Efficient computation of electromagnetic wave scattering for inhomogeneous bodies using a model order reduction approach

P. Bradley  C. Brennan  M. Condon

RF Modelling and Simulation Group, Research Institute for Networks and Communications Engineering (RINCE), School of Electronic Engineering, Dublin City University, Dublin, Ireland
E-mail: bradleyp@eeng.dcu.ie; bradleypatrickj@gmail.com

Abstract: This study presents a model order reduction algorithm for the volume integral equation formulation of electromagnetic wave scattering. The authors apply the Arnoldi algorithm to circumvent the computational complexity associated with the repeated solution of the forward electromagnetic scattering problem for varying material parameters. The authors discuss practical implementation issues regarding procedures for the implementation and termination of the Arnoldi iteration. An approximate extension of the Arnoldi algorithm to the problem of wave scattering from an inhomogeneous body is introduced and implemented. This approximation is shown to be exact in the limit as the level of reduction approaches zero. Numerical examples are presented which demonstrate the accuracy and efficiency of their approximate extension.

1 Introduction

In many applications ranging from medical imaging [1, 2] to geoscience exploration [3, 4], integral equation formulations are used for the analysis of electromagnetic scattering from bodies of both arbitrary shape and inhomogeneity. These problems can require the repeated solution of the forward electromagnetic scattering problems for varying material properties, where the approximate shape and location of the objects are known. The relevant integral equation is typically solved using the method of moments and results in a series of dense linear equations. The repeated solution of full-scattering problems for the total fields at each step in material property is inherently computationally prohibitive. Developments in iterative computational techniques which incorporate fast algorithms can alleviate these problems. The most widely used approaches to solve the integral equations are the Conjugate Gradient Fast Fourier Transform [5], wavelet transform techniques [6] and the Fast Multipole Method [7, 8] methods. These are capable of reducing the cost of a matrix vector multiplication from $O(m^2)$ to $O(m \log_2 m)$ to, $O(m)$ and $O(m)$ operations, respectively, where $m$ is the number of basis functions.

An alternative approach is to develop approximate solutions to expedite the solution of electromagnetic (EM) scattering problems. Several approximations of the integral equation formulation are discussed in literature, including the Born approximations [9, 10] and the family of model order reduction techniques [7, 11]. It has been well documented that the Born approximation can efficiently simulate the EM response of dielectric problems. However, these techniques are restricted to problems of relatively low frequencies and low contrast [9, 10].

Algorithms based on model order reduction have, to date, been typically applied to the problem of solving scattering or circuit problems over a wide frequency range [12, 13]. These techniques produce a reduced-order model which approximates the behaviour of the original system. The use of Krylov subspace techniques is widely accepted as being the most flexible and computationally efficient approach to model order reduction (MOR) and has been widely used in various formulations and applications. Since the essential features of the original system are captured at the early stage of the iteration, Krylov subspace algorithms can produce very accurate low-order models.

The Lanczos [14, 15] and Arnoldi [15, 16] algorithms are the most popular variants of the Krylov subspace approaches to model reduction. A set of vectors that span the Krylov subspace are used to construct the reduced-order matrix model. By imposing an orthogonality relation among the vectors, linear independence can be maintained (note that owing to finite precision, computation loss of orthogonality between the computed vectors can occur [14, 15, 17]) and so high-order approximations can be constructed.

In this paper, we apply the Arnoldi model order reduction techniques to the problem of efficiently performing scattering computations over a wide range of contrast. Contrast-sweep problems are associated with scattering analysis where the material properties such as the permittivity, permeability and conductivity are varied over a range to produce the scattered fields. Recently published work [16, 18] circumvented this particular computational problem by...
using Krylov subspace methods to produce a ROM for a homogeneous structure. The concept is to use the Arnoldi algorithm to build a Krylov subspace that is independent of the contrast term. In doing so, the same Krylov subspace can be used for different contrast terms. A reduced-order model is then constructed, where the dimension is dependent on the number of iterations of the Arnoldi algorithm. The main computational effort associated with computing solutions for another contrast profile consists of solving a much-reduced-order matrix.

In this work, an approximate extension that accounts for wave scattering from an inhomogeneous object using a two-dimensional volume integral formulation is presented. This approximation is the central contribution of this paper, which is shown to be exact in the limit as the level of reduction approaches zero. In our analysis, the shape of the object is known a priori. For inhomogeneous structures, this requires the shape of the homogenities embedded in the domain of the scatterer to be fixed. As such, the method outlined in this text can be applied to scatterers having a not-connected support. For scattering problems where multiple approximate solutions for varying contrast with fixed-source location are required, it will be shown that significant computational saving can be achieved as compared to accelerated solver techniques.

This paper is organised as follows. In Section 2, the volume integral equation formulation is discussed. In Section 3, the basic Arnoldi algorithm is reviewed. The approximate extension of the Arnoldi algorithm to wave scattering from an inhomogeneous object is introduced in Section 4. Computational issues associated with the Arnoldi algorithm are also outlined in this section. Numerical results are presented in Section 5. Some concluding remarks and observations are offered in Section 6.

