

Arnoldi model order reduction for electromagnetic wave scattering computation

P. Bradley* C. Brennan M. Condon

Abstract — This paper presents a model order reduction (MOR) algorithm for the volume integral equation formulation of electromagnetic wave scattering. We apply the Arnoldi algorithm to circumvent the computational complexity associated with the numerical solution of such formulations. An approximate extension of the Arnoldi algorithm to the problem of wave scattering from an inhomogeneous body is introduced and implemented. Numerical examples are presented to demonstrate the accuracy of our approximate extension.

1 INTRODUCTION

Inverse scattering problems involve the determination of the shape, location and constitutive parameters of an object from measurements of the scattered wave field generated by the illumination of an object by an incident wave field. An iterative solution to the inverse problem for high contrast cases can require the solution of multiple forward problems where the shape and location of the object is known. However, due to the inherent high computational cost of full-wave simulation for scattering from large structures possessing high contrast, a variety of approaches have been developed, which use various approximations to allow rapid simulations [1]. The primary difficulty of full-wave methods, such as integral equation based solvers, is the computational complexity of dense matrix manipulations. These require the use of iterative solver techniques such as the Conjugate Gradient method (CG) which requires $\mathcal{O}(n^2)$ operations per iteration, where n is the number of basis functions used to discretise the problem. This computational cost becomes increasingly problematic when one must solve for a range of source locations, frequencies and contrasts. Accelerated techniques such as the Conjugate Gradient Fast Fourier Transform (CG-FFT) and the Fast Multipole Method (FMM) methods are capable of reducing the cost of a matrix vector multiplication to $\mathcal{O}(n \log_2 n)$ and $\mathcal{O}(n)$ operations, respectively.

An alternative approach is to develop a reduced order model which approximates the behavior of the original system. In this paper, we apply a MOR

technique to the problem of efficiently performing scattering computations over a wide range of contrasts. In orthogonalised Krylov subspace model reduction approaches, such as the Arnoldi algorithm, a reduced order matrix model is constructed from a set of vectors that span the Krylov subspace. By imposing an orthogonality relation among the vectors, linear independence can be maintained and hence high order approximations can be constructed [2]. This circumvents the numerical instability associated with MOR algorithms based on explicit moment matching techniques, such as the Asymptotic Waveform Evaluation (AWE) [2]. Recently, the Arnoldi algorithm has been presented as a means of speeding up solutions of problems involving scattering from a homogeneous body over a range of contrasts [3, 4]. The primary contribution of this work is the approximate extension of the Arnoldi algorithm to scattering from inhomogeneous bodies.

2 CONFIGURATION

The Volume Electric Field Integral Equation (VE-FIE) formulation is commonly applied to the problem of wave scattering from inhomogeneous objects. The work presented in this paper examines a 2-D TM^z time-harmonic configuration which is invariant in the z -direction. The scattering body is characterized by its permittivity $\epsilon(\mathbf{r})$, conductivity σ and permeability μ . An expression for the total wave-field can be generated in terms of a convolution between the total wave-field and a suitable Greens function [1]. We assume that the problem is discretised using the method of moments with suitable basis functions. The object is illuminated by a line source \mathbf{x} and the scattered field \mathbf{e} can be expressed as [3]:

$$\mathbf{e} = (\mathbf{I} + \mathbf{GA})^{-1} \mathbf{x} \quad (1)$$

where \mathbf{I} is a $n \times n$ identity matrix and \mathbf{G} is a $n \times n$ matrix containing coupling information between the basis functions. \mathbf{A} is a $n \times n$ diagonal matrix whose diagonal elements contain the contrast:

$$\zeta = \frac{\epsilon(\mathbf{r}')}{\epsilon_b} - 1 \quad (2)$$

*RF modelling and simulation group, Research Institute for Networks and Communications Engineering (RINCE), School of Electronic Engineering, Dublin City University, Ireland, e-mail: bradley@eeng.dcu.ie, tel.: +353 1 7005856, fax: +353 1 7005508.

at each point. Equation 1 can be solved for \mathbf{e} to determine the fields $E_z^{sc}(\mathbf{r})$ throughout the scatterer.

