A fast direct solver for two dimensional quasi-periodic multilayered media scattering problems

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Abstract
This manuscript presents a fast direct solution technique for solving two dimensional wave scattering problems from quasi-periodic multilayered structures. When the interface geometries are complex, the dominant term in the computational cost of creating the direct solver scales $O(NI)$ where $N$ is the number of discretization points on each interface and $I$ is the number of interfaces. The bulk of the precomputation can be re-used for any choice of incident wave. As a result, the direct solver can solve over 200 scattering problems involving an eleven layer geometry with complex interfaces 100 times faster than building a new fast direct solver from scratch for each new set of boundary data. An added benefit of the presented solver is that building an updated solver for a new geometry involving a replaced interface or a change in material property in one layer is inexpensive compared to building a new fast direct solver from scratch.

Keywords Scattering · Multilayered media · Quasi-periodic · Fast direct solver · Boundary integral equation

1 Introduction
This manuscript considers the $I + 1$ layered scattering problem defined by

$$(\Delta + \omega_i^2)u_i(x) = 0 \quad x \in \Omega_i$$
$$u_1 - u_2 = -u_{inc}(x) \quad x \in \Gamma_1$$

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Fig. 1 A five layered periodic geometry. Seven periods are shown

\[
\frac{\partial u_1}{\partial v} - \frac{\partial u_2}{\partial v} = -\frac{\partial u^{\text{inc}}}{\partial v} \quad x \in \Gamma_1 \\
 u_i - u_{i+1} = 0 \quad x \in \Gamma_i, \ 1 < i < I + 1 \\
 \frac{\partial u_i}{\partial v} - \frac{\partial u_{i+1}}{\partial v} = 0 \quad x \in \Gamma_i, \ 1 < i < I + 1
\]

where \( u_i \) is the unknown solution in the region \( \Omega_i \in \mathbb{R}^2 \), the wave number in \( \Omega_i \) is given by \( \omega_i \) for \( i = 1, \ldots, I + 1 \), and \( v(x) \) is the normal vector at \( x \). The interface \( \Gamma_i \) for \( i = 1, \ldots, I \) between each layer is periodic with period \( d \). The boundary conditions enforce continuity of the solution and its flux through the interfaces \( \Gamma_i \).

The incident wave \( u^{\text{inc}} \) is defined by \( u^{\text{inc}}(x) = e^{ik \cdot x} \) where the incident vector is \( k = (\omega_1 \cos \theta^{\text{inc}}, \omega_1 \sin \theta^{\text{inc}}) \) and the incident angle is \(-\pi < \theta^{\text{inc}} < 0\). Figure 1 illustrates a five layered periodic geometry. The incident wave \( u^{\text{inc}} \) is quasi-periodic up to a phase, i.e. \( u^{\text{inc}}(x + d, y) = \alpha u^{\text{inc}}(x, y) \) for \( (x, y) \in \mathbb{R}^2 \), where \( \alpha \) is the Bloch phase defined by

\[
\alpha := e^{i\omega_1 d \cos \theta^{\text{inc}}}
\]

In the top and bottom layer, the solution satisfies a radiation condition that is characterized by the uniform convergence of the Rayleigh–Bloch expansions (see Sect. 2 of [1]).

Multilayered periodic geometries are important in the design of optical and electromagnetic devices as well as select inverse scattering applications. Some specific
devices that involve scattering from multilayered media are solar cells (thin-filmed photovoltaic cells [2–5] and solar thermal power [6]), dielectric gratings for high-powered laser [7–9] and wideband [10] applications. Most of these applications require solving a scattering problem for a large number of incident angles $\theta^{\text{inc}}$. For example, in many engineering applications, a Bragg diagram created from the solution of 200 boundary value problems is desirable [11]. In optimal design applications and inverse scattering, solving a scattering problem is nested inside of an optimization loop. At each step in the loop, a new scattering problem needs to be solved for many incident angles. When the geometry and material properties are close to the optimal choice or there are sufficient constraints on the material and/or interface properties the changes in the scattering problem are localized to a few layer.

This paper presents a fast direct solver for the multilayered media integral equation formulation presented in [12]. This integral formulation is robust even at the so-called Wood’s anomalies. The computational cost of the proposed fast direct solver scales linearly with respect to the number of discretization points on the interfaces. When a layer is changed with new material properties and/or a new interface geometry, the cost of updating the direct solver scales linearly with respect to the number of discretization points affected by the modification. For changing an interface, updating the direct solver has a cost that scales linearly with respect to the number of discretization points on the new interface. For updating a wave number in $\Omega_i$, the cost scales linearly with respect to the number of discretization points on the interfaces bounding $\Omega_i$. This makes the solution technique a good option for optimal design and inverse scattering applications.

### 1.1 Related work

Direct discretization of (1.1) is possible via finite difference or finite element methods [13] but it faces two challenges: (i) meshing to the interfaces to maintain accuracy and (ii) enforcing the radiation condition. Meshing to the interfaces can be effectively handled using mesh generation software such as GMSH [14]. Techniques such as perfectly matched layers [15] can artificially enforce radiation conditions but can introduce artificial reflections and suffer from high condition numbers. Another challenging aspect of using finite element methods is that there is a loss in accuracy if the points per wavelength remains fixed (the so-called pollution effect) [16]. Another alternative method for directly discretizing (1.1) is the rigorous-coupled wave analysis (RCWA) or Fourier Modal Method. It is designed for multilayer gratings [17] and it depends on an iterative solve. While a Fourier factorization method [18,19] can be used to accelerate the convergence of an iterative solver, this solution approach is not ideal for problems with many right hand sides that arise in applications. RCWA also has difficulty solving problems with interfaces that cannot be defined as a graph of a function of the x-coordinate such as the “hedgehog” interface in Fig. 8b. Most often RCWA is used for geometries like cones and pillars. There is a concern that the method is too simplified to capture complex structures [20–23].

When each layer is comprised of constant coefficient (i.e. not heterogeneous) medium, it is possible to recast (1.1) as a collection of boundary integral equations
where the unknowns lie on the interfaces between layers. There has been much work towards the use of boundary integral equations for quasi-periodic scattering problems including [24–28]. Reviews of boundary integral equation techniques for scattering off a quasi-periodic array of obstacles are presented in [11,12,29]. The review in this paper focuses on techniques for layered media. A boundary integral technique utilizing a fast direct solver for two layered media with periodic structures was presented in [30]. The integral formulation utilized the quasi-periodic Green’s function which is defined as an infinite series. For some choices of boundary data, this series does not converge even though the problem is well posed. An incident angle $\theta^{\text{inc}}$ that causes the quasi-periodic Green’s function not to converge is called a Wood’s anomaly. There have been many techniques suggested to avoid these anomalies (such as [11,31]). A fast direct solver was constructed for quasi-periodic scattering off an infinite array of scatterers in [29] for the robust integral formulation presented in [11]. The work in this paper is an extension of that work to multilayered media problems. This paper builds on the robust integral formulation in [12] though it is likely possible to build similar direct solvers for other formulations that are robust at Wood’s anomalies. The integral formulation in [12] makes use of the free space Helmholtz Green’s function, avoids the infinite sum and uses auxiliary unknowns to enforce periodicity. The radiation condition is satisfied by enforcing continuity of the integral equation solution with the Rayleigh–Bloch expansions.

Recently, [32] replaced the boundary integral formulation in this approach to a technique based on the method of fundamental solutions. This exchanges a second kind integral equation for a formulation that results in a system that is exponentially ill-conditioned.

### 1.2 High level view of the solution technique

Due to the problems associated with the quasi-periodic Green’s function and a desire to exploit the constant coefficient medium, the fast direct solver is built for the robust boundary integral formulation proposed in [12]. Each interface has a boundary integral equation that has “structural” similarities to a boundary integral equation for scattering off a single closed curve. The structural similarity is that a block matrix in the discretized boundary integral equation is amenable to fast direct solution techniques such as Hierarchically Block Separable (HBS) methods [33–35] which are closely related to the Hierarchically Semi-Separable (HSS) [36–38], the Hierarchical interpolative factorization (HIF) [39], the $H$ and $H^2$-matrix methods [40,41]. Roughly speaking these fast direct solvers utilize the fact that the off-diagonal blocks of the discretized integral equation are low rank to create compressed representations of the matrix and its inverse.

The linear system resulting from the discretization of the integral formulation in [12] is rectangular where the principle sub-block is a block tridiagonal matrix. Each block in this tridiagonal matrix corresponds to a discretized boundary integral operator that (in the low frequency regime) is amenable to compression techniques such as those in fast direct solvers. Utilizing this and separating the matrices that depend on Bloch phase allows for the precomputation of the direct solver to be utilized for all choices.
of incident angle. The Bloch phase dependence of many of the other block matrices in the rectangular system can be separated out in a similar manner allowing them to be reused for multiple solves. Further acceleration is gained by exploiting the block diagonal or nearly block diagonal sparsity pattern of all the matrices. The combination of all these efforts dramatically reduces the cost of processing the many solves needed in applications.

The fast direct solver presented in this paper is ideally suited for applications that require many solves per geometry, involve solving problems where there are changes in a subset of the layers (material properties and/or interface geometries), or a combination of many solves per geometry and changes in the geometry. Applications where the solver can be of benefit include optimal design of layered materials and inverse scattering problems where the goal is to recover the thickness and/or the material properties of intermediate layers. While the problems under consideration are acoustic scattering, the solution technique can be extended to transverse electric (TE) and transverse magnetic (TM) wave problems.