2 Volume electric field integral equation formulation

The volume electric field integral equation (EFIE) formulation is commonly applied to the problem of wave scattering from inhomogeneous objects. The work presented in this paper examines a 2D transverse magnetic (TM) configuration, where scattering structures and fields are assumed invariant in the z-direction. The scattering body is characterised by its permittivity $\varepsilon(r)$, conductivity (For this work we consider just changes in permittivity. The ideas are easily applicable to problems involving contrast in permeability and conductivity.) $\sigma$ and permeability $\mu$. A time dependence of $\exp(\mathbf{i} \omega t)$ is assumed and suppressed in what follows. The object is illuminated by a line source and the scattered field $E_z^s(r)$ can be expressed in terms of the following EFIE [19, 20]

$$E_z^s(r) = E_z(r) - E_z^{inc}(r)$$

$$= \frac{1}{\pi} \int V \int H_z^0(k_0|r-r'|)O(r')E_z(r') \, \mathrm{d}V$$

(1)

where $O(r')$ is the object function at point $r'$ given by

$$O(r') = k_0^2(r') - k_0^2$$

(2)

The background wave number is given by $k_0$, while $k(r')$ is the wave number at a point in the scatterer. $H_z^0$ is the zero-order Hankel function of the second kind. $E_z$ is the total electric field strength.

Using $m$ pulse basis functions and Dirac-Delta testing functions [19, 20], (1) can be discretised by employing the method of moments. Taking due care to the treatment of the singularity associated with the Hankel function leads to the following matrix equation

$$(I + GA)x = b$$

(3)

where $b$ is the incident field vector at the centre of each basis domain, $I$ is the $m \times m$ identity matrix and $G$ is an $m \times m$ matrix containing coupling information between the basis functions. $A$ is an $m \times m$ diagonal matrix whose diagonal elements contain the contrast at the centre of each basis domain, defined as

$$\zeta = \frac{\varepsilon(r')}{\varepsilon_0} - 1$$

(4)

Equation (3) must be solved to determine the total fields $E_z(r)$ throughout the scatterer and elsewhere. For each step in contrast value $\zeta$ requires the repeated solution of the full-scattering problems for $x$. The Arnoldi iteration will circumvent this particular computational problem to produce a reduced-order model that can be efficiently solved over the entire parameter range.

3 Arnoldi iteration

The Arnoldi method is an orthogonal projection method that iteratively builds an orthonormal basis for the Krylov subspace $K_q$ [15, 17, 21, 22] (We build the subspace $K_q$ in terms of $G$ instead of $GA$ to maintain a Krylov matrix, $Q$ which is not exclusive to a single problem configuration; this will be further discussed later in this work.)

$$K_q(G, u_1) = \text{span}\{u_1, Gu_1, \ldots, G^{q-1}u_1\}$$

(5)

for $G$ generated by the vector $u_1$. This algorithm generates a Hessenberg reduction

$$H_{q+q} = U_q^H GU_q$$

(6)

where $H_q$ is an upper Hessenberg matrix [15]. To derive the columns of

$$U_q = [u_1, u_2, \ldots, u_q]$$

(7)

iteratively, the Arnoldi process in Fig. 1 [15, 17, 21, 22] is applied.

The $u_q$ computed by the Arnoldi algorithm are called the Arnoldi vectors and they define an orthonormal basis for the Krylov subspace $K_q(G, u_1)$. The Arnoldi procedure can be essentially viewed as a modified Gram–Schmidt (MGS) process for building an orthogonal basis for the Krylov space $K_q(G, u_1)$. The procedure has the advantage that it can be stopped part-way, leaving a partial reduction to Hessenberg form that is exploited to provide a reduced-order model for (3). After $q$-steps, the Arnoldi process can
\[ u_1 = b/\|b\|_2 \]

for \( n = 1, \ldots, q \)

\[ w_n = G u_n \]

\[ v_n = \|w_n\|_2 \]

for \( i = 1, \ldots, n \)

\[ y_{i,n} = u_i^T w_n \]

\[ w_n = w_n - u_i y_{i,n} \]

end \( i \)

if \( \|w_n\|_2 < \eta \cdot v_n \)

for \( i = 1, \ldots, n \)

\[ h_{i,n} = u_i^T w_n \]

\[ w_n = w_n - u_i h_{i,n} \]

end \( i \)

\[ h_{n+1,n} = h_{n+1,n} + y_{n,n} \]

cendif

\[ h_{n+1,n} = \|w_n\|_2 \]

if \( h_{n+1,n} = 0 \) Quit

\[ u_{n+1} = w_n/h_{n+1,n} \]

end \( n \).

\[ H = h(1 : q,:) \]

Fig. 1 Arnoldi – MGS algorithm with re-orthogonalisation

be summarised by the \( q \)-step Arnoldi factorisation

\[ G U_q = U_q H_q + u_{q+1} h_{q+1,q} e_q^T \]

(8)

\[ = U_q H_q + w_q e_q^T \]

(9)

where \( e_q = I(. , q) \), \( h_{q+1,q} \) is the \((q + 1, q)\) entry of the Hessenberg matrix \( H_q \), and the vector \( h_{q+1,q} u_{q+1} \) is the Arnoldi residual \( w_q \) of the \( q \)-step Arnoldi factorisation and is orthogonal to the columns of \( U_q \).

