived.

The analysis is simplified if we assume for all levels that $m_l = 1 + \gamma^l(m_0 - 1)$. Let $\tilde{m}_l$ be the number of unknown solutions at level l. It follows that

$$m_l = 1 + \gamma(m_{l-1} - 1),\ \tilde{m}_l = m_l - m_{l-1} = \gamma^{l-1}(\gamma - 1)(m_0 - 1). \tag{16}$$

The relation between M, L, and γ is $M - 1 = \gamma^L(m_0 - 1)$. Hence, the number of levels L grows as $\log M / \log \gamma$ when M increases. At level l the separation between the angles is $\Delta\phi_l = \phi_I/(m_l - 1) = \phi_I/(\gamma^l(m_0 - 1))$. The computational work to interpolate the initial guess for one vector at level l from data at level $l - 1$ is denoted by w_{int}. The work for one iteration with the Krylov method to compute one solution at level l and the updating of the **QR**-decomposition is denoted by w_{it} which is much greater than w_{int}. The total work to compute the unknown $\tilde{m}_l$ solutions at level l is

$$\tilde{m}_l(w_{int} + K_l w_{it}) = \gamma^{l-1}(\gamma - 1)(m_0 - 1)(w_{int} + K_l w_{it}), \tag{17}$$

where K_l is the number of iterations for one right hand side at level l. Under certain assumptions there is an upper bound on the work spent on iterations in (17) independent of the level and M.

Assume that the interpolation (6) from level $l - 1$ to l introduces an error in the initial residual $\mathbf{r}^{(0)}$ for the iterative solver so that

$$\|\mathbf{r}^{(0)}\| \leq c\Delta\phi_{l-1}^p = c(\Delta\phi_0/\gamma^{l-1})^p, \tag{18}$$

where p is the number of $\mathbf{b}_i$ involved in the interpolation and c is independent of p, l, and $\Delta\phi_0$. For simplicity we assume in the analysis in this section that p is constant. This is not necessary in Algorithm 1 and p varies in the numerical experiments in the last section.

With a constant convergence rate θ independent of l, the norm of the residual after k iterations is

$$\|\mathbf{r}^{(k)}\| \leq \theta^k \|\mathbf{r}^{(0)}\|, \ \theta < 1, \tag{19}$$

for the solution corresponding to one right hand side at level l. From (19) and (18) we conclude that for the residual to satisfy a convergence criterion $\|\mathbf{r}^{(0)}\| \leq \varepsilon$ if no iterations are necessary and $\|\mathbf{r}^{(k)}\| \leq \varepsilon_I \leq \varepsilon$ if the iterative solver is invoked we need at most K_{lmax} iterations where K_{lmax} is the smallest integer greater than or equal to

$$\max(0, (c_1 - \log \varepsilon_I - p(l-1)\log\gamma)/|\log\theta|), \ c_1 = \log c + p \log \Delta\phi_0. \tag{20}$$

Since $\gamma > 1$ the criterion is satisfied immediately by the interpolated values if $l \geq 1 + (c_1 - \log\varepsilon)/(p \log\gamma)$. No iterations are necessary when

$$l \geq l_{max} = \max(0, 1 + (c_1 - \log\varepsilon_I)/(p\log\gamma)). \tag{21}$$

This bound increases with smaller ε_I and decreases with larger γ and p. The total amount of work for the iterations at level l follows from (17) and (20):

$$w_{maxit}(l) = \gamma^{l-1}(\gamma - 1)(m_0 - 1)K_{lmax} w_{it}. \tag{22}$$

We are now prepared to show that the work for the iterative solution is bounded independently of l and M.

Theorem 1
Assume that the number of vectors at each level l grows as in (16) with $\gamma \geq 2$, that the interpolation of the initial guess for the iteration satisfies (18) with p constant, and that the convergence rate of the iterations is θ (19). Then the computational work in (22) at level $l \geq 1$ is bounded independently of l by

$$w_{itbnd} = p \exp(p^{-1}(c_1 + |\log\theta| - \log\varepsilon_I) - 1)(\gamma - 1)(m_0 - 1)w_{it}/|\log\theta|.$$

Let the iterative work at the initial level be $w_0 w_{it}$. An upper bound on the total work to solve (1) for the M right hand sides is

$$w_{total} \leq (M - m_0)w_{int} + w_0 w_{it} + w_{l_{max}} w_{it},$$

where w_0 and $w_{l_{max}}$ are independent of M.
Proof
The iterative work $w_{maxit}(l)$ in (22) is bounded by

$$w_{maxit}(l) \leq \gamma^{l-1}(\gamma - 1)(m_0 - 1)\max(0, \alpha - \beta l),$$
$$\alpha = 1 + (c_1 - \log\varepsilon_I + p\log\gamma)/|\log\theta|,\ \beta = p\log\gamma/|\log\theta|.$$

The maximum of the right hand side is found at $l_* - 1 = ((c_1 + |\log\theta| - \log\varepsilon_I)/p - 1)/\log\gamma$. Hence, $w_{maxit}(l) \leq w_{itbnd} = w_{maxit}(l_*)$.