The direct solver presented in this paper is built for the robust boundary integral formulation proposed in [12] which enforces continuity of the solution and flux through interfaces. The integral formulation can be extended to problems where there are jumps in the solution and flux as long as these jumps are consistent with the quasi-periodicity conditions.

1.3 Outline

The paper begins by reviewing the integral formulation from [12] in Sect. 2. Next, Sect. 3 presents the proposed fast direct solver. Numerical results in Sect. 4 illustrate the performance of the direct solver. Section 5 summarizes manuscript and reviews the key features of the presented work.

2 Periodizing scheme

This section provides a review of the boundary integral formulation presented in [12]. The necessary integral operators are presented in Sect. 2.1. Then the full representation is presented in Sect. 2.2. Finally, the linear system resulting from enforcing continuity and quasi-periodicity of the solution is presented in Sect. 2.3.

The integral formulation proposed in [12] solves (1.1) in an infinite vertical unit strip of width $d$. Because the solution is known to be quasi-periodic, the solution outside of the unit strip can be found by scaling the solution by the appropriate Bloch phase factor. Let $x = L$ and $x = R$ denote the left and right bounds for the unit strip. The solution technique further partitions space by introducing artificial top and bottom walls to the unit strip at $y = y_U$ and $y = y_D$ respectively. Figure 2a illustrates this partitioning. The box bounded by these artificial boundaries is called the unit cell. Inside the unit cell the solution is represented via an integral formulation. Above and below the unit cell, (i.e. for points in the unit strip where $y > y_U$ or $y < y_D$), the solution is given by Rayleigh–Bloch expansions. Specifically, for $x = (x, y)$ in the unit strip where $y > y_U$, the solution is given by
Fig. 2 This figure illustrates a five layered periodic geometry with artificial walls and proxy circles. Only three periods of the infinite periodic geometry are shown. The period contained within the unit cell is in black while the other two periods are in blue. **a** Notation for the unit cell with left, right, upper, and lower boundary \( L, R, U, \) and \( D \) shown in red lines. **b** Proxy circles \( P_i \) for each layer. The color of the proxy circles alternates between green and magenta (color figure online)

\[
u(x, y) = \sum_{n \in \mathbb{Z}} a_n^U e^{i \kappa_n x} e^{i k_n^U (y - y_U)} \quad (2.1)
\]

and, for \( x = (x, y) \) in the unit strip where \( y < y_D \), the solution is given by

\[
u(x, y) = \sum_{n \in \mathbb{Z}} a_n^D e^{i \kappa_n x} e^{i k_n^D (-y + y_D)} \quad (2.2)
\]

where \( \kappa_n := \omega_1 \cos \theta^\text{inc} + \frac{2 \pi n}{d}, k_n^U = \sqrt{\omega_1^2 - \kappa_n^2}, k_n^D = \sqrt{\omega_{I+1}^2 - \kappa_n^2} \) and the sets \( \{a_n^U\} \) and \( \{a_n^D\} \) are coefficients to be determined. The square root can be either a positive real or positive imaginary number.

### 2.1 Integral operators

This section presents the integral operators needed to represent the solution inside the unit cell.

Let \( \Gamma_i \) for \( i = 1, \ldots, I \) denote the interfaces inside the unit cell and \( \Omega_i \) denote the regions in between for each layer in the unit cell. Both are numbered from the top down. Figure 2a illustrates the numbering of the five layered geometry within the unit cell.
Let $G_\omega(x, y) = \frac{i}{4} H_0^{(1)}(\omega \|x - y\|)$ denote the two dimensional free space Green’s function for the Helmholtz equation with wave number $\omega$ where $H_0^{(1)}$ is the Hankel function of zeroth order [42].

The standard Helmholtz single and double layer integral operators defined on a curve $W$ [43] are

$$(\mathcal{S}_W \omega \rho)(x) = \int_W G_\omega(x, y) \rho(y) dl(y) \quad \text{and} \quad (\mathcal{D}_W \omega \rho)(x) = \int_W \partial_{\nu_y} G_\omega(x, y) \rho(y) dl(y),$$

respectively, where $\nu_y$ denotes the normal vector at the point $y \in W$.

For the periodizing scheme, integral operators involving the unit cell and its neighbors (left and right) are needed.

These operators, denoted with tilde, are defined as follows

$$(\tilde{\mathcal{S}}_W \omega \rho)(x) = \sum_{l=-1}^{1} \alpha^l \int_W G_\omega(x, y + ld) \rho(y) dl(y) = (\mathcal{S}_W \omega \rho)(x) + (\mathcal{S}_W \omega, \text{pm} \rho)(x) \quad \text{(2.3)}$$

and

$$(\tilde{\mathcal{D}}_W \omega \rho)(x) = \sum_{l=-1}^{1} \alpha^l \int_W \partial_{\nu_y} G_\omega(x, y + ld) \rho(y) dl(y) = (\mathcal{D}_W \omega \rho)(x) + (\mathcal{D}_W \omega, \text{pm} \rho)(x) \quad \text{(2.4)}$$

where

$$(\mathcal{S}_W \omega, \text{pm} \rho)(x) = \sum_{l=-1, l \neq 0}^{1} \alpha^l \int_W G_\omega(x, y + ld) \rho(y) dl(y) \quad \text{(2.5)}$$

and

$$(\mathcal{D}_W \omega, \text{pm} \rho)(x) = \sum_{l=-1, l \neq 0}^{1} \alpha^l \int_W \partial_{\nu_y} G_\omega(x, y + ld) \rho(y) dl(y). \quad \text{(2.6)}$$

The notation $\text{pm}$ stands for plus–minus referring to the left and right neighboring copies of $W$.

These integral operators are not sufficient to enforce quasi-periodicity. They are missing information from the infinite copies that are “far” from the unit cell. A proxy basis is used to capture the missing information. For simplicity, consider a layer $\mathcal{O}_l$.

Let $\{y_j\}_{j=1}^{P}$ denote a collection of uniformly distributed points on a circle $P_l$ of radius $2d$ that is centered in $\mathcal{O}_l$. The proxy circle needs to be large enough to shield the interface in the unit cell from its far-field copies, which are more than $\frac{3d}{2}$ away from the center of $\mathcal{O}_l$ in the horizontal direction. It is proved in [44] that larger proxy radius
leads to higher order convergence rate with respect to the number of basis functions \( P \). However, the radius cannot be arbitrarily large, as the magnitude of the coefficients grows exponentially with respect to the ratio between the proxy radius and \( \frac{3d}{2} \). We set the radius of the proxy circle to be \( R_{\text{proxy}} \in \left[ \frac{3d}{2}, 2d \right] \) as in [12]. The elements of the proxy basis used to capture the far field information are defined by

\[
\phi_{\omega l}^{ij} = \frac{\partial G_{\omega l}(x, y_j)}{\partial n_j} + i \omega l G_{\omega l}(x, y_j) \quad (2.7)
\]

where \( n_j \) is the normal vector at \( y_j \) on \( P_l \). This choice of basis results in smaller coefficients when compared to using just the single or double layer potential as a basis [12]. If the layer has a high aspect ratio (i.e. taller than \( d \)), the proxy surface should be taken to be an ellipse; see p. 8 of [12]. Figure 2b illustrates the proxy circles for a five layered geometry.

The boundary integral equations involve additional integral operators which we define in this section for simplicity of presentation. Specifically, an integral operator defined on an interface \( W \) will need to be evaluated at \( x \in V \) where \( V \) is an interface (the same or a vertical neighbor of \( W \)). For \( x \in V \) where \( V \) is an interface, let \( (\tilde{S}_{V[W]}^{\omega} \rho) \) denote the evaluation of (2.3) at \( x \), i.e.

\[
(\tilde{S}_{V[W]}^{\omega} \rho)(x) = \frac{1}{\alpha l} \int_W G_{\omega}(x, y + l d) \rho(y) d l(y).
\]

Likewise, let \( (\tilde{D}_{V[W]}^{\omega} \rho) \) denote the evaluation of (2.4) at \( x \in V \), i.e.

\[
(\tilde{D}_{V[W]}^{\omega} \rho)(x) = \frac{1}{\alpha l} \int_W \partial_{\nu_y} G_{\omega}(x, y + l d) \rho(y) d l(y).
\]

The pm notation for the neighbor interactions follows in a similar fashion. For example, the operator \( (\tilde{S}_{V,W}^{\omega} \rho)(x) \) can be written as the following sum

\[
(\tilde{S}_{V,W}^{\omega} \rho)(x) = (S_{V,W}^{\omega} \rho)(x) + (S_{V,W}^{\omega, pm} \rho)(x),
\]

where

\[
(S_{V,W}^{\omega, pm} \rho)(x) = \frac{1}{\alpha l} \sum_{l=-1, l \neq 0} \int_W G_{\omega}(x, y + l d) \rho(y) d l(y).
\]

In order to enforce continuity of the fluxes, the normal derivatives of these integral operators are required. For \( x \in V \) where \( V \) is an interface, let \( (\tilde{D}_{V,W}^{\omega, \nu} \rho) \) denote the evaluation of the normal derivative of the single layer operator (2.3) at \( x \), i.e.
(\tilde{D}_{W,V}^{\alpha_0,\rho})(x) = \sum_{l=-1}^{1} \alpha^l \int_{W} \partial_{v_x} G_{\omega}(x, y + ld) \rho(y) dl(y)

where \(v_x\) is the normal vector at \(x \in V\). Similarly, let \((\tilde{T}_{W,V}^{\alpha_0,\rho})\) denote the evaluation of the normal derivative of the double layer operator (2.4) at \(x\), i.e.