3 THE ARNOLDI ITERATION

The Arnoldi algorithm outlined in Table 1 builds an orthogonal basis for the Krylov subspace \mathcal{K}_k :

$$\mathcal{K}_k(\mathbf{G}, \mathbf{q}) = \text{span} [\mathbf{q} \mathbf{G} \mathbf{q} \mathbf{G}^2 \mathbf{q} \dots \mathbf{G}^{k-1} \mathbf{q}]. \quad (3)$$

Generation of the Krylov sequence of vectors \mathbf{q}_k employs a modified Gram-Schmidt with re-orthogonalisation (MGSR) process [3, 5]. The vectors \mathbf{q}_k are mutually orthonormal and have the property that the generated \mathbf{Q} matrix:

$$\mathbf{Q}_k = [\mathbf{q}_1 \mathbf{q}_2 \dots \mathbf{q}_k] \quad (4)$$

spans the Krylov subspace \mathcal{K}_k . We can compute as many leading columns of \mathbf{Q}_k as are needed to obtain an accurate solution. After k iterations, we have the following summarising equation [3, 5]:

$$\mathbf{G} \mathbf{Q}_k = \mathbf{Q}_k \mathbf{H}_k + h_{k+1,k} \mathbf{q}_{k+1} \mathbf{e}_k^T \quad (5)$$

where \mathbf{e}_k is the k^{th} column of the $k \times k$ identity matrix \mathbf{I}_k , $h_{k+1,k}$ is the $(k+1, k)$ entry of the Hessenberg matrix \mathbf{H}_k . The vector $h_{k+1,k} \mathbf{q}_{k+1}$ is the Arnoldi residual \mathbf{f}_k of the k -step Arnoldi factorisation and is orthogonal to the columns of \mathbf{Q}_k . Using the identity $\mathbf{Q}_k^H \mathbf{Q}_k = \mathbf{I}_k$ and the fact that $\mathbf{Q}_k \mathbf{q}_{k+1} = 0$, an expression for \mathbf{H}_k can be derived:

$$\mathbf{H}_k = \mathbf{Q}_k^H \mathbf{G} \mathbf{Q}_k \quad (6)$$

where \mathbf{H}_k is an upper Hessenberg matrix of order k . It can be shown that \mathbf{H}_k is the orthogonal projection of \mathbf{G} onto a k -dimensional subspace, whose leading eigenvalues are approximations to those of \mathbf{G} [3, 5]. The modified Gram-Schmidt procedure present in Table 1 orthonormalises each vector sequentially by computing the orthogonal projection of \mathbf{w}_j onto, $\text{span}\{\mathbf{q}_1 \mathbf{q}_2 \dots \mathbf{q}_j\}$. This projection is subtracted from the original vector and the result is normalised to obtain \mathbf{q}_{j+1} . This is by construction orthogonal to all previously computed Arnoldi vectors $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_j$ with unit norm [3, 5].

4 MOR FOR SCATTERING FROM AN INHOMOGENEOUS BODY

The MOR technique outlined in [4, 3] is applied to wave scattering from homogeneous bodies. This section extends the MOR technique to the case of scattering from inhomogeneous bodies. Solution of the scattering problem over a range of contrasts therefore necessitates the ability to compute the quantity:

$$\mathbf{e} = (\mathbf{I} + \mathbf{G} \mathbf{A})^{-1} \mathbf{x}. \quad (7)$$

Input: Matrix \mathbf{G} , number of steps k , initial vector $\mathbf{q}_1 = \mathbf{x}/\|\mathbf{x}\|_2$ and orthogonalisation parameter $\eta = 1/\sqrt{2}$,

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For  $j = 1, \dots, k$ 
   $\mathbf{w}_j = \mathbf{G} \mathbf{q}_j$ 
   $\beta_j = \|\mathbf{w}_j\|_2$ 
  For  $i = 1, \dots, j$ 
     $\alpha_{i,j} = \mathbf{q}_i^H \mathbf{w}_j$ 
     $\mathbf{w}_j = \mathbf{w}_j - \mathbf{q}_i \alpha_{i,j}$ 
  End  $i$ 
  If  $\|\mathbf{w}_j\|_2 < \eta * \beta_j$ 
    For  $i = 1, \dots, j$ 
       $h_{i,j} = \mathbf{q}_i^T \mathbf{w}_j$ 
       $\mathbf{w}_j = \mathbf{w}_j - \mathbf{q}_i h_{i,j}$ 
    End  $i$ 
     $h_{j,j} = h_{j,j} + \alpha_{j,j}$ 
  EndIf
   $h_{j+1,j} = \|\mathbf{w}_j\|_2$ 
  If  $h_{j+1,j} = 0$  Quit
   $\mathbf{q}_{j+1} = \mathbf{w}_j / h_{j+1,j}$ 
End  $j$ .
 $\mathbf{H} = h(1 : k, :)$ 

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Table 1: Arnoldi - modified Gram-Schmidt algorithm with re-orthogonalisation (MGSR).