It follows from (21) that no iterations are required when the level exceeds l_{max}. The total iterative work for $l \geq 1$ is bounded by

$$w_{ittot} \leq \sum_{l=1}^{l_{max}+1} w_{maxit}(l) \leq (\gamma - 1)(m_0 - 1)w_{it} \sum_{l=1}^{l_{max}+1} \gamma^{l-1}(\alpha - \beta l).$$

The sum is bounded independently of M and therefore, $w_{ittot} = w_{l_{max}} w_{it}$ is independent of M. The work at level 0 depends on m_0, w_{it}, and the initial residual. Initial data are interpolated for all M vectors except for the m_0 vectors at level 0. The bound on the total work is proved. ■

The conclusion from the theorem is that the work grows linearly with the number of right hand sides and there is an upper bound on the total work spent in the iterative method. The linear growth is slow thanks to the inexpensive MRI. The work $w_{int} = \mathcal{O}(pN)$ is small compared to $w_{it} = \mathcal{O}(KN\log N)$ also for FMM, since the multiplying factor in front of the leading term is large there. This is confirmed in the numerical examples in the last section. Problems with sparse matrices where matrix-vector multiplications use $\mathcal{O}(N)$ operations will also benefit from MRI as long as $w_{int} \ll w_{it}$. The work w_{itbnd} increases with smaller ε_I and decreases with larger p.

In the next theorem, a sufficient condition on the regularity of $\mathbf{b}(\phi)$ is derived such that the leading term of the initial residual behaves as in (18) as required in the previous theorem.

Theorem 2
Assume that the components in the right hand side vectors $\mathbf{b}_i = \mathbf{b}(\phi_i)$ *have* p *continuous derivatives in* ϕ, $\|\mathbf{r}_i\| \leq \varepsilon_I$, *and that an approximation to* $\mathbf{b}_\alpha$ *at* ϕ_α *is computed at level* l *by the minimization*

$$\min_{\mathbf{y}} \|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\|.$$

Then

$$\|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\| \leq \sqrt{N} b_{max}^{(p)} \Delta\phi_{l-1}^{p} + \sqrt{p}\|\mathbf{l}\|\varepsilon_I,$$

where $b_{max}^{(p)} = \max_j \max_\phi |b_j^{(p)}(\phi)|$, $b_j^{(p)}$ *is the* p*:th derivative of* b_j, *and* $\mathbf{l}$ *consists of the coefficients of the Lagrange polynomial at the point* ϕ_α.
Proof
Let γ_i be a set of coefficients different from y_i. The triangle inequality together with the equality $\mathbf{s}_i = \mathbf{b}_i - \mathbf{r}_i$ yields

$$\|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\| \leq \|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i \gamma_i\| \leq \|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{b}_i \gamma_i\| + \|\sum_{i=1}^{p} \mathbf{r}_i \gamma_i\|.$$

To obtain an estimate of the first part we let $l(\phi)$ be the interpolating polynomial of degree less than p of the j:th component of b through the points ϕ_i, $i = 1 \ldots p$. By an interpolation theorem [3] we have for all j

$$|b_j(\phi_\alpha) - l(\phi_\alpha)| = |b_j(\phi_\alpha) - \sum_{i=1}^{p} b_j(\phi_i) l_{\alpha i}| \leq |b_j^{(p)}||W_\alpha|/p!.$$

where $|b_j^{(p)}| = \max_\phi |b_j^{(p)}(\phi)|$, $W_\alpha = \prod_{i=1}^{p}(\phi_\alpha - \phi_i)$, and $l_{\alpha i}$ are the coefficients of the Lagrange polynomial. Thus, if $\gamma_i = l_{\alpha i}$ then

$$\begin{aligned}&\|\mathbf{b}_\alpha - \textstyle\sum_{i=1}^{p} \mathbf{b}_i l_{\alpha i}\|^2 = \sum_{j=1}^{N} |b_j(\phi_\alpha) - \sum_{i=1}^{p} b_j(\phi_i) l_{\alpha i}|^2 \\ &\leq \textstyle\sum_{j=1}^{N} |b_j^{(p)} W_\alpha/p!|^2 = (W_\alpha/p!)^2 \sum_{j=1}^{N} |b_j^{(p)}|^2 \leq (W_\alpha/p!)^2 N (b_{max}^{(p)})^2.\end{aligned}$$

Since $\phi_\alpha \in [\phi_1, \phi_M]$, an upper bound on $|W_\alpha|/p!$ is $\Delta\phi_{l-1}^{p}$.

With $\mathbf{R} = [\mathbf{r}_1 \ldots \mathbf{r}_p]$, the choice of Lagrange coefficients in the first part together with Cauchy-Schwartz' inequality gives the estimate of the second part since

$$\begin{aligned}\|\textstyle\sum_{i=1}^{p} \mathbf{r}_i l_{\alpha i}\|^2 &= \textstyle\sum_{j=1}^{N} |\mathbf{R}_{j,:}\mathbf{l}|^2 \leq \sum_{j=1}^{N} \|\mathbf{l}\|^2 \|\mathbf{R}_{j,:}\|^2 \leq \|\mathbf{l}\|^2 \sum_{i=1}^{p} \sum_{j=1}^{N} |R_{ji}|^2 \\ &\leq p\|\mathbf{l}\|^2 \max_i \|\mathbf{r}_i\|^2 \leq p\|\mathbf{l}\|^2 \varepsilon_I^2,\end{aligned}$$

and the theorem is proved. ■

If $\varepsilon_I \leq \varepsilon$ and $\mathbf{b}$ varies smoothly with ϕ, then it is possible to satisfy $\|\mathbf{r}_{m+1}\| \leq \varepsilon$ in (5) without any iterations. It is important here that ε_I is not chosen greater than ε, i.e. the vectors $\mathbf{s}_i$ in the basis are close to the corresponding $\mathbf{b}_i$. However, one should note that the proof is based on interpolation, while the method is based on least squares. The method works adaptively and tries to reduce the largest term in the estimate. Therefore it is likely that the method is able to predict the correct residual even if $\varepsilon_I = \varepsilon$, which is indicated in the numerical experiments.

The theorems will be applied to Maxwell's equations with multiple right hand sides in the next section. We choose the special case of scattering from plane waves.