\((\tilde{T}_{W,V}^{\alpha_0,\rho})(x) = \sum_{l=-1}^{1} \alpha^l \int_{W} \partial_{v_x} v_y G_{\omega}(x, y + ld) \rho(y) dl(y)\).

### 2.2 Integral formulation

The periodizing scheme within the unit cell is based on a modified version of the combined field boundary integral formulation [45,46]. Specifically, the solution in the unit cell is expressed as

\[ u_1(x) = (\tilde{\mathcal{J}}_{\Gamma_1}^{\omega}) \sigma_1(x) + (\tilde{\mathcal{D}}_{\Gamma_1}^{\omega}) \tau_1(x) + \sum_{j=1}^{P} c^1_j \phi_j^{\omega_1}(x) \quad \text{for} \ x \in \Omega_1, \quad (2.8) \]

\[ u_{I+1}(x) = (\tilde{\mathcal{J}}_{\Gamma_{I+1}}^{\omega}) \sigma_{I+1}(x) + (\tilde{\mathcal{D}}_{\Gamma_{I+1}}^{\omega}) \tau_{I+1}(x) + \sum_{j=1}^{P} c^{I+1}_j \phi_j^{\omega_{I+1}}(x) \quad \text{for} \ x \in \Omega_{I+1}, \quad \text{and} \]

\[ u_{i}(x) = (\tilde{\mathcal{J}}_{\Gamma_{i-1}}^{\omega}) \sigma_{i-1}(x) + (\tilde{\mathcal{D}}_{\Gamma_{i-1}}^{\omega}) \tau_{i-1}(x) + (\tilde{\mathcal{J}}_{\Gamma_i}^{\omega}) \sigma_i(x) + (\tilde{\mathcal{D}}_{\Gamma_i}^{\omega}) \tau_i(x) + \sum_{j=1}^{P} c^{i}_j \phi_j^{\omega_i}(x) \quad (2.10) \]

for \(x \in \Omega_i, 2 \leq i \leq I\) where \(\sigma_i\) and \(\tau_i\) are unknown boundary charge distributions and \(\{c^i_j\}_{j=1}^{P}\) are unknown constants, for \(i = 1, \ldots, I\).

Enforcing the transmission condition in equation (1.1) corresponding to continuity of the solution through the interfaces results in the following integral equations:

\[-\tau_1 + (\tilde{D}_{\Gamma_1}^{\omega_1} - \tilde{D}_{\Gamma_1}^{\omega_2}) \tau_1 + (\tilde{S}_{\Gamma_1}^{\omega_1} - \tilde{S}_{\Gamma_1}^{\omega_2}) \sigma_1 - \tilde{D}_{\Gamma_1}^{\omega_2} \tau_2 - \tilde{S}_{\Gamma_1}^{\omega_2} \sigma_2 + \sum_{p=1}^{P} (c^1_p \phi_p^{\omega_1} - c^2_p \phi_p^{\omega_2}) |_{\Gamma_1} = -u^{\text{inc}} \quad \text{on} \ \Gamma_1, \quad (2.11)\]

\[-\tau_I + (\tilde{D}_{\Gamma_I}^{\omega_I} - \tilde{D}_{\Gamma_I}^{\omega_{I+1}}) \tau_I + (\tilde{S}_{\Gamma_I}^{\omega_I} - \tilde{S}_{\Gamma_I}^{\omega_{I+1}}) \sigma_I - \tilde{D}_{\Gamma_I}^{\omega_{I+1}} \tau_{I-1} - \tilde{S}_{\Gamma_I}^{\omega_{I+1}} \sigma_{I-1} + \sum_{p=1}^{P} (c^I_p \phi_p^{\omega_I} - c^{I+1}_p \phi_p^{\omega_{I+1}}) |_{\Gamma_I} = 0 \quad \text{on} \ \Gamma_I, \quad (2.12)\]
and

\[-\tau_i + (\tilde{D}^{0}_{\Gamma_i, \Gamma_i} - \tilde{D}^{0+1}_{\Gamma_i, \Gamma_i})\tau_i + (S^{0}_{\Gamma_i, \Gamma_i} - S^{0+1}_{\Gamma_i, \Gamma_i})\sigma_i + \tilde{S}^{0}_{\Gamma_i, \Gamma_i - \Gamma_i - 1} + \tilde{S}^{0+1}_{\Gamma_i, \Gamma_i - 1} = 0 \text{ on } \Gamma_i \text{ for } 1 < i < I\]

where \(\tilde{S}^{0}_{\Gamma_i, \Gamma_i - 1}\) denotes the periodized single layer integral operator (2.3) defined on \(\Gamma_i\) evaluated on \(\Gamma_i - 1\), etc.

Likewise, enforcing the transmission condition in Eq. (1.1) corresponding to continuity of the flux through the interfaces results in the following boundary integral equations:

\[-\sigma_i + (\tilde{T}^{0}_{\Gamma_i, \Gamma_i} - \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i})\tau_i + (\tilde{D}^{*, 0}_{\Gamma_i, \Gamma_i} - \tilde{D}^{*, 0+1}_{\Gamma_i, \Gamma_i})\sigma_i + \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i - 1}\tau_i - \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i} = 0 \text{ on } \Gamma_i, \quad (2.14)\]

\[-\sigma_I + (\tilde{T}^{0}_{\Gamma_i, \Gamma_i} - \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i})\tau_I + (\tilde{D}^{*, 0}_{\Gamma_i, \Gamma_i} - \tilde{D}^{*, 0+1}_{\Gamma_i, \Gamma_i})\sigma_I + \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i - 1}\tau_I - \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i} = 0 \text{ on } \Gamma_I, \quad (2.15)\]

and

\[-\tau_i + (\tilde{D}^{*, 0}_{\Gamma_i, \Gamma_i} - \tilde{D}^{*, 0+1}_{\Gamma_i, \Gamma_i})\tau_i + (\tilde{D}^{*, 0}_{\Gamma_i, \Gamma_i} - \tilde{D}^{*, 0+1}_{\Gamma_i, \Gamma_i})\sigma_i + \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i - 1}\tau_i - \tilde{T}^{0+1}_{\Gamma_i, \Gamma_i} = 0 \text{ on } \Gamma_i \text{ for } 1 < i < I. \quad (2.16)\]

### 2.3 The linear system

Once the representation of the solution has been determined and the boundary integral equations are derived, the unknown densities, periodicity constants \(c^l\) for the proxy surfaces and the coefficients of the Rayleigh–Bloch expansion need to be approximated. This is done by approximating the boundary integral equations, enforcing the quasi-periodicity of the solution and its flux on the left and right walls, and enforcing the continuity of the solution through the top and bottom of the unit cell.

In this paper, the boundary integral equations are discretized via a Nyström method but the fast direct solver can be applied to the linear system arising from other discretizations. Let \(N_l\) denote the number of discretization points on interface \(\Gamma_l\). As in
[12], the quasi-periodicity is enforced at points that lie on Gaussian panels between each interface on the left and right walls of the unit cell. Let \( M_w \) denote the number of points used to enforce periodicity in a layer. (For simplicity of presentation, we assume this number is the same for all the layers.) Lastly, the continuity of the integral representation and the Rayleigh–Bloch expansions is enforced at collection of \( M \) uniformly distributed points on the top and bottom of the unit cell. The Rayleigh–Bloch expansions are truncated at \( \pm K \).

The rectangular linear system that arises from these choices has the form

\[
\begin{bmatrix}
A & B & 0 \\
C & Q & 0 \\
Z & V & W
\end{bmatrix}
\begin{bmatrix}
\hat{\sigma} \\
c \\
a
\end{bmatrix}
= \begin{bmatrix}
f \\
0 \\
0
\end{bmatrix}
\]  

(2.17)

where \( A \) is a matrix of size \( 2N \times 2N \) where \( N = \sum_{i=1}^{I} N_i \), \( B \) is a matrix of size \( 2N \times P \) where \( P = \sum_{i=1}^{I+1} P_i \), \( C \) is a matrix of size \( 2(I+1)M_w \times 2N \), \( Q \) is a matrix of size \( 2(I+1)M_w \times P \), \( Z \) is a matrix of size \( 4M \times 2N \), \( V \) is a matrix of size \( 4M \times P \), and \( W \) is a matrix of size \( 4M \times 2(2K+1) \). The first row equation enforces the continuity of the scattered field and its flux through the interfaces. The second row equation enforces the quasi-periodicity of the solution and the flux. The last row equation enforces continuity of the integral representation and the Rayleigh–Bloch expansions.

When the interface geometries are complex, a large number of discretization points \( N \) are needed to achieve a desired accuracy. Because the number of discretization points on an interface \( N_i \) is significantly larger than \( M_w \), \( M \), \( K \), and \( P \) in this scenario, the cost of inverting a matrix the size of \( A \) dominates the cost of building a direct solver. For this reason, it is best to build the direct solver in a manner that allows for the bulk of the computational cost associated with matrices of the size \( 2N \times 2N \) to be reused.