After k steps of the Arnoldi algorithm an approximation \mathbf{u}_k , to \mathbf{e} , can be made in terms of the k orthonormal vectors generated by the Arnoldi algorithm for a range of \mathbf{A} , specifically [3]:

$$\mathbf{u}_k = \alpha_1 \mathbf{q}_1 + \alpha_2 \mathbf{q}_2 + \dots \alpha_k \mathbf{q}_k = \mathbf{Q}_k \mathbf{a}_k \quad (8)$$

where $\mathbf{a}_k = [\alpha_1 \alpha_2 \dots \alpha_k]^T$ is a vector of expansion coefficients. The residual \mathbf{r}_k that corresponds to this approximation is introduced as:

$$\mathbf{r}_k = \mathbf{x} - (\mathbf{I} + \mathbf{G} \mathbf{A}) \mathbf{u}_k. \quad (9)$$

The reduced order model chooses a starting vector \mathbf{q}_1 and an expansion vector \mathbf{a}_k , to ensure this residual has components in the Krylov space \mathcal{K}_{k+1} , by making all β_i vanish except for β_{k+1} , where β is defined in Equation 13. Specifically we note:

$$\mathbf{r}_k = \mathbf{x} - \mathbf{Q}_k \mathbf{a}_k - \mathbf{G} \mathbf{A} \mathbf{Q}_k \mathbf{a}_k \quad (10)$$

$$\approx \mathbf{x} - \mathbf{Q}_k \mathbf{a}_k - \mathbf{G} \mathbf{Q}_k \tilde{\mathbf{A}} \mathbf{a}_k \quad (11)$$

$$\approx \mathbf{x} - \mathbf{Q}_k \mathbf{a}_k - \mathbf{Q}_k \mathbf{H}_k \tilde{\mathbf{A}} \mathbf{a}_k - h_{k+1,k} \mathbf{q}_{k+1} \mathbf{e}_k^T \tilde{\mathbf{A}} \mathbf{a}_k \quad (12)$$

where $\tilde{\mathbf{A}} = \mathbf{Q}_k^H \mathbf{A} \mathbf{Q}_k$. Choosing the first Arnoldi vector to be $\mathbf{q}_1 = \|\mathbf{x}\|^{-1} \mathbf{x}$ yields:

$$\mathbf{r}_k \approx \mathbf{Q}_k \left(\|\mathbf{x}\|_2 \mathbf{e}_1 - (\mathbf{I}_k + \mathbf{H}_k \tilde{\mathbf{A}}) \mathbf{a}_k \right) - h_{k+1,k} \mathbf{q}_{k+1} \mathbf{e}_k^T \tilde{\mathbf{A}} \mathbf{a}_k \approx \mathbf{Q}_k \beta_k - \beta_{k+1} \mathbf{q}_{k+1}. \quad (13)$$

We set

$$\mathbf{a}_k = \|\mathbf{x}\|_2 \left(\mathbf{I}_k + \mathbf{H}_k \tilde{\mathbf{A}} \right)^{-1} \mathbf{e}_1 \quad (14)$$

then the residual becomes $\mathbf{r}_k = -\beta_{k+1} \mathbf{q}_{k+1}$ as required with $\mathbf{r}_k \in \mathcal{K}_{k+1}$. The reduced order model for \mathbf{u}_k is thus:

$$\mathbf{u}_k = \|\mathbf{x}\|_2 \mathbf{Q}_k \left(\mathbf{I}_k + \mathbf{H}_k \tilde{\mathbf{A}} \right)^{-1} \mathbf{e}_1. \quad (15)$$

Substituting this into Equation 1 yields the reduced order model for the total field:

$$\tilde{\mathbf{e}} = \mathbf{Q}_k \|\mathbf{x}\|_2 \left(\mathbf{I}_k + \mathbf{H}_k \tilde{\mathbf{A}} \right)^{-1} \mathbf{e}_1. \quad (16)$$