4 Integral equations

Consider the time-harmonic electromagnetic scattering from a perfect electric conductor (PEC). Combining the Electric Field Integral Equation (EFIE) and the Magnetic Field Integral Equation (MFIE) in variational form yields the Combined Field Integral Equation (CFIE) [12]

$$\begin{aligned} &\alpha \int_\Gamma \int_\Gamma G(\mathbf{x}, \mathbf{x}') \left(\mathbf{J} \cdot \mathbf{J}' - \frac{1}{\kappa^2} \boldsymbol{\nabla}_\Gamma \cdot \mathbf{J} \boldsymbol{\nabla}_\Gamma \cdot \mathbf{J}' \right) d\Gamma d\Gamma \\ &+ (1-\alpha) \frac{\imath}{\kappa} \int_\Gamma \hat{\mathbf{n}} \times \int_\Gamma \boldsymbol{\nabla}_{\mathbf{x}'} G(\mathbf{x}, \mathbf{x}') \times \mathbf{J} \cdot \mathbf{J}' d\Gamma d\Gamma \\ &= -\alpha \frac{1}{\imath \kappa Z} \int_\Gamma \mathbf{E}_a \cdot \mathbf{J}' d\Gamma + (1-\alpha) \frac{\imath}{\kappa} \int_\Gamma \hat{\mathbf{n}} \times \mathbf{H}_a \cdot \mathbf{J}' d\Gamma. \end{aligned} \tag{23}$$

Here, $\mathbf{J}$ is the unknown electric current on the surface Γ of the scatter, $\mathbf{J}'$ is the test current, κ is the wavenumber, Z is the impedance in free space, $\hat{\mathbf{n}}$ is the unit normal pointing outward from Γ, and $\imath = \sqrt{-1}$. The function $G(\mathbf{x}, \mathbf{x}')$ is the free-space Green's function for Helmholtz' equation. The parameter α can vary between 0 (MFIE) and 1 (EFIE). The right hand side depends on the applied electric field $\mathbf{E}_a$ and the applied magnetic field $\mathbf{H}_a$.

The equations are discretized with the Galerkin method and the rooftop or RWG basis functions [13]. The discretization leads to a dense, complex system of equations of the form (1). If $\alpha = 1$ then $\mathbf{A}$ is complex symmetric but not Hermitian. The unknowns in $\mathbf{x}$ are the coefficients for each basis function and the right hand side $\mathbf{b}$ depends on the applied fields $\mathbf{E}_a$ and $\mathbf{H}_a$. A change in the applied field affects only the right hand side, while $\mathbf{A}$ is unchanged.

Gaussian elimination has been used for problems with up to the order of 10^5 unknowns, but beyond that computing time and memory requirements are prohibitive. Our iterative solver is the GMRES method [14] with the fast multipole

method [5] for the matrix-vector multiplications. The major cost in the iterations is the multiplication of an arbitrary vector by the matrix. The matrix is preconditioned with a modified Sparse Approximate Inverse Preconditioner (SPAI) as in [10], [11], which improves the convergence rate especially for EFIE. For several right hand sides, the block version of GMRES accelerates the convergence as in [15].

The applied electric and magnetic fields in (23) at $\mathbf{x}$ can be written

$$\mathbf{E}_a(\mathbf{x}, \hat{\boldsymbol{\kappa}}_a) = \mathbf{E}_0 \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}),\ \mathbf{H}_a(\mathbf{x}, \hat{\boldsymbol{\kappa}}_a) = \mathbf{H}_0 \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}), \tag{24}$$

for a plane wave traveling in the direction given by the unit vector $\hat{\boldsymbol{\kappa}}_a$. With the Cartesian unit vectors $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$, and the spherical angles ϕ and θ defining $\hat{\boldsymbol{\kappa}}_a$

$$\hat{\boldsymbol{\kappa}}_a = \sin\theta\cos\phi\hat{\mathbf{x}} + \sin\theta\sin\phi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}},$$

$\mathbf{E}_0$ in (24) is expressed as

$$\mathbf{E}_0(\hat{\boldsymbol{\kappa}}_a) = (E_\theta\cos\theta\cos\phi - E_\phi\sin\phi)\hat{\mathbf{x}} + (E_\theta\cos\theta\sin\phi + E_\phi\cos\phi)\hat{\mathbf{y}} - E_\theta\sin\theta\hat{\mathbf{z}}. \tag{25}$$

The electric and magnetic fields are coupled in a plane wave so that

$$\mathbf{H}_0(\hat{\boldsymbol{\kappa}}_a) = Z^{-1}\hat{\boldsymbol{\kappa}}_a \times \mathbf{E}_0(\hat{\boldsymbol{\kappa}}_a).$$

Then the right hand side in (23) is

$$\begin{aligned} b(\phi,\theta) &= \frac{\iota}{\kappa Z}\int_\Gamma (\alpha\mathbf{E}_0 + (1-\alpha)\hat{\mathbf{n}} \times (\hat{\boldsymbol{\kappa}}_a \times \mathbf{E}_0)) \cdot \mathbf{J}' \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}) d\Gamma \\ &\equiv \int_\Gamma \mathbf{K}(\hat{\boldsymbol{\kappa}}_a) \cdot \mathbf{J}' \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}) d\Gamma. \end{aligned} \tag{26}$$

After Galerkin discretization with the test functions $\mathbf{j}_j$ and approximation of the integral with a quadrature rule with q positive weights w_{jk}, the j:th component of the discretized right hand side is

$$b_j(\phi,\theta) = \sum_{k=1}^{q} w_{jk}\mathbf{K}(\hat{\boldsymbol{\kappa}}_a) \cdot \mathbf{j}_j(\mathbf{x}_{jk}) \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}_{jk}). \tag{27}$$

For plane waves one can prove a sharper bound on the interpolation error than in Theorem 2. The bound is independent of the number of unknowns. In order to show that b_j in (27) is well approximated by MRI we need a bound on the derivatives of the angles.