Using the identity \( U_q^H U_q = I \) and the fact that \( U_q^H U_{q+1} = 0 \), an expression for \( H_q \) can be derived

\[ U_q^H G U_q = H_q \]

(10)

The matrix \( H_q \) is the orthogonal similarity transformation of the matrix \( G \) to Hessenberg form. This matrix can be interpreted as the orthogonal projection of \( G \) onto the \( q \)-dimensional subspace \( K_q \), whose leading eigenvalues are approximations to those of \( G \).

It is clear that \( G \) and \( H_q \) are approximately unitarily similar if \( q \neq m \). As \( q \to m \), the number of eigenvalues \( \lambda_q(H_q) \) that constitute a good approximation for corresponding eigenvalues \( \lambda_q(G) \) will improve. If \( q = m \) then \( G \) and \( H_q \) are unitarily similar and \( \lambda_q(H_q) = \lambda_q(G) \). This eventuality is characterised by the residual \( \|w_q\|_2 = 0 \) (calculated in line 8 of Fig. 1), at which point the algorithm is terminated. This signals the fact that \( w_{q+1} \) is linearly dependent with respect to \([w_1 \ w_2 \cdots \ w_q]\) [21–23]. However, this situation is very unlikely to occur in practice, because of finite-precision arithmetic. In this scenario \( \|w_q\|_2 = 0 \), \( K_q(G, u_1) \) is an exact invariant subspace of \( G \).

It should be noted that because of finite-precision arithmetic each newly computed vector \( u_{n+1} \) may not be orthogonal to the columns of \( U_q \) [15, 21, 23, 24]. If subsequent Arnoldi vectors are not forced to be orthogonal to the previous vectors, then spurious eigenvalues will appear in the spectrum of the projected matrix \( H_q \).

A computational procedure that monitors and enforces orthogonality is implemented on line 9 of the Arnoldi-modified Gram–Schmidt algorithm with re-orthogonalisation (MGSR) algorithm Fig. 1. A value for the parameter \( \eta = 1/\sqrt{2} \) has been proposed by [25] which results in a good compromise maintaining an orthogonal set of Arnoldi vectors without an unnecessary amount of re-orthogonalisation. Loss of orthogonality of the matrix \( U_q \) at each iteration step can be bounded [24, 26]

\[ \|I - U_q^H U_q\|_2 \leq \text{tolerance} \]

(11)

4 Model-order reduction for an inhomogeneous body

The MOR technique outlined in [18] is applied only to wave scattering from homogeneous bodies. In this work we extend this technique to the case of scattering from inhomogeneous bodies where application of a surface IE is not appropriate. The applicability of the Arnoldi approach to producing a reduced-order model for an inhomogeneous body is contingent on the approximation made in (20). This approximation will be shown to be exact in the limit as the level of reduction approaches zero (Section 4.1). The main computational cost of our approach is outlined in Section 4.2. Practical implementation issues are addressed in Section 4.3 where a simple example is given to re-enforce the concepts of the following sections.

Solution of the scattering problem over a range of contrasts necessitates the ability to compute in an efficient manner the quantity

\[ x = (I + G A)^{-1} b \]

(12)

where \( A \) is the diagonal contrast matrix whose diagonal elements contain the contrast at the centre of each basis domain. The Arnoldi algorithm achieves this by iteratively computing the Hessenberg reduction

\[ H_q = U_q^H G U_q \]

(13)

and using it to develop a ROM for the total field. After \( q \)-steps of the Arnoldi algorithm, an approximation \( \hat{x}_q \), to \( x \), can be made in terms of the \( q \) basis vectors

\[ x \simeq \hat{x}_q = \sum_{n=1}^{q} u_q a_q = U_q a_q \]

(14)

where \( a_q = [\alpha_1 \ \alpha_2 \ \ldots \ \alpha_q]^T \) is a vector of expansion coefficients for the Arnoldi basis vectors \( u_q \) that span the Krylov subspace. The residual \( r_q \) that corresponds to this approximation is introduced as

\[ r_q = b - (I + G A) \hat{x}_q \]

(15)

To find the optimal approximate solution, \( \hat{x}_q \) is constrained to minimise the residual \( r_q \). Specifically, the residual vector is constrained to be orthogonal to the \( q \) linearly independent vectors \( u_q \), this is known as the orthogonal residual...
property or a Galerkin condition

\[ r_q \perp K_q \quad U_q^H r_q = 0 \quad (16) \]