It should be noted that Equation 11 is exact only if the range $\mathcal{R}(\mathbf{Q}_k)$ of \mathbf{Q}_k is an invariant subspace of \mathbf{A} . However, due to the independence of the columns of \mathbf{Q}_k imposed by the re-orthogonalisation process, Equation 11 can be shown to be a valid approximation. As prescribed in [6], if the columns of \mathbf{Q}_k are independent and the norm of the residual matrix:

$$\mathbf{R} = \mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S} \quad (17)$$

has been minimised for some \mathbf{S} , then the columns of \mathbf{Q}_k define an approximate invariant subspace of \mathbf{A} . The selection of $\mathbf{S} = \mathbf{Q}_k^T \mathbf{A} \mathbf{Q}_k = \tilde{\mathbf{A}}$ results in the Frobenius norm of the residual being minimised:

$$\min \|\mathbf{A}\mathbf{Q}_k - \mathbf{Q}_k\mathbf{S}\|_F = \|(\mathbf{I} - \mathbf{Q}_k \mathbf{Q}_k^H) \mathbf{A} \mathbf{Q}_k\|_F. \quad (18)$$

As such Equation 11 becomes an valid approximation with the property, that as $k \rightarrow n$, we procure a better approximation. This is validated numerically in the results section. Note when $k = n$, Equation 11 is an exact approximation as:

$$\mathbf{Q}^H \mathbf{Q} = \mathbf{Q} \mathbf{Q}^H = \mathbf{I}. \quad (19)$$

As a corollary of creating the Krylov subspace \mathcal{K}_k in terms of \mathbf{G} instead of $\mathbf{G}\mathbf{A}$, Equation 16 can be used to solve any inhomogeneous domain with the same dimension and discretisation. It should be noted that Equation 16 is posed for an explicit source location and as such would require the generation of a new Krylov vector \mathbf{Q}_k for any deviation of source location. This procedure results in an efficient solution which requires $\mathcal{O}(4n^2k)$ flops to generate the initial Krylov matrix \mathbf{Q}_k and once stored can be applied to any inhomogeneous domain with the same configuration [5]. All subsequent solutions for domains with different contrast configuration require only the formation of a new $\tilde{\mathbf{A}}$. It can be shown that an additional worst case scenario of $\mathcal{O}(k^2n)$ flops is required to form $\tilde{\mathbf{A}} = \mathbf{Q}_k^H \mathbf{A} \mathbf{Q}_k$, where \mathbf{A}

is a $n \times n$ diagonal matrix and \mathbf{Q}_k is a $n \times k$ matrix. This computational cost can be shown to be significantly reduced to $\mathcal{O}(k^2m)$, for $m \ll k$, for scenarios whereby we restrict our analysis to objects where we assume the shape of the object is known *a priori* and only the contrast is varying in a weakly inhomogeneous body. The resultant matrix equation can be solved using any iterative solver requiring the inversion of a matrix of order $k \ll n$. The main drawback of this approach is the initial computational cost to generate the Krylov matrix \mathbf{Q}_k , but once generated and stored, it can be applied to any scattering problems as outlined above.

5 RESULTS

In the first example, an inhomogeneous circular cylinder composed of four concentric regions centred at the origin with radii $r_1 = 2\lambda$, $r_2 = 1.5\lambda$, $r_3 = \lambda$ and $r_4 = \lambda/2$. The cylinder is illuminated by waves emanating from a line source located at $(-10, 0)$, radiating at a frequency of $f = 300$ MHz and assumed to be embedded in free space. The cylinder was discretised using $n = 2000$ cells and the mono-static backscattered field E_z^{sc} was computed over a range of contrast values $\zeta_4 = 0 : 6$ while keeping $\zeta_3 = 3$, $\zeta_2 = 4$, $\zeta_1 = 5$ constant exactly and using the MOR techniques described in this paper. The bi-static field was also computed for a fixed value of contrast and for a varying observation angle $\phi = 0 : 360$. Figures 1 and 2 shows the results obtained in comparing the MGSAR Arnoldi algorithm against the exact solution for varying k values. In both cases, the MGSAR procedure shows a 90% reduction in n for both the mono-static and bi-static setup, incurring an approximate relative error of 0.7% and 1% respectively for the calculated scattered field. Figure 3 substantiates the argument for the approximation of Equation 11, clearly showing that this approximation converges to working precision linearly as k increases with a 0.6% relative error for a 90% reduction. The second example used a completely inhomogeneous domain where the contrast $\zeta_n = 0 : 6$, is chosen randomly for each basis domain. As seen in Figure 4, the MGSAR Arnoldi expansion closely matches the exact results, executing a 87.5% reduction in n with a 10% relative error in the scattered field.