Lemma 3
Let

$$\mathbf{f}_{jk}(\phi,\theta) = \mathbf{K}(\hat{\boldsymbol{\kappa}}_a) \exp(-\iota\kappa\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}_{jk})$$

in (27) and $x_{max} = \max_{jk} \|x_{jk}\|$. *Then for* $\psi = \phi$ *or* θ

$$\|\frac{\partial^p \mathbf{f}}{\partial \psi^p}\| \leq \sum_{i=0}^{p} c_i^{\psi} (\kappa x_{max})^i,$$

where c_i^{ψ} *depends only on* ϕ *and* θ.

Proof

In spherical coordinates we have

$$\mathbf{x}_{jk} = r_{jk}(\sin\theta_{jk}\cos\phi_{jk}\hat{\mathbf{x}} + \sin\theta_{jk}\sin\phi_{jk}\hat{\mathbf{y}} + \cos\theta_{jk}\hat{\mathbf{z}}).$$

The scalar product between $\hat{\boldsymbol{\kappa}}_a$ and x_{jk} is

$$\hat{\boldsymbol{\kappa}}_a \cdot \mathbf{x}_{jk} = r_{jk} g(\phi, \theta, \phi_{jk}, \theta_{jk}),$$

where g is a sum of products of sine and cosine of the angles. The same holds true for all derivatives of g. From the definition of $\mathbf{K}(\hat{\boldsymbol{\kappa}}_a)$ in (26) and (25) we infer the same property for all derivatives of $\mathbf{K}$. By induction it follows that

$$\frac{\partial^p}{\partial \psi^p} \exp(-\iota\kappa r_{jk} g) = \sum_{i=1}^{p} (-\iota\kappa r_{jk})^i G_i(\phi, \theta) \exp(-\iota\kappa r_{jk} g), \tag{28}$$

where G_i is a sum of products of sine and cosine of ϕ and θ. From Leibnitz' differentiation rule, (28), and $\partial^j \mathbf{K}/\partial\psi^j$ we arrive at the estimate for $\partial^p \mathbf{f}/\partial\psi^p$. ■

The lemma and the techniques in the proof of Theorem 2 are applied to the discretized right hand side (27) in the following theorem. The object Γ is centered around the origin so that x_{max} is a relevant measure of its size. Otherwise it can be translated there by a coordinate transformation.

Theorem 4

Assume that the components in the right hand side vectors are computed by the Galerkin discretization (27) so that

$$\mathbf{b}_i = \mathbf{b}(\phi_i) = (b_1(\phi_i, \theta), \ldots b_N(\phi_i, \theta))^T,$$

for a given θ *and let* $\Delta\phi = \phi_{i+1} - \phi_i$. *Assume that an approximation to* $\mathbf{b}_\alpha$ *at* ϕ_α *is computed by minimization*

$$\min_{\mathbf{y}} \|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\|,$$

and that $\kappa x_{max} \geq \eta > 1$. *Let* $j_{max} = \max_{\mathbf{x}} \max_j |\mathbf{j}_j(\mathbf{x})|$ *and the area of* Γ *be* A. *Then there is a constant* C *independent of* κ, x_{max}, *and* $\Delta\phi$ *such that*

$$\|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\| \leq C A j_{max} (\kappa x_{max} \Delta\phi)^p + \sqrt{p}\|\mathbf{l}\|\varepsilon_I.$$

Proof
In the same manner as in the proof of Theorem 2 we have with the coefficients $l_{\alpha i}$ of the Lagrange polynomial l

$$\|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{s}_i y_i\| \leq \|\mathbf{b}_\alpha - \sum_{i=1}^{p} \mathbf{b}_i l_{\alpha i}\| + \sqrt{p}\|\mathbf{l}\|\varepsilon_I.$$

Inserting the expression (27) and letting the summand in (27) be $w_{jk}\mathbf{f}_{jk}(\phi)\cdot\mathbf{j}_j(\mathbf{x}_{jk})$ we obtain

$$\begin{aligned}
&\|\mathbf{b}_\alpha - \textstyle\sum_{i=1}^{p} \mathbf{b}_i l_{\alpha i}\|^2 = \sum_{j=1}^{N} |\sum_{k=1}^{q} w_{jk}(\mathbf{f}_{jk}(\phi_\alpha) - \sum_{i=1}^{p} l_{\alpha i}\mathbf{f}_{jk}(\phi_i))\cdot\mathbf{j}_j(\mathbf{x}_{jk})|^2 \\
&\leq \textstyle\sum_{j=1}^{N} (\sum_{k=1}^{q} w_{jk}|\mathbf{f}_{jk}(\phi_\alpha)\cdot\mathbf{j}_j(\mathbf{x}_{jk}) - \sum_{i=1}^{p} l_{\alpha i}\mathbf{f}_{jk}(\phi_i)\cdot\mathbf{j}_j(\mathbf{x}_{jk})|)^2 \\
&\leq \textstyle\sum_{j=1}^{N} \left(\sum_{k=1}^{q} w_{jk} \max_\phi \|\mathbf{f}_{jk}^{(p)}\|\|\mathbf{j}_j(\mathbf{x}_{jk})\| \prod_{i=1}^{p}|\phi_\alpha - \phi_i|/p!\right)^2 \\
&\leq \max_j \max_k \max_\phi \|\mathbf{f}_{jk}^{(p)}\|^2 \Delta\phi^{2p} \left(\textstyle\sum_{j=1}^{N}\sum_{k=1}^{q} w_{jk}\|\mathbf{j}_j(\mathbf{x}_{jk})\|\right)^2.
\end{aligned}$$