We choose to build a fast direct solver for (2.17) via the following block solve:

\[
\hat{\sigma} = -A^{-1} \left( [B \ 0] \begin{bmatrix} c \\ a \end{bmatrix} + A^{-1} f \right)
\]  

(2.18)

\[
\begin{bmatrix} c \\ a \end{bmatrix} = - \left( \left[ \begin{array}{cc} Q & \theta \\ V & W \end{array} \right] - \begin{bmatrix} C \\ Z \end{bmatrix} A^{-1} [B \ 0] \right)^{\dagger} \begin{bmatrix} C \\ Z \end{bmatrix} A^{-1} f
\]  

(2.19)

where \( \dagger \) denotes the Penrose pseudo-inverse.

**Remark 2.1** A linear scaling direct solver can be built by processing the block solve in the same order as in [12]; i.e. solving for \( \begin{bmatrix} c \\ a \end{bmatrix}^T \) first. The matrix that needs to be inverted in order to solve for \( \hat{\sigma} \) is an approximation of the quasi-periodic Green’s function and thus can be ill-conditioned when the incident angle is a Wood’s anomaly.

Each of the matrices in (2.17) has a sparsity pattern that can be used to accelerate the block solve. The bulk of the acceleration comes from a fast direct solver for the matrix \( A \) (see Sect. 3.1).

The matrix \( A \) is block tridiagonal. The diagonal blocks of \( A \) denoted by \( A_{ii} \) can be written as the sum of two matrices \( A_{ii}^s \) and \( A_{ii}^{pm} \) where \( A_{ii}^s \) corresponds to the integral operator on \( \Gamma_i \) in the unit cell evaluated on \( \Gamma_i \), i.e.
\[ A^p_{ii} = \begin{bmatrix} -I + D^{\alpha_1}_{1,1}, & -D^{\alpha_1+1}_{1,1} \\ T^{\alpha_1}_{1,1} - T^{\alpha_1+1}_{1,1} & I + D^{*,\alpha_1}_{1,1} - D^{*,\alpha_1+1}_{1,1} \end{bmatrix}, \]

where \( I \) denotes the identity operator, and \( A^p_{ii} \) is the contributions from the left and right neighboring copies, i.e.

\[ A^p_{ii} = \begin{bmatrix} D^{\alpha_1}_{1,1} - D^{\alpha_1+1}_{1,1} & -S^{\alpha_1}_{1,1} \\ T^{\alpha_1}_{1,1} - T^{\alpha_1+1}_{1,1} & D^{*,\alpha_1}_{1,1} - D^{*,\alpha_1+1}_{1,1} \end{bmatrix}, \]

for \( i = 1, \ldots, I \). The upper diagonal block \( A_{i,i+1} \) corresponds to the integral operators on \( \Gamma_{i+1} \) being evaluated on \( \Gamma_i \), i.e.

\[ A_{i,i+1} = \begin{bmatrix} -\tilde{D}^{\alpha_1+1}_{1,1} & -\tilde{S}^{\alpha_1}_{1,1} \\ -\tilde{T}^{\alpha_1+1}_{1,1} & -\tilde{D}^{*,\alpha_1+1}_{1,1} \end{bmatrix}, \]

for \( i = 1, \ldots, I - 1 \). The lower diagonal blocks \( A_{i,i-1} \) corresponds to the integral operators on \( \Gamma_{i-1} \) being evaluated on \( \Gamma_i \), i.e.

\[ A_{i,i-1} = \begin{bmatrix} \tilde{D}^{\alpha_1}_{1,1} & \tilde{S}^{\alpha_1}_{1,1} \\ \tilde{T}^{\alpha_1}_{1,1} & \tilde{D}^{*,\alpha_1}_{1,1} \end{bmatrix}, \]

for \( i = 2, \ldots, I \).

The matrix \( B \) is upper block diagonal with block defined by

\[ B_{i} = \begin{bmatrix} \phi^0_1 | r_i & \cdots & \phi^0_P | r_i \\ \frac{\partial \phi^0_1}{\partial n} | r_i & \cdots & \frac{\partial \phi^0_P}{\partial n} | r_i \end{bmatrix}, \]

and \( B_{i,i+1} = \begin{bmatrix} -\phi^{\alpha_1+1}_1 | r_i & \cdots & -\phi^{\alpha_1+1}_P | r_i \\ -\frac{\partial \phi^{\alpha_1+1}_1}{\partial n} | r_i & \cdots & -\frac{\partial \phi^{\alpha_1+1}_P}{\partial n} | r_i \end{bmatrix} \]

for \( i = 1, \ldots, I \). The matrix \( C \) is lower block diagonal with blocks defined by

\[ C_{i,i} = \begin{bmatrix} \alpha^{-2}D^{\alpha_1}_{1,1} - \alpha D^{\alpha_1+1}_{1,1} & \alpha^{-2}S^{\alpha_1}_{1,1} - \alpha S^{\alpha_1+1}_{1,1} \\ \alpha^{-2}T^{\alpha_1}_{1,1} - \alpha T^{\alpha_1+1}_{1,1} & \alpha^{-2}D^{*,\alpha_1}_{1,1} - \alpha D^{*,\alpha_1+1}_{1,1} \end{bmatrix}, \]

and

\[ C_{i,i-1} = \begin{bmatrix} \alpha^{-2}D^{\alpha_1}_{1,1} - \alpha D^{\alpha_1+1}_{1,1} & \alpha^{-2}S^{\alpha_1}_{1,1} - \alpha S^{\alpha_1+1}_{1,1} \\ \alpha^{-2}T^{\alpha_1}_{1,1} - \alpha T^{\alpha_1+1}_{1,1} & \alpha^{-2}D^{*,\alpha_1}_{1,1} - \alpha D^{*,\alpha_1+1}_{1,1} \end{bmatrix}, \]

for \( i = 1, \ldots, I \).
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for $i = 1, \ldots, I$ and $i = 2, \ldots, I + 1$, respectively. The matrix $Q$ is block diagonal with blocks given by

$$Q_{ii} = \begin{bmatrix}
\alpha^{-1} \phi_{1i}^0 | R_i - \phi_{1i}^0 | L_i \\
\alpha^{-1} \frac{\partial \phi_{1i}^0}{\partial n} | R_i - \frac{\partial \phi_{1i}^0}{\partial n} | L_i \\
\ddots
\end{bmatrix}$$

(2.23)

for $i = 1, \ldots, I + 1$.

The matrices $Z$, $V$, and $W$ are sparse matrices of the form

$$Z = \begin{bmatrix}
Z_U & 0 & \cdots & 0 \\
0 & \cdots & 0 & Z_D
\end{bmatrix},
\quad V = \begin{bmatrix}
V_U & 0 & \cdots & 0 \\
0 & \cdots & 0 & V_D
\end{bmatrix},
\quad W = \begin{bmatrix}
W_U & 0 \\
0 & W_D
\end{bmatrix}$$

where

$$Z_U = \begin{bmatrix}
\tilde{D}_{U,1}^0 & \tilde{S}_{U,1}^0 \\
\tilde{T}_{U,1}^0 & \tilde{D}_{U,1}^* & \tilde{S}_{U,1}^*
\end{bmatrix},
\quad Z_D = \begin{bmatrix}
\tilde{D}_{D,1}^{i+1} & \tilde{S}_{D,1}^{i+1} \\
\tilde{T}_{U,1}^{i+1} & \tilde{D}_{U,1}^{i+1} & \tilde{S}_{U,1}^{i+1}
\end{bmatrix},$$

(2.24)

$$V_U = \begin{bmatrix}
\phi_{1i}^0 | U \\
\phi_{1i}^0 \frac{\partial}{\partial v} | U
\end{bmatrix},
\quad V_D = \begin{bmatrix}
\phi_{1i}^{i+1} | D \\
\phi_{1i}^{i+1} \frac{\partial}{\partial v} | D
\end{bmatrix},$$

(2.25)

$$W_U = \begin{bmatrix}
-e^{ik^{1-k}x} | U \\
-ie^{ik^{1-k}x} | U
\end{bmatrix},
\quad W_D = \begin{bmatrix}
-e^{ik^{1-k}x} | D \\
-ie^{ik^{1-k}x} | D
\end{bmatrix},$$

(2.26)

The matrices $W_U$ and $W_D$ correspond to the evaluation of the terms in the Rayleigh–Bloch expansions at points on the top and bottom of the unit cell where continuity of the solution is enforced.

### 3 The fast direct solver

While exploiting the sparsity of the matrices can accelerate the construction of a direct solver, the speed gains are not sufficient for applications when the interface geometries are complex. When the interface geometries are complex, the cost of building a direct solver for the rectangular system is dominated by the cost of inverting $A$. The fast direct solver proposed in this section exploits not only the sparsity but also the data sparse nature of the matrix $A$.

The foundation of the fast direct solver is a fast inversion technique for $A$ presented in Sect. 3.1. The fast inversion of $A$ allows for $\hat{\sigma}$ to be computed for a cost that scales linearly with respect to $N$ via equation (2.18). Constructing and applying an approximation of the pseudo-inverse of the Schur complement
\[
S = - \left( \begin{bmatrix} Q & 0 \\ V & W \end{bmatrix} - \begin{bmatrix} C \\ Z \end{bmatrix} A^{-1} [B \ 0] \right)
\]  

(3.1)

is needed to find \( c \) and \( a \) via (2.19). The approximate pseudo-inverse is created by first computing an \( \epsilon_{\text{Schur}} \)-truncated singular value decomposition (SVD) and then applying the pseudo-inverse of this factorization.