The residual \( r_q \) is minimised when the residual vector is orthogonal to the space \( K_q \). This requires substituting (14) into (15)

\[ r_q = b - (I + G A) U_q a_q \quad (17) \]

and performing a Galerkin test, to give

\[ U_q^H r_q = U_q^H b - (I + G A) U_q a_q \]

\[ = U_q^H b - (I + U_q^H G A U_q) a_q \quad (19) \]

\[ \simeq U_q^H b - (I + U_q^H G U_q U_q^H A_q) a_q \]

\[ = U_q^H b - (I + H_q \tilde{A}_q) a_q \quad (20) \]

where

\[ \tilde{A}_q = U_q^H A U_q \quad (22) \]

As a result of setting

\[ a_q = (I + H_q \tilde{A}_q)^{-1} U_q^H b \quad (23) \]

the residual has been minimised

\[ U_q^H r_q = U_q^H b - (I + H_q \tilde{A}_q)(I + H_q \tilde{A}_q)^{-1} U_q^H b = 0 \quad (24) \]

For exclusive contrast sweep problems, this formulation can be further simplified by choosing the first Arnoldi vector to be \( u_1 = \|b\|_2^{-1} b \)

\[ U_q^H b = e_1 \|b\|_2 = \begin{pmatrix} \|b\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (25) \]

as all the remaining columns of \( U_q \) are orthogonal to \( b \). As a result, the reduced form for the total field is given by

\[ x \simeq x_q = U_q (I + H_q \tilde{A}_q)^{-1} e_1 \|b\|_2 \quad (26) \]

It should be noted that the contrast \( \zeta \) appears as a parameter and neither \( U_q \) nor matrix \( H_q \) depends on \( \zeta \). As such, the \( U_q \) matrix need only be generated once in a contrast-sweep analysis. Subsequently, (26) can be used for the solution of any inhomogeneous domain of the same dimension and discretisation. Clearly, (26) permits efficient solution for the total field over a wide range of contrasts as it requires the inversion of a matrix of order \( q = m \) for each contrast value.

### 4.1 Equation (20) approximation

In this section, the approximation of (20) will be substantiated. As stated earlier, for \( q \neq m \) the following relations hold

\[ U_q^H U_q = I \quad U_q U_q^H \neq I \quad (27) \]

However, owing to the independence of the columns of \( U_q \) imposed by the re-orthogonalisation process, (20) can be shown to be a reasonable approximation. As prescribed in [15], if the columns of \( U_q \) are independent and the norm of the residual matrix

\[ R = AU_q - U_q S_q \quad (28) \]

has been minimised for some choice of \( S_q \) then the columns of \( U_q \) define an approximate subspace. The selection of \( S_q = U_q^H A U_q = A_q \) results in the norm of the residual being minimised

\[ \min \|A U_q - U_q S_q\|_2 = \|I - U_q U_q^H A U_q\|_F \quad (29) \]

Thus, (20) becomes a valid approximation with the property that, as \( q \to m \), a better approximation is procured. This is validated numerically in the results section. Note that, when \( q = m \), (20) is exact as

\[ U_q^H U_m = U_m U_q^H = I \quad (30) \]

### 4.2 Computational analysis

In this analysis, the shape of the object is known a priori. For inhomogeneous structures, this requires the shape of the homogeneities embedded in the domain of the scatterer to be fixed. As such, the method outlined in this text can be applied to scatterers having a not-connected support. For scattering problems where multiple approximate solutions for varying contrast with fixed-source location are required, it will be shown that significant computational saving can be achieved as compared with accelerated solver techniques, such as the Conjugate Gradient Normal Equation-Fast Fourier Transform (CGNE-FFT) [19]. Additionally, considerable time savings can be obtained for scattering with fixed contrast profiles when compared with such accelerated solvers.

The main computational cost of this approach is incurred in generating the Krylov matrix \( U_q \). However, once generated it is stored and can be applied to scattering problems with the same geometry but different contrast configuration. The computation of the \( U_q \) involves the multiplication of \( G \) by \( q - 1 \) Arnoldi vectors \( u_n \), at a cost of \( O(2m^2 q) \) operations. If a second orthogonalisation is performed at each iteration, the operation count is doubled (line 8 of Fig. 1). This represents the worst-case scenario.