The quadrature rule is such that

$$\sum_{k=1}^{q} w_{jk} = \int_{\Delta_j} d\Gamma = A_{\Delta_j},$$

where A_{Δ_j} is the area of the two triangles supporting $\mathbf{j}_j$. At most three $\mathbf{j}_j$ are nonzero in every triangle. Hence,

$$\sum_{j=1}^{N}\sum_{k=1}^{q} w_{jk} \leq 3A,$$

and

$$\begin{aligned}
\textstyle\sum_{j=1}^{N}\sum_{k=1}^{q} w_{jk}\|\mathbf{j}_j(\mathbf{x}_{jk})\| &\leq \textstyle\sum_{k=1}^{q} \max_j \|\mathbf{j}_j(\mathbf{x}_{jk})\| \sum_{j=1}^{N} w_{jk} \\
&\leq j_{max}\textstyle\sum_{k=1}^{q}\sum_{j=1}^{N} w_{jk} = 3j_{max}A.
\end{aligned}$$

The conclusion from Lemma 3 is

$$\begin{aligned}
\|\mathbf{f}_{jk}^{(p)}\| \leq \|\tfrac{\partial^p \mathbf{f}}{\partial\phi^p}\| &\leq (\kappa x_{max})^p \textstyle\sum_{i=0}^{p} c_i^\phi (\kappa x_{max})^{i-p} \\
&\leq (\kappa x_{max})^p \max_i c_i^\phi/(1-\eta^{-1}) \leq C(\kappa x_{max})^p/3,
\end{aligned}$$

when $\kappa x_{max} \geq \eta > 1$ and the theorem is proved. ■

The interpolation condition (18) in Theorem 1 is fulfilled by a Galerkin discretization of (23). If the other assumptions there also are satisfied, then the work in the iterative solver is bounded independently of M. The error in the initial guess depends on the wavenumber, the size of the object, and the difference between the angles.

The radar cross section (RCS) is a measure of the electromagnetic field for an observer at $\mathbf{x}$ far from the source. Let $\mathbf{x} = r\hat{\boldsymbol{\kappa}}$, where $\hat{\boldsymbol{\kappa}}$ is a unit vector and let the scattered field be $\mathbf{E}_s(\mathbf{x}, \hat{\boldsymbol{\kappa}})$. Then the bistatic RCS is defined by

$$\sigma(\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a) = \lim_{r\to\infty} 4\pi r^2 \frac{|\mathbf{E}_s(r\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a)|^2}{|\mathbf{E}_a(r\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a)|^2}. \tag{29}$$

The monostatic RCS is the special case with $\hat{\boldsymbol{\kappa}} = \hat{\boldsymbol{\kappa}}_a$. The RCS is often computed in decibels (dB) by the relation $\sigma_{dB}(\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a) = 10 \log_{10} \sigma(\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a)$. For large r, $\mathbf{E}_s$ is well approximated by the far field pattern $\boldsymbol{\Phi}$

$$\begin{aligned} \mathbf{E}_s(r\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a) &\approx r^{-1} \exp(\iota\kappa r)\boldsymbol{\Phi}(\hat{\boldsymbol{\kappa}}, \mathbf{J}) \\ &= r^{-1} \exp(\iota\kappa r)\hat{\boldsymbol{\kappa}} \times (\textstyle\int_\Gamma \exp(-\iota\hat{\boldsymbol{\kappa}} \cdot \mathbf{x}')\mathbf{J}(\mathbf{x}')d\Gamma \times \hat{\boldsymbol{\kappa}}), \end{aligned} \tag{30}$$

and consequently,

$$\sigma(\hat{\boldsymbol{\kappa}}, \hat{\boldsymbol{\kappa}}_a) = 4\pi |\boldsymbol{\Phi}(\hat{\boldsymbol{\kappa}}, \mathbf{J})|^2 / |\mathbf{E}_0|^2.$$

The current $\mathbf{J}$ is the solution of (23) and depends on $\hat{\boldsymbol{\kappa}}_a$.

It follows from (30) that $\boldsymbol{\Phi}$ can be written as in (12) with $S = 2$, because the far field has no radial component, and $\mathbf{x}_i$ is the solution of the discretized integral equation. This is the case when the RCS is computed at one position $r\hat{\boldsymbol{\kappa}}$ for many incidence fields $\hat{\boldsymbol{\kappa}}_a$. If the number of different $\hat{\boldsymbol{\kappa}}_a$ is M, then with the dual approach (12)-(14) only two systems of equations have to be solved compared to solution of M systems for $\mathbf{J}$ in the usual strategy. For EFIE $\mathbf{A}^T = \mathbf{A}$ and the dual equation can be solved with the same FMM solver as the primal equation.

If the wavenumber κ in (23) is not constant then we have the situation in (15) when both the matrix and the right hand side depend on a parameter.

5 Numerical experiments

To illustrate some characteristics of the method we perform a few numerical experiments with Maxwell's equations in integral form (23). The aim of the experiments is to find out what kind of performance that can be expected for realistic objects and different parameters in the method.

In the first experiment, we consider scattering from a small airplane model called RUND, see Fig. 2. The equations are solved by GMRES iteration [14], [15]. The matrix-vector products in the Krylov method are computed by an implementation of FMM [5], [11]. The size of the model is $0.8 \times 0.8 \times 0.2$ m. Let ϕ be defined in the wing plane with $\phi = 90^o$ at the nose.