**Definition 3.1** Let \( U \Sigma T^* \) be the SVD of the Schur complement matrix \( S \) of size \((2(I + 1)M_w + 4M) \times (P + 2(2K + 1)) \) where \( \Sigma \) is a diagonal rectangular matrix with entries of the singular values of \( S \) and matrices \( U \) and \( T \) are unitary matrices of size \((2(I + 1)M_w + 4M) \times (2(I + 1)M_w + 4M) \) and \((P + 2(2K + 1)) \times (P + 2(2K + 1)) \), respectively. Then the \( \epsilon_{\text{Schur}} \)-truncated SVD is

\[
\hat{U} \hat{\Sigma} \hat{T}^*
\]

where \( \hat{\Sigma} \) is a diagonal square matrix of size \( l \times l \) where \( l \) is the number of singular values of \( S \) that are larger than \( \epsilon_{\text{Schur}} \), \( \hat{U} \) is an \((2(I + 1)M_w + 4M) \times l \) matrix and \( \hat{T} \) is an \((P + 2(2K + 1)) \times l \) matrix.

In practice, we found \( \epsilon_{\text{Schur}} = 10^{-13} \) is a good choice when the desired accuracy for the solution is \( 10^{-10} \).

Then \( c \) and \( a \) can be approximated by

\[
\begin{bmatrix} c \\ a \end{bmatrix} \approx \hat{T} \hat{\Sigma}^{-1} \hat{U}^* \begin{bmatrix} C \\ Z \end{bmatrix} A^{-1} f.
\]

The most efficient way to find \( c \) and \( a \) is to apply the matrices from right to left in this equation meaning that the vectors are found via a collection of matrix vector multiplies.

**Remark 3.1** The cost of constructing the truncated SVD for \( S \) scales cubically with respect to the number of interfaces \( I \) but is constant with respect to the number of points on the interfaces.

Combining the fact that many of the matrices (less scalar factors) in (2.17) can be re-used for multiple incident angles (see Sect. 3.2) with a fast direct solver for \( A \) results in a fast direct solver that is ideal for problems where many solves are required. An additional key feature of the fast direct solver is that the bulk of the precomputation can be re-used if an interface \( \Gamma_j \) or a wave number \( \omega_j \) is changed (see Sect. 3.3).

### 3.1 Fast inversion of \( A \)

The key to building the fast direct solver for the block system (2.17) is having a fast way of inverting \( A \). This technique is designed to make solves for different Bloch phases as efficient as possible.
The solver considers the matrix $A$ written as the sum of two matrices

$$
A = A_0 + \hat{A}.
$$

(3.2)

where the block diagonal matrix $A_0$ whose entries are self-interaction matrices and $\hat{A}$ is the block tridiagonal matrix where the diagonal blocks correspond to the interaction of an interface with its left and right neighbors and the off-diagonal blocks correspond to the interactions between the interfaces directly above and below each other. Since the submatrices in $\hat{A}$ correspond to “far” interactions, they are numerically low rank. Let $LR$ denote the low rank factorization of $\hat{A}$ where $L$ and $R^T$ are $2N \times k_{\text{tot}}$ matrices and $k_{\text{tot}}$ is the numerical rank of $\hat{A}$. Section 3.1.1 presents a technique for constructing this factorization. Then $A$ can be approximated by

$$
A \approx A_0 + LR.
$$

The advantage of this representation is that the factors $L$ and $R$ can be computed in a way that is independent of Bloch phase as presented in Sect. 3.1.1. Additionally, the inverse can be formulated via a Woodbury formula [47]

$$
A^{-1} \approx (A_0 + LR)^{-1} = A_0^{-1} - A_0^{-1}L\left(1 + RA_0^{-1}L\right)^{-1}RA_0^{-1}.
$$

(3.3)

Not only is the matrix $A_0$ block diagonal but each of the diagonal blocks is amenable to a fast direct solver such as Hierarchically Block Separable (HBS) methods [33–35] which are closely related to the Hierarchically Semi-Separable (HSS) [36–38], the Hierarchical interpolative factorization [39], the $H^1$ and $H^2$-matrix methods [40,41].

Thus an approximate inverse of $A_0$ can be constructed and applied for a cost that scales linearly with respect to the number of discretization points on the interfaces. This computation is independent of Bloch phase.

The condition number of $(I + RA_0^{-1}L)$ is bounded above by the product of the condition number of $A_0$ and $(A_0 + LR)$ [48]. Since both $A$ and $A_0$ result from the discretization of second kind boundary integral equations, they are well-conditioned. Thus applying the Woodbury formula is numerically stable.
It is never necessary to construct the approximation of $A^{-1}$. It is only necessary to have a fast algorithm for applying it to a vector $f \in \mathbb{C}^{2N \times 1}$, i.e. a fast algorithm is needed for evaluating

$$A^{-1}f \approx A_0^{-1}f - A_0^{-1}L\left(1 + RA_0^{-1}L\right)^{-1}RA_0^{-1}f. \quad (3.4)$$

The fast direct solver for $A_0$ and the block structure of the matrices $L$ and $R$ allow for $A_0^{-1}L$ and $RA_0^{-1}f$ to be evaluated for a cost that scales linearly with $N$. Thanks to the sparsity pattern of the matrices, the intermediate matrix $S_2 = I + RA_0^{-1}L$ of size $k_{tot} \times k_{tot}$ that needs to be inverted is block tridiagonal. “Appendix A” reports on the construction of $S_2$. Since $k_{tot}$ is much smaller than $N$ in practice, the inverse of $S_2$ can be applied rapidly using a block variant of the Thomas algorithm. This computation needs to be done for each new Bloch phase since $L$ and $R$ are dependent on Bloch phase.

**Remark 3.2** To achieve nearly optimal ranks in the construction of the fast direct solver, it is advantageous to reorder the matrices in $A$ according to the physical location of the unknowns. For example, if there are $N_1$ discretization points on $\Gamma_1$, the unknowns are $\sigma_{1,1}, \ldots, \sigma_{1,N_1}$ and $\tau_{1,1}, \ldots, \tau_{1,N_1}$, etc. Then the matrices should be ordered so that $\hat{\sigma}$ is as follows

$$\hat{\sigma}^T = [\sigma_{1,1}, \tau_{1,1}, \ldots, \sigma_{1,N_1}, \tau_{1,N_1}, \ldots, \sigma_{I,1}, \tau_{I,1}, \ldots, \sigma_{I,N_I}, \tau_{I,N_I}].$$

### 3.1.1 Low rank factorization of $\hat{A}$

The technique for creating the low rank factorizations of the blocks in $\hat{A}$ is slightly different depending on whether or not the block is on the diagonal. This section begins by presenting the technique for creating low rank factorizations of the diagonal blocks. Then the technique for creating the low rank factorizations of the off-diagonal blocks is presented.

Recall the diagonal blocks of $\hat{A}$ are $A_{ii}^{pm}$ corresponding to the discretized version of

$$(\mathcal{S}_{\omega, \Gamma_i, \Gamma_i}^{\omega, pm} \rho)(x) = \alpha \int_{\Gamma_i} G_{\omega}(x, y + d) \rho(y) dl(y) + \alpha^{-1} \int_{\Gamma_i} G_{\omega}(x, y - d) \rho(y) dl(y).$$

The matrix $A_{ii}^{pm}$ can be written as the sum of two matrices that are independent of Bloch phase: $A_{ii}^{pm} = \alpha A_{ii}^p + \alpha^{-1} A_{ii}^m$. Thus by creating low rank factorizations of $A_{ii}^p$ and $A_{ii}^m$ independently, the factorizations can be used for any Bloch phase $\alpha$. Let $L_{ii}^p R_{ii}^p$ and $L_{ii}^m R_{ii}^m$ denote the low rank approximations of $A_{ii}^p$ and $A_{ii}^m$ respectively. These two approximations are combined to create a low rank approximation of $A_{ii}^{pm}$ as follows:
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\[ A_{pm}^{ii} \approx [L_i^p, L_i^m] \begin{bmatrix} \alpha R_i^p \\ \alpha^{-1} R_i^m \end{bmatrix} \]

The technique used to create the low rank factorizations is similar to the one used in [49]. The new technique has an extra step to keep the rank \( k_{tot} \) small.

For brevity, this manuscript only presents the technique for compressing the interaction with the left neighbor (i.e. computing the low rank factorization of \( A_{m}^{ii} \)). The technique for compressing the interaction with the right neighbor follows directly.

We choose to build the factorization via the interpolatory decomposition [50,51] defined as follows.

**Definition 3.2** The interpolatory decomposition of a \( m \times n \) matrix \( M \) that has rank \( l \) is the factorization

\[ M = PM(1 : J, :) \]

where \( J \) is a vector of integers \( j \) such \( 1 \leq j \leq m \), and \( P \) is a \( m \times l \) matrix that contains a \( l \times l \) identity matrix. Namely, \( P(J(1 : l), :) = l \).

Creating the low rank factorization of \( A_{m}^{ii} \) by directly plugging it into the interpolatory decomposition has a computational cost of \( O(N^2i k_i) \) where \( k_i \) is the numerical rank of \( A_{m}^{ii} \). This would result in a solution technique that has a computational cost that scales quadratically, not linearly, with respect to \( N \). To achieve the linear computational complexity, we utilize potential theory.

Recall \( \Gamma_i \) denotes the part of the \( i \)th interface in the unit cell. Let \( \Gamma_i^{m} \) denote the part of the \( i \)th interface in the left neighboring cell. First \( \Gamma_i \) is partitioned into a collection of \( S \) segments \( \gamma_j \) via dyadic refinement where the segments get smaller as they approach \( \Gamma_i^{m} \) so that \( \Gamma_i = \bigcup_{j=1}^{S} \gamma_j \). Figure 3 illustrates a partitioning when compressing the interaction of \( \Gamma_i \) with \( \Gamma_i^{m} \). The refinement is stopped when the segment closest to \( \Gamma_i^{m} \) has less than \( n_{\text{max}} \) points on it. Typically, \( n_{\text{max}} = 45 \) is a good choice.