For inhomogeneous scattering problems, the computational cost is increased by the need to formulate the matrix \( A_q \) in (22). This requires an initial operation cost of \( O((0.5q)^2 m) \) flops for the preliminary contrast configuration, which can be attributed to the sparse nature of the matrix \( A_q \) and the symmetry of the matrix multiplication, \( U_q^H A_q U_q \). All subsequent solutions for domains with different contrast configurations require only the formation of an amended matrix \( A_q \). To demonstrate the computational overhead associated with the calculation of a new \( A_q \), a simple example is considered. The homogeneous Region 1 (\( \xi_1 = \xi_2 \)) in Fig. 2 is kept constant, while the contrast in Region 2 (\( \xi_3 = \xi_4 = \xi_5 \)) is varied. For this simple case of two homogeneous regions as illustrated in Fig. 2, the
The computational time associated with the generation and approximation residual error be defined as

\[ r_q = \frac{\| b - (I + G\lambda )x_q \|_2}{\| b \|_2} \]  

(34)

If \( r_q \leq \text{tol}_q \) for some pre-specified error tolerance value \( \text{tol}_q \), the iteration process is terminated and hence, the ROM is considered to have converged to this tolerance.

In addition to monitoring the residual error, a procedure to detect when the process has stagnated is required. This means that \( u_{q+1} \) will essentially offer no new information and therefore is not expected to improve the approximation. As discussed earlier, the Arnoldi algorithm approximates the eigenvalues of the \( G \) in order of magnitude. The eigenvalues of largest magnitude are classified as the most dominant and contain the maximum amount of information describing the system. After the most dominant eigenvalues have been approximated, there is a decrease in the amount of new information introduced into the reduced-order model. Consequently, there is a need to monitor the reduction in new information being gained by approximating any new eigenvalues. This can be achieved by monitoring the convergence of the eigenvalues of the approximation matrix \( \lambda (I_q) \) to the eigenvalues of \( \lambda (G) \). The Arnoldi technique seeks an approximate eigenvalue \( \tilde{\lambda} \) and eigenvector \( \tilde{y} \) that minimise the eigenvalue problem

\[ \| (G - \tilde{\lambda} J) \tilde{y} \|_2 \]  

(35)

When the Arnoldi residual \( \| w_q \|_2 = 0 \), then the columns of \( U_q \) define an exact invariant subspace of \( G \) and the approximate eigenvalues and eigenvectors are exact. Otherwise, by using the relation

\[ H_q \tilde{y} = \lambda \tilde{y} \]  

(36)

and the Arnoldi factorisation, a bound for the error of the approximation can be derived [15]. These yield the relation

\[ GU_q = U_q H_q + u_{q+1} b_{q+1} e_q^T \]  

(37)

\[ GU_q = U_q H_q + w_q e_q^T \]  

(38)

\[ GU_q \tilde{y} = U_q \lambda \tilde{y} + w_q \tilde{e}_q^T \tilde{y} \]  

(39)

\[ GU_q \tilde{y} = U_q \lambda \tilde{y} + w_q \tilde{e}_q^T \tilde{y} \]  

(40)

\[ (G - \tilde{\lambda} I) U_q \tilde{y} = w_q \tilde{e}_q^T \tilde{y} \]  

(41)

The Ritz residual norm is subsequently given by [15, 22]

\[ \| (G - \tilde{\lambda} I) x \|_2 = \| w_q e_q^T \tilde{y} \|_2 \]  

(42)

\[ \| e_q \|_2 = \| w_q e_q^T \tilde{y} \|_2 \]  

(43)

where \( x = U_q \tilde{y} \) and is known as the Ritz approximate eigenvector. Although this residual norm is not indicative of the actual error in the approximation of the eigenvalues, it is useful in monitoring the stagnation of the Arnoldi process [15, 21]. Additionally, obtaining the residual norm, as the algorithm progresses, is inexpensive because of the associated vectors being already generated within the
Arnoldi algorithm. As $q$ increases, the approximate eigenvalues will converge to the corresponding eigenvalues of the $G$ matrix and subsequently, the size of the residual norm will decrease. Typically, the process will start to stagnate after the most dominant eigenvalues have been approximated. Consequently, no additional useful information will be added by the generation of a new vector $u_{q}$. To justify the generation of $u_{q+1}$, the residual norm can be used to compare the current value of residual to that of $s$ steps previous

$$\text{if} \left( \| t_q - t_{q-s} \| \leq \text{tol}_q \right) \text{ stagnation} = \text{True} \quad (44)$$

Typically, a value for the tolerance $\text{tol}_q = 10^{-4}$ is used to determine stagnation and the subsequent termination of the Arnoldi algorithm.

In order to improve the range of the Arnoldi iteration in a contrast-sweep analysis, the size of the ROM must increase, as such a balance needs to be struck between the $q$ and range of $\zeta$ for which the approximation is good. As indicated earlier, the Arnoldi algorithm rapidly approximates well-separated external eigenvalues better than the internal eigenvalues. Since the external eigenvalues are the most dominant eigenvalues of the MoM matrix $G$, an accurate approximation can be achieved from a relative low-order subspace. However, often the eigenvalues are clustered, leading to slower convergence and an unacceptable number of steps are required to achieve an accurate approximation.