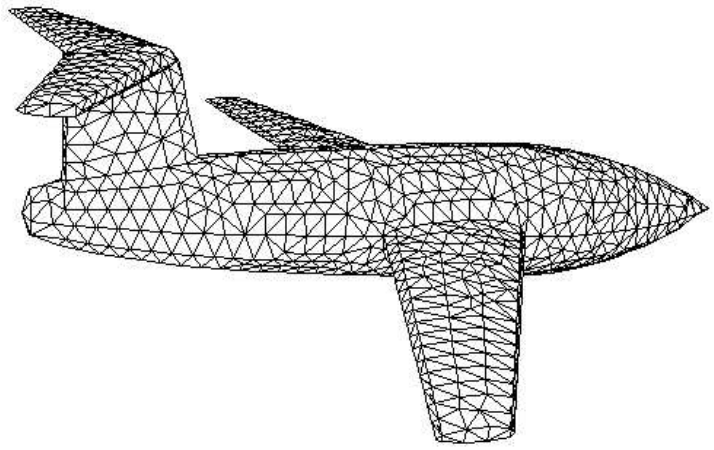

Figure 2: The trianglated RUND model with about 4000 edges.

In Fig. 3 the method is validated by comparing the monostatic RCS σ_{dB} for RUND at 6 GHz corresponding to $\kappa = 40\pi$. Our method (FMM–MRI) using CFIE and $\alpha = 0.5$ is compared with with measurements from FOI, The Swedish Defence Research Agency, a time-domain hybrid method (FD–FE) [6], and a straightforward MoM method using EFIE. The fine surface grid has approximately 65000 edges yielding an edge length of about 5 mm or ten points per wavelength. The termination criteria are $\varepsilon = \varepsilon_I = 10^{-3}$. The difference between our method and the MoM solution is plotted. The difference is mainly due to the different integral equations CFIE and EFIE.

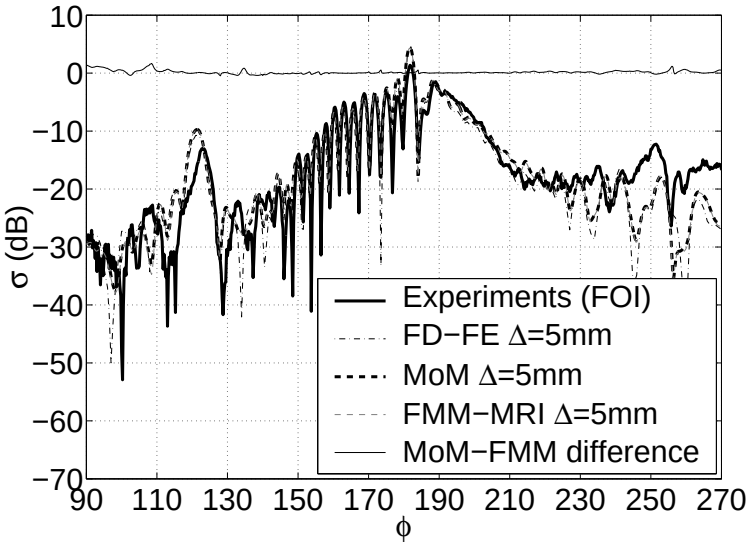

Figure 3: Comparison between different monostatic RCS solutions obtained for RUND at 6 GHz.

In Fig. 4 the method is verified by computing the monostatic RCS for RUND

at 1.5 GHz with $\Delta\phi = 0.4^o$ and two different grids. One grid is composed of about 16000 edges as in Fig. 2 and the other grid is same as in the previous experiment. The termination criteria are as above. The symmetry of the airplane explains the symmetric result around the nose at $\phi = 90^o$. The solution is almost grid independent.

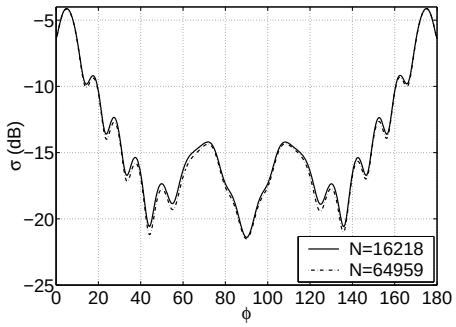

Figure 4: The monostatic RCS for RUND at 1.5 GHz.

The monostatic RCS is computed at $\phi = 45^o$ on the port side using interpolation with p vectors separated by $\Delta\phi$ and centered around $\phi = 45^o$. The polarization of the incoming plane wave is such that $E_\theta = 1$ and $E_\phi = 0$ in (25). The purpose of these experiments is to validate the convergence theory from the previous sections. The convergence rate of the relative residual $\|\mathbf{r}^{(0)}\|/\|\mathbf{b}\|$ is shown to the left in Fig. 5 for different $\Delta\phi$. We choose $\varepsilon_I = 10^{-9}$ small enough so that $\mathbf{r}^{(0)}$ is unaffected by that part. To the right in Fig. 5, the quotient between two different $\mathbf{r}^{(0)}$ is computed with $2\Delta\phi$ and $\Delta\phi$. The expected asymptotic behavior of $\|\mathbf{r}^{(0)}(2\Delta\phi)\|/\|\mathbf{r}^{(0)}(\Delta\phi)\|$ when $\Delta\phi \to 0$ is 2^p, see Theorem 4. The real convergence rate is even slightly higher than the predicted one, once $\Delta\phi$ is small enough.