6 CONCLUSION

The contribution of this paper is to extend the use of the Arnoldi MOR algorithm to inhomogeneous structures using the volume electric field integral

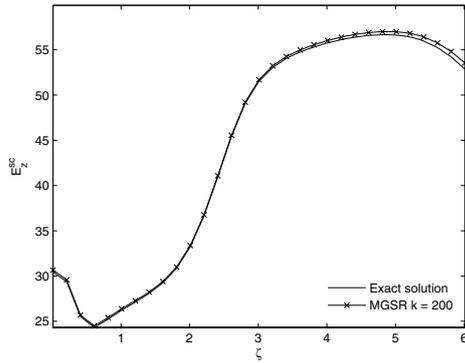


Figure 1: E_z^{sc} magnitude for mono-static scattering over range of contrast $\zeta_4 = 0 : 6, \zeta_3, \zeta_2, \zeta_1 =$ constant.

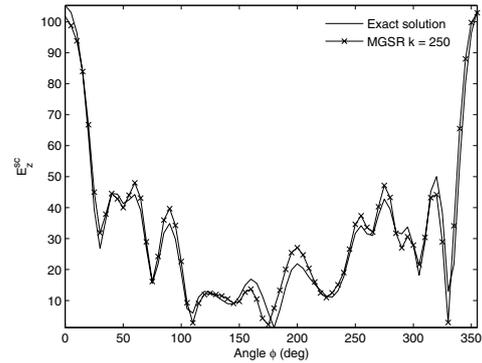


Figure 4: E_z^{sc} magnitude for bi-static scattering over range of angle $\phi = 0:360$, completely inhomogeneous domain for $\zeta_n = 0 : 6$.

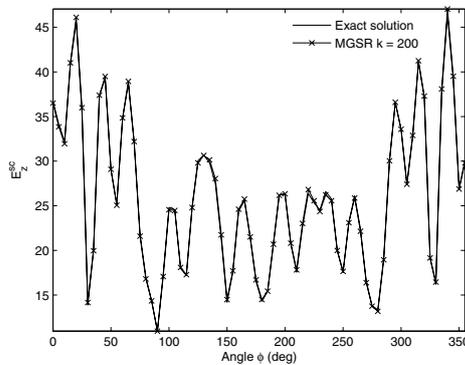


Figure 2: E_z^{sc} magnitude for bi-static scattering over range of angle $\phi = 0:360, \zeta_4 = 1, \zeta_3 = 3, \zeta_2 = 4, \zeta_1 = 5$.

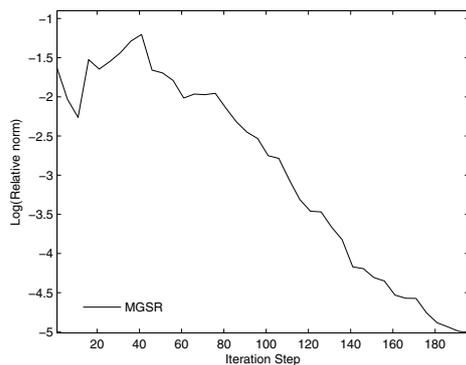


Figure 3: Equation 11 r_k approximation.

equation formulation. Through implicitly matching the moments of the original system we are able to obtain a reduced model without the need to directly calculate the moments. Hence, we do not suffer

from the same numerical ill-conditioning that is associated with direct moment matching algorithms. Notably, we have demonstrated that a significant reduction in system size can be achieved for an inhomogeneous structure while still resulting in an accurate approximation over a wide contrast range. The computational expense for any subsequent simulation with an alternative contrast distribution is reduced to the formation of a revised $\tilde{\mathbf{A}}$ and the inversion of a matrix of order $k \ll n$.

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