Even if the size of the $q$ is increased, the MGSR reduced-order-scaled matrix $H_q$ approximation to the MoM $G$ decreases as the $\zeta$ value is increased. To illustrate this point we consider a homogeneous cylinder of radius $r_1 = 1.5$ m illuminated by a TM$_{0}$ plane wave radiating at a frequency of $f = 300$ MHz. The cylinder was discretised using $m = 2472$ cells and the MoM $G$, MGSR ROM $H$ matrices are computed. The first $q = 250$ eigenvalues of the MoM $G$ matrix are compared against the $q$ eigenvalues of the MGSR $H$ matrix for varying values of $\zeta$. Fig. 3 clearly shows that as we scale the $G$ matrix by the constant $\zeta$ from 1.1:6.1, the error between $\lambda(G)$ and $\lambda(H_q)$ linearly increases

$$\beta_q = \| \lambda(G) - \lambda(H_q) \|_2 \quad \text{For } \zeta_q = 1.1:6.1 \quad (45)$$

The effect of this reduction of accuracy to the external eigenvalues results in the MGSR being subject to a linear decrease in accuracy as the contrast values rises, in effect limiting this approach to relative low values of $\zeta$.

5 Numerical results and validations

In this section, the scattered field $E^s$ is calculated from a circular cylinder for a variety of contrast profiles. The numerical performance of the reduced-order model, generated using the Arnoldi algorithm, is compared against the Born series and an accelerated solver. Subsequently, these are validated against the direct solution using the MoM and Mie series [10]. We compare the proposed algorithm against the Born series as a means to highlight the limitation of the Born approximation. Although the Born series has been shown to be an efficient formulation in the electromagnetic scattering by dielectric objects, its limitations have been well documented [3, 9]. Specifically, when the frequency is high, the contrast of the dielectric object is large or when applied to large-scale problems the Born approximation becomes inaccurate.

5.1 Case study 1: bi-static scattering from an inhomogeneous cylinder – medium 1, 2

We initially consider a structure of two concentric cylinders of radii $r_1 = 0.16$ m, $r_2 = 0.08$ m centred at the origin and assumed to be embedded in free space (see Fig. 4). It is illuminated by a TM$_{0}$ plane wave radiating at a frequency of $f = 100$ MHz. The cylinder is discretised using $m = 316$ cells and a bi-static backscattered field $E^s$ is created using the MGSR as presented in this paper for $q = 6$, extended Born [3] and the high-order Born [9] (fifth-order). The MGSR achieves a 98% reduction in system size while yielding a maximum relative error of 0.005% over the entire observation angle range. Equivalently, the extended Born

---

**Fig. 3** Error analysis of the approximate eigenvalues of the ROM created using the MGSR for a range of $\zeta$ values

**Fig. 4** Case study 1 setup – inhomogeneous cylinder illuminated by a TM$_{0}$ plane wave
and the high-order Born achieve a maximum relative error of 0.086 and 0.025%, respectively.

Next we consider an inhomogeneous cylinder of radii $r_1 = 1.5 \text{ m}$, $r_2 = 0.75 \text{ m}$ illuminated by a TM$_z$ plane wave radiating at a frequency of $f = 300 \text{ MHz}$. The cylinder was discretised using $m = 2472$ cells and a bi-static backscattered field $E^s_z$ field is computed for the particular case of contrast $\zeta_1 = 2.5$ and $\zeta_2 = 1.5$ over an observation angle of $\varphi = 0.2\pi$ using a fixed source location.

Figs. 6a and b show the scattered field and associated error obtained from the MoM, Mie series, extended Born, high-order Born and the MGSR technique for $q = 250$, representing a 90% reduction in system size. It is clear from these figures that the MGSR outperforms the Born approximations, replicating the reference solution over the entire contrast range to within a maximum error of 0.77%. As expected the extended Born and high-order Born approximations are ineffective at the higher frequency when applied to a large-scale simulation, archiving a maximum error of 1680 and 302%, respectively.

5.2 Case study 2: bi-static scattering from an inhomogeneous cylinder – medium 1, 2, 3, 4

In this section, we consider an inhomogeneous circular cylinder composed of four concentric regions centred at the origin, with radii $r_1 = 1.5 \text{ m}$, $r_2 = 1.125 \text{ m}$, $r_3 = 0.75 \text{ m}$, $r_4 = 0.375 \text{ m}$, and assumed to be embedded in free space. The structure is illuminated by a TM$_z$ wave emanating from a line source located at $(-10x, 0)$ and radiating at a frequency of $f = 300 \text{ MHz}$. The cylinder was discretised using $m = 2472$ cells and the bi-static backscattered field $E^s_z$ is computed for the particular case of $\zeta_1 = 4$, $\zeta_2 = 3$, $\zeta_3 = 1.5$ and $\zeta_4 = 1.25$.
$\xi_3 = 2$, $\xi_1 = 1.1$, over an observation angle of $\varphi = 0.2\pi$ with a fixed source location.