For each segment \( \gamma_j \) not touching \( \Gamma_i^{m} \), consider a circle concentric with the bounding box containing \( \gamma_j \) with a radius slightly less than the distance from the center of the bounding box to \( \Gamma_i^{m} \). Figure 3a illustrates the proxy surface for \( \gamma_1 \) when there are 5 levels of dyadic refinement toward \( \Gamma_i^{m} \). From potential theory, we know that any field generated by sources outside of this circle can be approximated to high accuracy by placing enough equivalent charges on the circle. In practice, it is enough to place a small number of proxy points evenly on the circle. Let \( n_{\text{proxy}} \) denote the number of proxy points on the circle. For problems where the direct solver scales linearly, \( n_{\text{proxy}} \) is small and chosen to be a constant independent of \( \omega_i \). For the experiments in this paper, it is sufficient to set \( n_{\text{proxy}} = 80 \). Let \( n_j \) denote the number of points on \( \gamma_j \). An interpolatory decomposition can be constructed for the matrix \( A_{\text{proxy}}^{ii} \) capturing the interaction between \( \gamma_j \) and the proxy points. The result is an index vector \( J_j \) and an interpolation matrix \( P_{j} \) of size \( n_j \times k_j \) where \( k_j \) is the numerical rank of \( A_{\text{proxy}}^{ii} \). For \( \gamma_S \) (the segment touching \( \Gamma_i^{m} \)), \( n_{\text{proxy}} \) proxy points are placed uniformly on a circle of radius 1.75 times larger than the radius of the smallest circle containing all the points.
Fig. 3  Illustration of the dyadic refinement partitioning of $\Gamma_i$ with 5 levels refinement and geometries for compressing $A_{ii}^m$.  

(a) Illustration of the proxy surface (dashed circle) used to compress neighbor interactions when $\gamma_1$ is far from $\Gamma_i$.  

(b) Illustration of the proxy surface (dashed circle) and near points (bold blue curve on $\Gamma_i$) when $\gamma_1$ is touching $\Gamma_i$ (color figure online).

The points on $\Gamma_i$ corresponding to the index vector $J$ are called the skeleton points.  

on $\gamma_S$. All the points on $\Gamma_i$ inside the circle are labeled near points and indexed $I_{\text{near}}$.  

Figure 3b illustrates the proxy circle and near points for $\gamma_S$ when there are 5 levels of dyadic refinement toward $\Gamma_i$. An interpolatory decomposition is then performed on $[A_{ii}^m(\gamma_S, I_{\text{near}}) | A_{\text{proxy}}^m]$. The result is an index vector $J_S$ and an interpolation matrix $P_S$ of size $n_S \times k_S$.

The low rank factorization of the matrix $A_{ii}^m$ can be constructed with the result of this compression procedure. Let $J = [J_1(1 : k_1), \ldots, J_S(1 : k_S)]$ denote an index vector consisting of the index vectors for each segment. Then $L_i^m$ is a block diagonal matrix with block entries $P_j$ for $J = 1, \ldots, S$ and $P_j^m = A_{ii}^m(J, :)$.

The rank of this factorization is far from optimal and will result in an excessively large constant prefactor in the application of the Woodbury formula (3.3). A recompression step is necessary to resolve this problem. Let $k_{\text{orig}}$ denote the rank of the original approximate factorization, i.e. the length of $J$. If $k_{\text{orig}}$ is small enough, applying the interpolatory decomposition to $A_{ii}^m(J, :)$ can be done efficiently resulting in an index vector $J_{\text{up}}$ and interpolation matrix $P_{\text{up}}$ of size $k_{\text{orig}} \times k_{\text{up}}$. Let $L_{\text{up}} = P_{\text{up}}$. Otherwise, the interpolatory decomposition can be applied to the submatrices corresponding to a lump of the segments at a time. For example, suppose $S$ is even, then the
segments can bunched two at a time. The interpolatory decomposition can be applied to $\mathbf{A}^m_{ij}([J_j(1:k_j), J_{j+1}(1:k_{j+1})], :)$ for odd values of $j$. The resulting interpolation matrices are the block entries for the block diagonal matrix $L$. The corresponding index vector $J_{up}$ is formed in a similar manner to the vector $J$. Finally the low rank factorization of $\mathbf{A}^m_{ij}$ can be formed by multiplying $L = L_{up}$ and using the updated skeleton of $J(J_{up}, :)$. In other words, $L = L_{up}$ and $R = A_{ij}^m(J(J_{up}, :)$. The technique for constructing the low rank factorization of the off-diagonal blocks of $\hat{A}$ is similar. Recall that each off-diagonal block $A_{ij}$, for $i \neq j$, corresponds to the discretization of the following integral operator where $x \in \Gamma_i$:

$$
(\mathcal{F}_{\Gamma_i \Gamma_j} \rho)(x) = \int_{\Gamma_j} G_\omega(x, y) \rho(y) dl(y) + \alpha \int_{\Gamma_j} G_\omega(x, y+d) \rho(y) dl(y)
$$

$$
+ \alpha^{-1} \int_{\Gamma_j} G_\omega(x, y-d) \rho(y) dl(y).
$$

It is natural to write $A_{ij}$ as the summation of three parts,

$$
A_{ij} = A_{0,ij} + \alpha A_{ij}^p + \alpha^{-1} A_{ij}^m,
$$

where $A_{0,ij}, A_{ij}^p,$ and $A_{ij}^m$ are the discrete approximations of the corresponding integral operators.

While the actual matrix entries of $A_{ij}$ are dependent on $\alpha$, the low rank factorization can be computed independent of $\alpha$ since the matrices need only be scaled by $\alpha$. As with the diagonal blocks, building the factorization of $A_{ij}$ directly is computationally prohibitive. (The computational cost of the direct factorization is $O(N_i N_j k_{ij}$) where $k_{ij}$ is the numerical rank of $A_{ij}$.) Potential theory is again utilized to decrease the computational cost. Consider an ellipse horizontally large enough to enclose $\Gamma_i$ and vertically shields $\Gamma_i$ from its top and bottom neighbor interface. A collection of $n_{\text{proxy}}$ equivalent charges are evenly distributed on the ellipse in parameter space. Figure 4 illustrates a proxy surface used for compressing $A_{i+i+1}$. The interpolatory decomposition is applied to the matrix characterizing the interactions between the points on $\Gamma_i$ and the proxy surface, $A^\text{proxy}$. The index vector $J_i$ and the $N_i \times k_{\text{proxy}}$ interpolation matrix $P_{\text{orig},ij}$ are returned. Let $J_{\text{orig}} = J_i(1:k_{\text{proxy}})$.

As with the diagonal block factorization, $k_{\text{proxy}}$ is far from the optimal rank. To reduce the rank, we apply the interpolatory decomposition to $[A_{0,ij} | A_{ij}^p | A_{ij}^m](J_{\text{orig}}, :)$. An $k_{\text{proxy}} \times k_{\text{new}}$ interpolation matrix $P_{\text{new},ij}$ and index vector $J_{\text{new}}$ are returned. Then the low rank factorization is complete. One factor can be used for all Bloch phases; $L_{ij} = P_{\text{orig},ij}P_{\text{new},ij}$. The other factor is simply a matrix evaluation; $R_{ij} = A_{ij}(J_{ij}, :)$. The rank of the factorizations of $A_{ij}$ will depend on the distance between the interfaces. If the interfaces are space filling, the interaction between the interfaces is not low rank.
3.2 The Bloch phase and incident angle dependence

Beyond the matrix $A$ and exploiting the sparsity of the other matrices in (2.17), additional acceleration can be gained for problems where the solution is desired for multiple incident angles.

The matrix $B$ has block entries (2.20) that are independent of Bloch phase and thus need only be computed once. This is also the case for $V$. The non-zero block matrices in $C$ (2.21) and (2.22) are dependent on $\alpha$ but only as a constant multiple. Thus the submatrices of $C$ can be precomputed and used for all incident angles. The same statement is true for $Q$ and $Z$.

The only matrix that has entries that are dependent on incident angle is $W$. In fact, the matrix $W$ is only dependent on the Bloch phase $\alpha$. Recall that the Bloch phase is defined as $\alpha = e^{i d \omega_1 \cos \theta_{\text{inc}}}$. This means that for all incident angles that share a Bloch phase, there exist a representative angle $\hat{\theta}$ such that $\omega_1 \cos \theta_{\text{inc}} = \hat{\theta} + \frac{2\pi m}{d}$ for some $m \in \mathbb{Z}$. Since the entries of $W$ involve $e^{i \kappa_{j} x} = e^{i (\omega_1 \cos \hat{\theta}_{\text{inc}} + \frac{2\pi j}{d}) x}$

for $j = -K, \ldots, K$, for angles with a shared Bloch phase, the entries of $W$ are the same up to a shift in the index. For example, suppose that we know that 12 incident angles $\{\theta_{\text{inc}}^{1}, \ldots, \theta_{\text{inc}}^{12}\}$ share a Bloch phase and $\omega_1 \cos \theta_{\text{inc}}^{j} = \hat{\theta} + \frac{2\pi (j-1)}{d}$ for $j = 1, \ldots, 12$. The matrix $W$ is constructed so that it has entries with $\kappa_j$ indexed from $-K$ to $K + 12$. This allows the singular value decomposition of $S$ to be used for all angles that share a Bloch phase which results in substantial savings. To evaluate the solution using the resulting coefficients for the Rayleigh–Bloch expansion above or below the unit cell, it is only necessary to use the terms that correspond to $-K, \ldots, K$ for that incident angle.
3.3 Extensions

Many applications consider boundary value problem (1.1) for a collection of geometries where the variation is in a single interface or wave number in a layer. The proposed direct solver can efficiently update an existing fast direct solver for these localized changes in the geometry.