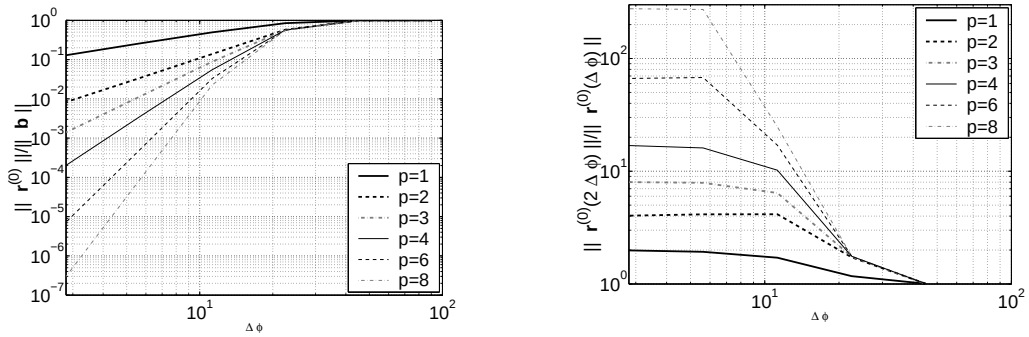

Figure 5: The relative residual (left) and the quotient $\|\mathbf{r}^{(0)}\,(2\Delta\phi)\,\|/\|\mathbf{r}^{(0)}\,(\Delta\phi)\,\|$ (right) as a function of $\Delta\phi$ for different numbers of interpolating vectors .

To the left in Fig. 6 we examine the number of iterations required to reach convergence for different p and $\Delta\phi$ when $\varepsilon = \varepsilon_I = 10^{-3}$. To the right in Fig. 6,

$\Delta\phi = 5.6^o, \varepsilon_I = 10^{-5}$, and the objective is to compare the convergence rate θ in (19) of the iterative solver and a single right hand side for different interpolations in the initial guess. The results indicate that the rate is insensitive to p and it is almost constant, which is one of the assumptions in the theorems in the previous section.

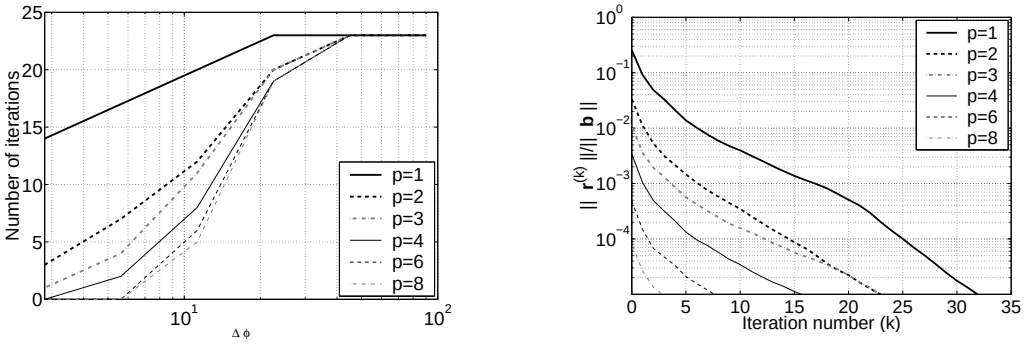

Figure 6: The number of iterations required for convergence with different $\Delta\phi$ (left). The convergence history of the GMRES-solver for different numbers of interpolation vectors (right).

The monostatic RCS in Fig. 4 is computed with $k = 1$ in Algorithm 1. The number of vectors p in the interpolation is displayed to the left in Fig. 7 for different values of ϕ. The order in which the solutions are computed is shown by combining two consecutive data points with a solid line for the coarse grid and a dashed line for the fine grid. They overlap each other in the left panel of Fig. 7. As soon as a new solution $\mathbf{x}_i$ is computed the corresponding $\mathbf{s}_i$ is added to the basis $\mathbf{S}$. At most 32 right hand sides were used in the interpolation.

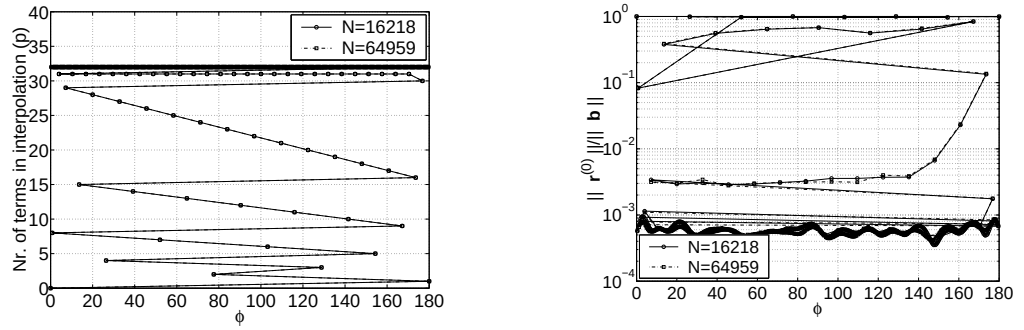

Figure 7: Number of vectors used for interpolation in MRI (left). The relative residual of the initial guess from MRI (right).

The right plot in Fig. 7 shows the relative residual $\|\mathbf{r}^{(0)}\|/\|\mathbf{b}\|$ of the initial guess. After 58 of 451 right hand sides the interpolated initial guess is so accurate that no more iterations are necessary. The difference between the fine and the

coarse grid is small as is expected from Theorem 4 where the error estimate is independent of N.

The number of iterations to obtain convergence is recorded to the left in Fig. 8 for the coarse and the fine grids. Most of the right hand sides do not need any iterations at all. For the smaller case a total of 403 iterations was required while the larger case required 422 iterations. On the other hand, from Fig. 4 it is evident that a sampling density $\Delta\phi$ of approximately 1^o is sufficient to represent the monostatic RCS. Hence, about $420/180 \approx 2.3$ iterations per important right hand side suffice. Adding more right hand sides only incurs a cost for the interpolation (cf. Theorem 1).