The scattered field and associated percentage relative error calculated by comparing the MoM against the MGSR for $q = 250$, are shown in Figs. 7a and b, respectively. The MGSR represents a 90% reduction in system size while yielding a maximum relative error of 5.917%.

When determining how to terminate the MGSR iteration, the approximation residual error $r_q$ (34) and the Ritz residual norm (43) are utilised. On the approximation residual error $r_q$ reaching the pre-specified tolerance of $\text{tol}_r = 10^{-3}$, the iteration is terminated. This indicates that the approximation solution $\hat{e}$ has converged to $e$, within the tolerance $\text{tol}_r$.

As identified from Fig. 8a, a value of $q = 200$ results in $r_q < 10^{-3}$. Fig. 8b clearly demonstrates that as $q$ increases the approximate eigenvalues will converge to the corresponding eigenvalues of the $G$ matrix and subsequently the size of the residual norm will decrease. Stagnation in the iteration can be bounded by monitoring the Ritz residual stagnation check (43). Termination of the iteration will occur when the pre-specified $\text{tol}_r = 10^{-4}$ is reached ($q = 200$), signalling that no additional useful information will be added by the generation of a new vector $u_q$ as illustrated in Fig. 9a.

By way of illustrating how the Arnoldi iteration process progresses, a plot of the $q = 250$ approximation eigenvalue $\lambda(H_q)$ and the corresponding eigenvalue $\lambda(G)$, in order of magnitude is compared in Fig. 9b. From this figure, it is clear that the Arnoldi iteration initially approximates the largest eigenvalues of the matrix $G$.

As $q$ is increased, the process rapidly approximates these external eigenvalues (eigenvalues of the largest magnitude located in the outer spectrum) to a higher level of accuracy than the internal eigenvalues (eigenvalues closest to the origin). Although the external eigenvalues are the most dominant, it was highlighted in the previous section that the poor approximation to the internal eigenvalues (located around the origin) results in a limited contrast sweep range.

Loss of orthogonality of the computed Krylov matrix $U_q$, utilising re-orthogonalisation at each iteration step is
\[ \| I_n - U_n^H U_n \|_2 \text{ for all } 1 \leq n \leq q \] (46)

where \( I_n \) is a \( n \times n \) identity matrix. We note the MGSR algorithm remains near-machine precision over the entire iteration process.

It should be noted that the stopping criterion, as discussed in this section, is subject to the ROM being analysed for a constant value of \( \xi_4 = 1.1 \). As \( \xi_4 \) increases, there is no guarantee that the above analysis will produce an accurate approximation response over a contrast range. Additionally, repeated calculation of the approximation residual error for each contrast profile and iteration step will become computationally expensive.

Finally, Fig. 10b depicts the subspace residual error

\[ \frac{\| (x - U_q a_q - GAU_q a_q) - (x - U_q a_q - GU_q A_q a_q) \|_2}{\| x - U_q a_q - GU_q A_q a_q \|_2} \] (47)

This plot substantiates the argument for the approximation of (20), by clearly showing that as \( q \) increases this approximation converges to working precision.

5.3 Case study 3: mono-static scattering from an inhomogeneous cylinder – medium 1, 2, 3, 4

In this section, the MGSR is applied to an inhomogeneous cylinder for a contrast-sweep analysis for \( m = 2472 \) cells. A similar numerical experiment is conducted where the mono-static backscattered field \( E_s \) is computed over a range of contrast values of \( \xi_4 = 1.1:0.1:4 \) while \( \xi_3 = 2 \), \( \xi_2 = 3 \), \( \xi_1 = 4 \) are kept constant, for a fixed line source location.

Figs. 11a and b show the scattered field and associated error obtained from the MoM and the MGSR technique for \( q = 250 \) and \( q = 150 \). From Table 1 and the above figures, a reduction in system size of 94\% results in a maximum relative error of 5.8\% and a Ritz residual norm of 0.10. A maximum relative error of 0.65\% over the entire contrast range can be achieved by a 90\% reduction in system size.
with a Ritz residual norm of 0.015. As discussed in the previous section, the Ritz residual norm \( r_q \) and approximation residual error \( t_q \) can be monitored to determine the optimum order of the Arnoldi iteration.

The CPU time associated with the solution of the scattered field for the MoM and MGSR for 45 samples is given in Table 1. These simulations were run on a 3.00 GHz Xeon CPU processor with 3.00 GB of RAM at 2.99 GHz. The MoM solution is solved using the accelerated solver CGNE-FFT. The CGNE-FFT can reduce the cost of matrix-vector multiplications from \( O(m^2) \) operations per iteration to \( O(m \log_2 m) \) operations.