For example, if a user wants to replace $\Gamma_i$, only the matrices corresponding to that interface need to be recomputed. This includes: the parts of the fast direct solver for $A$ corresponding to that block row and column, the corresponding block columns of $C$ and the corresponding block rows of $B$. If the replaced layer is either the top or the bottom, then sub-blocks in $V$ and $Z$ need to be updated as well. Independent of the interface changed, the cost of creating a new direct solver is linear with respect to the number of discretization points on the new interface.

If a user wants to change the wave number $\omega_i$ in $\Omega_i$ where $1 < i < I$, there are two interfaces affected $\Gamma_i$ and $\Gamma_{i+1}$. The corresponding block rows and columns of the fast direct solver of $A$ need to be recomputed. In addition to updating those matrices, the corresponding blocks in $B$, $C$ and $Q$ need to be updated. If the wave number is changed in the top or bottom layer, then the corresponding blocks in $Z$ and $V$ need to be updated as well. Again the cost of updating the direct solver scales linearly with number of discretization points on the interfaces affected, i.e. the cost of the update is $O(N_i + N_{i+1})$.

4 Numerical examples

This section illustrates the performance of the fast direct solver for several geometries with up to 11 layers, though the solution technique can be applied to geometries of arbitrary number of layers. Section 4.1 demonstrates the scaling of the fast direct solver for 3-layer and 9-layer geometries where the wave number alternates between 10 and $10\sqrt{2}$ in the layers. The ability for the solution technique to efficiently solve (1.1) for hundreds of incident waves is demonstrated in Sect. 4.2. Section 4.3 illustrates the performance of the solution technique when the problem has: an interface geometry that is changed or a wave number that is changed in one of the layers.

All the geometries considered in this section have period fixed at $d = 1$. The vertical separation between the neighbor interfaces is roughly 1 for the geometries considered in Sect. 4.1 and roughly 1.5 for the rest of the experiments. The interfaces are discretized via the Nyström method with a 16-point composite Gaussian quadrature. The diagonal blocks require specialized quadrature to handle the weakly singular kernels. For the experiments presented in this section generalized Gaussian quadrature [52] is utilized, but the fast direct solver is compatible with other specialized quadrature including Alpert [53], Helsing [54], Kapur–Rokhlin [55], and QBX [56]. The geometries under consideration involve both smooth interfaces and interfaces that have corners. In order to achieve high accuracy without over discretizing, each corner is discretized with five levels of dyadic refinement. Additionally, the integral operators are discretized in $L^2$ [57]. The artificial separation walls and proxy circles are discretized with parameter choices similar to those in [12]. Specifically, the left and
right (vertical) artificial walls for each layer are discretized by $M_w = 120$ composite Gaussian quadrature nodes, the (horizontal) upper and lower walls of the unit cell are sampled at $M = 60$ equispaced nodes and $P = 160$ equispaced nodes are chosen on the proxy circle for each layer. For the wave numbers under consideration in these experiments, it is sufficient to truncate the Rayleigh–Bloch expansions at $K = 20$.

For all experiments, a HBS fast direct solver with tolerance $\epsilon = 10^{-12}$ was used to construct the approximation of $A_0^{-1}$ in (3.3). The tolerance for all of the low rank factorizations was set to $10^{-12}$. The singular value decomposition of $S$ was truncated at $\epsilon_{\text{Schur}} = 10^{-13}$.

All experiments were run on a dual 2.3 GHz Intel Xeon Processor E5-2695 v3 desktop workstation with 256 GB of RAM. The code is implemented in MATLAB, apart from the interpolatory decomposition, which uses Fortran.

The computational cost of the direct solution technique is broken into four parts:

- Precomputation I: This consists of all computations for the fast linear algebra that are independent of Bloch phase. This includes the fast application of $A_0^{-1}$, and the low rank factors $L_{ij}$ and $R_{ij}$ needed to make $L$ and $R$ as presented in Sect. 3.1. The computational cost of this step is $O(N)$ where $N = \sum_{l=1}^{I} N_l$, and $N_l$ denotes the number of discretization points on interface $l$.

- Precomputation II: This consists of the remainder of the precomputation that is independent of Bloch phase as presented in Sect. 3.2. The computational cost of this step is $O(N)$.

- Precomputation III: This consists of all the precomputation that can be used for incident angles that share a Bloch phase $\alpha$, including scaling matrices by $\alpha$, construction of the matrix $W$ as explained in Sect. 3.2, constructing the fast apply of $A^{-1}$, evaluating the Schur complement matrix $S$ (3.1), and computing the $\epsilon_{\text{Schur}}$ SVD of $S$. The computational cost of this step is $O(N)$. For a fixed number of discretization points on an interface, the computational cost is $O(I^3)$.

- Solve: This consists of the application of the precomputed solver to the right hand side of (2.17) via (2.18) and (2.19). The computational cost of the solve is $O(N)$. For a fixed number of discretization points on an interface, the computational cost is $O(I^3)$.

The error is approximated via a flux error estimate as in [12] which measures conservation of energy. This has been demonstrated to agree with the relative error at any point in the domain.

### 4.1 Scaling experiment

This section illustrates the scaling of the fast direct solver for problems with 3-layers and 9-layers corresponding to two and eight interface geometries.

For the experiments in this section, the wave number in the layers remains fixed (alternating between 10 and $10\sqrt{2}$) while the number of discretization points per layer increases. The geometry consists of alternating the following two interface geometries: $\gamma_1 = (x_1(t), y_1(t))$ and $\gamma_2 = (x_2(t), y_2(t))$ defined as
Fig. 5 Three periods of the interface geometries $\gamma_1$ and $\gamma_2$ as defined in Eq. (4.1)

\[
\gamma_1 : \begin{cases} 
  x_1(t) = t - 0.5 \\
  y_1(t) = \frac{1}{60} \sum_{j=1}^{30} a_j \sin(2\pi j t)
\end{cases}
\]

and

\[
\gamma_2 : \begin{cases} 
  x_2(t) = t - 0.5 \\
  y_2(t) = \frac{1}{60} \sum_{j=1}^{30} b_j \cos(2\pi j t)
\end{cases}
\] (4.1)

for $t \in [0, 1]$, where $\{a_j\}_{j=1}^{30}$ and $\{b_j\}_{j=1}^{30}$ are random numbers in $[0, 1)$ sorted in descending order. Figure 5 illustrates the two interface geometries. In each experiment, $\gamma_1$ and $\gamma_2$ are discretized with the same number of points $N_i$. The run time in seconds and flux error estimates are reported in Table 1.

Each part of the solution technique scales linearly with respect to $N_i$. The factor of four increase in time for Precomputation I is expected since the cost scales linearly with the number of interfaces. Precomputation II should scale linearly with the number of layers and this is observed with a factor three increase in the timings for this portion of the solver. Precomputation III is expected to observe a factor nine increase in the computational cost as this step scales cubically with the number of layers. A factor of six is observed. This is likely because the problems under consideration are sub-asymptotic in the number of layers. The same statement is true for the solve step. As expected the precomputation dominates the cost of the solver for both experiments. Precomputation parts I, II and III account for approximately 90%, 3%, and 7% of the precomputation time, respectively. Thus the Bloch phase independent parts of the direct solver dominate the computational cost.

### 4.2 Sweep over multiple incident angles

Many applications require solving (1.1) for many incident angles (as discussed in Sect. 1). In this setting, Precomputation I and II only needs to be done once. Precomputation III can be utilized for all incident angles that share a Bloch phase $\alpha$. This section demonstrates the efficiency of the fast direct solver for handling scattering problems involving many incident angles. Specifically, we consider the geometry in Fig. 6 which has eleven layers. The interfaces consist of three different corner geome-
Table 1  Time in seconds and flux error estimates for applying the direct solver to a 3-layer and 9-layer geometry where the interfaces alternate between $\gamma_1$ and $\gamma_2$ defined in (4.1)

|                | $N_i$  | 1280 | 2560 | 5120 | 10,240 | 20,480 |
|----------------|--------|------|------|------|--------|--------|
| Precomp I      | 3-Layer| 50   | 100  | 185  | 337    | 569    |
|                | 9-Layer| 201  | 407  | 768  | 1390   | 2360   |
| Precomp II     | 3-Layer| 1.3  | 2.4  | 4.5  | 8.2    | 15.8   |
|                | 9-Layer| 3.8  | 7.6  | 13.4 | 26.1   | 51.4   |
| Precomp III    | 3-Layer| 2.5  | 5.9  | 10.6 | 21.4   | 41.9   |
|                | 9-Layer| 14.9 | 31.5 | 61.5 | 117.1  | 231.2  |
| Solve          | 3-Layer| 0.1  | 0.2  | 0.8  | 1.6    | 3.4    |
|                | 9-Layer| 0.6  | 2.5  | 4.9  | 13.5   | 27.9   |
| Flux error     | 3-Layer| 4.2e−5| 6.9e−6| 2.3e−8| 3.8e−10| 4.5e−10|
|                | 9-Layer| 2.1e−4| 1.2e−5| 1.5e−7| 4.6e−11| 4.6e−10|

$N_i$ denotes the number of discretization points for each boundary charge density on the interface. The wave number alternates between 10 and $10\sqrt{2}$

Fig. 6  Illustration of the real part of the total field of the solution to (1.1) for a geometry with 10 interfaces where the wave number alternates between 40 and $40\sqrt{2}$. The shown solution is for $\theta^{inc} = -0.845\pi$. The total number of discretization points was set to $N = 121, 136$, resulting in a flux error estimate of $2.3e−8$. Seven periods in the geometry are shown.

tries repeated in order. Each of the interfaces contains 40 to 50 right-angle corners. With the five levels of dyadic refinement into each corner there are 10,000 to 15,000 discretization points per interface. Figure 7 provides more details about the corner geometries including how many discretization points were used on each geometry.
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Fig. 7 The three different “corner” geometries in the 11-layer structure. Three periods are shown. See Fig. 6 for the full structure.