To the right in Fig. 8 we compare the total solution time T_k for all right hand sides for different step sizes k in Algorithm 1. The order of interpolation p increases with k up to 32. The solution times are normalized by the time T_1 for solving one right hand side at a time. The solution of one right hand side ($k = 1$) without an interpolated initial guess with a standard algorithm was 5.3 % of the total time. The relative time for this method would be $451 \cdot 5.3\,\% \approx 2390\,\%$ in Fig. 8. The total time T_{Ik} used by the interpolation part of the method is compared to the total solution time T_k for a given step size k. The fraction is 4 % of T_k or less for $k \geq 4$. Thus, the solution of 420 right hand sides was obtained in less than the same time as the solution of 1 right hand side with a standard method. Also note that if ε and ε_I are reduced the cost for the iterations is increased while the interpolation cost is constant (cf. Theorem 1). When the step size is greater than 32 there is an increase in solution time because it is more favorable to interpolate instead of iterate for the remaining solutions.

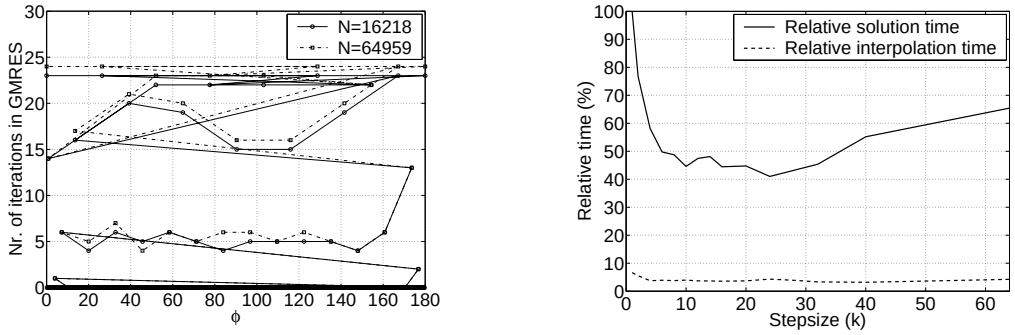

Figure 8: Number of iterations in GMRES for each right hand side (left) and the relative solution times T_k/T_1 and T_{Ik}/T_k for different step sizes k (right).

6 Conclusions

A method has been developed for iterative solution of systems of linear equations with many right hand sides with a smooth dependence of a parameter. The work in the iterations is bounded independently of the number of right hand sides

and the initial guess for the iterations is rapidly becoming so accurate that this guess is a satisfactory solution. The method is applied to a discretization of the integral equation satisfied by Maxwell's equation in the frequency domain. The theoretical properties of the method are corroborated by numerical calculations of the monostatic radar cross section of an airplane model.

References

[1] Richard Barrett, Michael Berry, Tony F. Chan, James Demmel, June Donato, Jack Dongarra, Victor Eijkhout, Roldan Pozo, Charles Romine, and Henk van der Vorst. *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*. SIAM, Society for Industrial and Applied Mathematics, Philadelphia, 1993.

[2] Åke Björck. *Numerical Methods for Least Squares Problems*. SIAM, Society for Industrial and Applied Mathematics, Philadelphia, 1996.

[3] E. W. Cheney. *Introduction to Approximation Theory*. McGraw-Hill, New York, p. 60, 1966.

[4] Weng Cho Chew, Jian-Ming Jin, Eric Michielssen, and Jiming Song. *Fast and Efficient Algorithms in Computational Electromagnetics*. Artech House, Inc., Norwood, 2001.

[5] Ronald Coifman, Vladimir Rokhlin, and Stephen Wandzura. The fast multipole method for the wave equation: A pedestrian prescription. *IEEE Trans. Antennas Prop.*, 35(3):7–12, June 1993.

[6] Fredrik Edelvik and Gunnar Ledfelt. A comparison of time-domain hybrid solvers for complex scattering problems. *Int. J. Numer. Modeling*, 15:475–487, 2002.

[7] Roland W. Freund and Manish Malhotra. A block–QMR algorithm for non–Hermitian linear systems with multiple right–hand sides. *Lin. Alg. Appl.*, 254:119–157, 1997.

[8] Anne Greenbaum. *Iterative Methods for Solving Linear Systems*. SIAM, Society for Industrial and Applied Mathematics, Philadelphia, 1997.

[9] Leslie Greengard and Vladimir Rokhlin. A new version of the fast multipole method for the Laplace equation in three dimensions. *Acta Numerica*, pages 229–269, 1997.

[10] Martin Nilsson. A fast multipole accelerated block quasi minimum residual method for solving scattering from perfectly conducting bodies. In *Proceedings of Antennas and Propagation Society International Symposium*, volume 4, pages 1848–1851, Salt Lake City, Utah, USA, July 2000.

[11] Martin Nilsson. *Iterative solution of Maxwell's equations in frequency domain.* Licentiate thesis No. 2002-004, Department of Information Technology, Uppsala University, May 2002. Available at: http://www.it.uu.se/research/reports/lic/2002-004/.

[12] Andrew F. Peterson, Scott L. Ray, and Raj Mittra. *Computational Methods for Electromagnetics.* IEEE Press and Oxford University Press, New York, Oxford, Tokyo, Melbourne, 1998.

[13] S. M. Rao, D. R. Wilton, and A. W. Glisson. Electromagnetic scattering by surfaces of arbitrary shape. *IEEE Trans. Antennas Prop.*, 30(3):409–418, May 1982.

[14] Youcef Saad and Martin H. Schultz. GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems. *SIAM J. Sci. Comput.*, 7:856–869, 1986.

[15] Yousef Saad. *Iterative Methods for Sparse Linear Systems.* PWS publishing, New York, 1996.

[16] V. Simoncini and E. Gallopoulos. An iterative method for nonsymmetric systems with multiple right-hand sides. *SIAM J. Sci. Comput.*, 16:917–933, 1995.