As is evident from Table 1, the MGSR algorithm can significantly decrease the computational expense associated with the direct solution of each contrast value in a sweep analysis. The main computational cost of this approach is incurred in generating the Krylov matrix \( U_q \) and the initial \( A_q \). However, once generated, the \( U_q \) matrix and non-varying components of \( A_q \) can be used in subsequent simulations. Specifically, only the component of \( A_q \) associated with each varying homogeneous region needs to be re-calculated. This is confirmed in this table where a combined time of 36.63 s is required to generate the initial \( U_q \) and \( A_q \). However, the CPU time is significantly reduced for all subsequent generation of the amended \( A_q \) at a cost of 0.4219 s. From this table, it is also clear that as the size of the ROM increases, the CPU overhead associated with the creation and updating of the contrast profile matrix significantly increases.

However, considerable CPU time saving can be achieved by utilising this method. For a 90% reduction in system size using the MGSR, near-machine precision in accuracy is observed over the entire contrast range. This reduction achieves a speed-up of 20.52 as compared with the MoM solution with FFT capability. Similarly, for a 94% reduction, the MGSR incurs an average percentage relative error of approximately 5.8% with a speed-up of 43.3 where

\[
\text{speed-up} = \frac{\text{total CPU time in seconds to generate and solve MoM solution}}{\text{total CPU time in seconds to generate and solve MGSR}}
\]

### Table 1 CPU time analysis

<table>
<thead>
<tr>
<th>Legend</th>
<th>Technique</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoM (CGNE-FFT)</td>
<td>Arnoldi MGSR (CGNE)</td>
</tr>
<tr>
<td>Order</td>
<td>( M = 2472 )</td>
</tr>
<tr>
<td>( c_n )</td>
<td>891.65</td>
</tr>
<tr>
<td>( n_o )</td>
<td>45</td>
</tr>
<tr>
<td>( t_s(s) )</td>
<td>–</td>
</tr>
<tr>
<td>( t_s(s) )</td>
<td>–</td>
</tr>
<tr>
<td>( t_o(s) )</td>
<td>–</td>
</tr>
<tr>
<td>( t_s(s) )</td>
<td>26.766</td>
</tr>
<tr>
<td>( n_t )</td>
<td>887</td>
</tr>
<tr>
<td>( o_o )</td>
<td>–</td>
</tr>
<tr>
<td>( t_r(s) )</td>
<td>1204.5</td>
</tr>
<tr>
<td>( r_o )</td>
<td>–</td>
</tr>
<tr>
<td>( p_o ), %</td>
<td>–</td>
</tr>
<tr>
<td>( e_o ), %</td>
<td>–</td>
</tr>
<tr>
<td>speed-up</td>
<td>–</td>
</tr>
</tbody>
</table>

Case study 3, 4 – inhomogeneous structure with four homogeneous regions, \( f = 300 \text{ MHz} \), free space wave number \( \lambda_0 = 1 \text{ m} \), \( n_t = 1.5\lambda_0 \). Region 4 – \( n = 1.1:0.1:4 \) \( (\xi_s, \xi_z, \xi_l = 3, 2) \), \( m \) = size of MoM matrix, \( q \) = size of ROM, \( c_n \) = condition number of MoM or ROM matrix accordingly, \( n_o \) = number of contrast samples, \( t_s \) = CPU time in seconds to generate Krylov \( U_q \) matrix, \( t_r \) = CPU time in seconds to generate initial \( A_q \), \( t_o \) = CPU time in seconds to generate the amended component of \( A_q \), \( t_v \) = average CPU time in seconds to solve for \( E_v \) at each contrast value using CGNE or CGNE-FFT accordingly, \( n_t \) = number of iteration of the solver required to reach the tolerance \( 10^{-5} \), \( o_o \) = value for the orthogonality check \( \| I - U_q^t U_q^{t+1} \|_2 \) at iteration \( q \), \( t_r \) = total CPU time in seconds to generate and solve case study problem, \( r_o \) = Ritz residual norm at iteration \( q \), \( p_o \) = ROM size reduction expressed in %, \( e_o \) = \( E_v \) max absolute error over the entire contrast range.

6 Conclusions

In this work the Arnoldi algorithm was introduced and the procedure for generating ROMs using this algorithm was outlined for a contrast-sweep configuration. An extension of
this algorithm to produce a ROM for inhomogeneous geometries using the volume EPFIE formulation was formulated. Notably, we have shown that the Arnoldi algorithm can produce accurate low-order approximations for a relatively low computational cost. The computational expense for any subsequent simulation with an alternative contrast distribution is reduced to the formation of a revised \( A \) and the inversion of a matrix of order \( q \ll m \).

The approximate extension of the Arnoldi algorithm has been shown to be a valid approximation owing to the independence of the columns of the generated orthonormal matrix, imposed by the re-orthogonalisation process. Notably, this approximation was demonstrated to produce a significant reduction in the system size for varying geometries, sizes and contrast profiles while still resulting in an accurate approximation over a wide contrast range.

Finally, a process for monitoring the linear independence of the generated Arnoldi vectors has been applied in conjunction with a relative residual to automate the termination of the Arnoldi iteration.

7 References