Table 2 Time in seconds for solving 287 incident angles and 24 distinct Bloch phases on an 11-layer geometry shown in Fig. 6

| $N_{total}$ | Precomp I | Precomp II | Precomp III | Solve |
|-------------|-----------|------------|-------------|-------|
| 121,136     | 2369.3    | 32.3       | 4517.4      | 482.2 |
|             |           |            | (188.2 per Bloch phase) | (1.7 per incident angle) |

The incident angles are sampled from $[-0.89\pi, -0.11\pi]$

The wave number in the layers alternates between 40 and $40\sqrt{2}$. Equation (1.1) was solved for 287 incident angles between $[-0.89\pi, -0.11\pi]$. This corresponds to 24 different Bloch phases. The average flux error estimate over the 287 incident angles is $2.4e-8$. Figure 6 illustrates the real part of the total field for the incident angle $\theta^{inc} = -0.845\pi$. The time for constructing and applying the fast direct solver for one incident angle is reported in the column labeled Original Problem in Table 3. Table 2 reports the time for applying the proposed solution technique to the 287 boundary value problems using the same Precomputation I and II for all solves and exploiting the shared Bloch phase accelerations. Since the first two parts of the precomputation dominate the computational cost for this geometry, significant speed up over building the direct solver for each angle independently is observed. For this problem, the proposed solution technique is 100 times faster than building a fast direct solver from scratch for each incident angle. There is a 10 times speed up in the time for applying the solver for the multiple incident angles. This results from the fact that angles that share a Bloch phase are processed together.

4.3 Local change to the geometry

This section illustrates the performance of the direct solver when there is a change in one layer of the geometry for the boundary value problem. Either there is
a change in an interface geometry or the wave number has been changed in a layer.

We consider an 11-layer geometry where the original set of interfaces are as illustrated in Fig. 6. As in the last section, the wave number alternates between 40 and $40\sqrt{2}$ in the layers of the original geometry. The incident angle for these experiments is fixed at $\theta_{inc} = -\frac{\pi}{5}$. In the first experiment, the fourth interface in the original geometry is changed to the “hedgehog” interface. Figure 8 illustrates the original and new geometries. The hedgehog geometry consists of 17 sharp corners and cannot be written as the graph of a function defined on the $x$-axis. The number of discretization points on the new interface needed to maintain the same accuracy as the original problem is $N_4 = 14,496$. In the second experiment, the wave number for the second layer is changed from $40\sqrt{2}$ to 30 but the interfaces are kept fixed with the geometry illustrated in Fig. 8a. As presented in Sect. 3.2, only a small number of the matrices in each step of the precomputation need to be recomputed.

Table 3 reports time in seconds for building a direct solver from scratch for the original problem, updating the solver when the fourth interface is replaced and updating the direct solver when there is a change in wave number in the second layer. The parts of Precomputation I and II that are needed in the updating scheme are smaller than building them from scratch. Precomputation I is approximately twice as expensive for the problem with the changed wave number because it requires updating matrices for two interfaces while the changed interface problem only involves one interface. Precomputation III needs to be redone for the new wave number problem. This is why it is nearly as expensive as for the original problem. There is slight savings because the ranks related to the replaced wave number are lower since the new wave number is smaller than the original. The cost savings for updating the solver is greater for the changed interface problem since more of the solver from the original problem can be re-used.

When an application requires many solves per new geometry and many new geometries need to be considered, the speed gains over building a solver from scratch for each new geometry will be significant.
5 Conclusion

This paper presents a fast direct solution technique for multilayered media quasi-periodic scattering problem. For low frequency problems, the computational cost of the direct solver scales linearly with the number of discretization points. The bulk of the precomputation can be used for all solves independent of incident angle and Bloch phase $\alpha$. For a problem where over 200 hundred incident angles are considered, the proposed fast direct solver is 100 times faster than building a direct solver from scratch.

An additional benefit of this solution technique is that modifications in the wave number of a layer or an interface geometry result in only having to update the matrices corresponding to that layer or interface. The cost of updating the precomputation parts scales linearly with the number of points on that interface. For a problem with a changed interface, the constant associated with the linear scaling is very small for the precomputation (relative to building a new direct solver from scratch). In optimal design and inverse scattering applications where the geometry will be changed many times and for each geometry many solves are required, the fast direct solver will have significant savings.
Two dimensional geometries have to be complex in order to justify the need for the fast direct solver. For three dimensional problems, a fast direct solver will be necessary for most geometries of interest in applications. The extension to three dimensional problems is not trivial but the work presented in this paper provides the foundations for that work.

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A The construction of $S_2$

This section presents an efficient technique for constructing the tridiagonal matrix $S_2 = I + RA^{-1}L$.

For simplicity of presentation, let the blocks of $S_2$ be denoted as follows

$X_i$ for $1 \leq i \leq I$ denotes the diagonal blocks,

$Y_i$ for $2 \leq i \leq I$ denotes the lower diagonal blocks, and

$Z_i$ for $1 \leq i \leq I - 1$ denotes the upper diagonal blocks.

The diagonal blocks are given by

$$X_1 = \begin{bmatrix} I + R_{11}^{pm}A_{0,11}^{-1}L_{11}^{pm} & R_{11}^{pm}A_{0,11}^{-1}L_{12}^{pm} \\ 0 & I \end{bmatrix},$$

$$X_i = \begin{bmatrix} R_{ii}^{pm}A_{0,ii}^{-1}L_{i,i}^{pm} & 0 \\ 0 & I \end{bmatrix},$$

and, for $2 \leq i \leq (I - 1)$,

$$X_i = \begin{bmatrix} I + R_{ii}^{pm}A_{0,ii}^{-1}L_{i,i}^{pm} & 0 \\ 0 & I \end{bmatrix}.$$

The lower diagonal blocks are given by

$$Y_2 = \begin{bmatrix} R_{21}A_{0,11}^{-1}L_{11}^{pm} & R_{21}A_{0,11}^{-1}L_{12}^{pm} \\ 0 & 0 \end{bmatrix},$$

and, for $3 \leq i \leq I$,

$$Y_i = \begin{bmatrix} R_{i-1,i}A_{0,(i-1)(i-1)}^{-1}L_{i-1,i-2}^{pm} & R_{i-1,i}A_{0,(i-1)(i-1)}^{-1}L_{i-1,i}^{pm} \\ 0 & 0 \end{bmatrix}.$$

Finally the upper diagonal blocks are defined by

$$Z_i = \begin{bmatrix} R_{i,i+1}A_{0,(i+1)(i+1)}^{-1}L_{i+1,i}^{pm} & 0 \\ 0 & R_{i,i+1}A_{0,(i+1)(i+1)}^{-1}L_{i+1,i+2}^{pm} \end{bmatrix}.$$
for $1 \leq i \leq (I - 2)$, and

$$Z_{I-1} = \begin{bmatrix} 0 & 0 \\ R_{I-1,I} A_{0,II}^{-1} \mathbf{L}_{I-1} & R_{I-1,I} A_{0,II}^{-1} \mathbf{L}_{II} \end{bmatrix}.$$  

The matrix $S_2$ can be inverted via a block variant of the Thomas algorithm. Let the sum of the ranks of the low-rank approximations be defined as $N_{i}^{\text{block}} = k_{pm,ii} + k_{i,i-1} + k_{i,i+1}$ for $2 \leq i \leq I - 1$, $N_{1}^{\text{block}} = k_{pm,11} + k_{1,2}$ and $N_{I}^{\text{block}} = k_{pm,I} + k_{I,I-1}$. The diagonal block $X_i$ is of size $N_{i}^{\text{block}} \times N_{i}^{\text{block}}$. The upper diagonal block $Z_i$ has size $N_{i}^{\text{block}} \times N_{i+1}^{\text{block}}$. The lower diagonal block $Y_i$ has size $N_{i}^{\text{block}} \times N_{i-1}^{\text{block}}$.

For the tested geometries and wave numbers, $N_{i}^{\text{block}}$ is only several hundreds and the diagonal blocks can be inverted rapidly via dense linear algebra. If all of the blocks are of similar size $N_{i}^{\text{block}} \approx N_{i}^{\text{block}}$, then the cost of inverting $S_2$ via the block Thomas algorithm is $O([N_{i}^{\text{block}}]^3 I)$, which is linear with respect to the number of interfaces.

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