ARE SPECTRAL COARSE SPACES SUFFICIENTLY ROBUST FOR HETEROGENEOUS HELMHOLTZ PROBLEMS?*

N. BOOTLAND† AND V. DOLEAN‡

Abstract. Numerical solution of heterogeneous Helmholtz problems presents various computational challenges, with descriptive theory remaining out of reach for many popular approaches. Robustness and scalability are key for practical and reliable solvers in large-scale applications, especially for large wave number problems. In this work we explore the use of a GenEO-type coarse space to build a two-level additive Schwarz method applicable to highly indefinite Helmholtz problems. Through a range of numerical tests on a 2D model problem, discretised by finite elements on pollution-free meshes, we observe robust, wave number independent convergence and scalability of our approach. We further provide results showing a favourable comparison with the DtN coarse space. Our numerical study shows promise that our solver methodology can be effective for challenging heterogeneous applications.

Key words. Helmholtz equation, domain decomposition, two-level method, coarse space, additive Schwarz method, heterogeneous problem, high frequency

1. Introduction. Consider solving the heterogeneous Helmholtz problem: for a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, we wish to find $u(x) : \Omega \rightarrow \mathbb{C}$ such that

\begin{align}
(1.1a) \quad -\Delta u - k^2 u &= f \quad \text{in } \Omega, \\
(1.1b) \quad C(u) &= 0 \quad \text{on } \partial\Omega,
\end{align}

where $C$ incorporates some appropriate boundary conditions. For the heterogeneous problem we suppose the wave number $k(x) > 0$ is a function of space, defined by the ratio $k = \omega/c$ of the angular frequency $\omega$ and the wave speed $c(x)$. In this work we investigate the use of an overlapping Schwarz preconditioner with a suitably chosen coarse space based on solving local eigenvalue problems on each subdomain.

The ability to compute solutions to the Helmholtz problem (1.1) is important across many disciplines of science and engineering. As the prototypical model for frequency-domain wave propagation, it features within the fields of optics, acoustics and seismology amongst others. Further applications can be found in imaging science, such as through medical imaging techniques and geophysical studies of the Earth’s subsurface within, for instance, the oil industry. Nonetheless, it is challenging to develop efficient computational methods to solve (1.1), particularly when the wave number $k$ becomes large.

Discretisation of (1.1) by standard approaches, such as Lagrange finite elements as we shall use here, results in large linear systems to be solved which are indefinite, non-self-adjoint, and ill-conditioned; see also [47]. These systems present various difficulties to solve, especially in the presence of complex heterogeneities, at high frequencies (large $k$), or when solutions include many wavelengths in the domain. Classical methods for solving such large systems typically fail for several reasons, as detailed in [25, 30], and specialist approaches must be employed for a robust solver. While much progress has been made for symmetric positive definite problems, such techniques cannot be applied out-of-the-box and extensions to tackle indefinite and

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*The authors gratefully acknowledge support from the EPSRC grant EP/S004017/1.
†Department of Mathematics and Statistics, University of Strathclyde, Glasgow, UK (niall.bootland@strath.ac.uk).
‡Department of Mathematics and Statistics, University of Strathclyde, Glasgow, UK and Laboratoire J.A. Dieudonné, CNRS, University Côte d’Azur, Nice, France (work@victoritadolean.com).
non-self-adjoint problems may not be clear. This has led to a number of approaches being developed in recent years, aiming to bridge this gap. For the Helmholtz problem this includes parallel direct solvers, such as [32, 54], and preconditioned iterative methods that utilise multigrid, such as [12, 41], or the so-called “shifted Laplace” approach [23, 24]. This latter (complex-)shifted Laplace preconditioner has seen much interest into its practical use [14] and further developments through deflation techniques, most recently in [20, 45].

Another broad class of solvers are domain decomposition methods, which provide a natural balance between using direct and iterative solvers. Specialist methods are again required for the Helmholtz problem, a popular set of which fall under the heading of “sweeping” methods [21, 22]. These are multiplicative domain decomposition methods and linked to a variety of other approaches, including optimised Schwarz methods, as detailed in the recent survey [30]. While sweeping is a conceptually serial approach, much work has been done to incorporate parallelism. Of particular note is the “L-Sweeps” method [53], stated to be the first parallel scalable preconditioner for high-frequency Helmholtz problems; a review of developments in this area is provided in the introductions of [17, 53]. Another popular approach are FETI methods, for the Helmholtz problem these include FETI-H [27] and FETI-DPH [26].

Within the domain decomposition community, there has also been renewed work on additive Schwarz methods, which offer a naturally parallel approach. Following on from the seminal work [18], which utilised Robin (or impedance) transmission conditions to provide a convergent Schwarz method for the Helmholtz problem, a wealth of non-overlapping Schwarz methods have been devised; see the introduction of [13] for a recent overview. In these methods one has to be careful to either avoid or treat cross points (where three or more subdomains meet), as can be done in the robust treatment of [13]. Many optimised approaches rely on deriving higher-order transmission conditions, such as through second order impedance operators in [29], absorbing boundary conditions (ABCs) [10], or non-local operators [15]. Ideally one would use the Dirichlet-to-Neumann (DtN) map (a Poincaré–Steklov operator) to provide transparent transmission conditions, but this is prohibitive in practice and so these optimised Schwarz methods in essence try to approximate this operator.

Overlapping Schwarz methods for the Helmholtz problem, see for example [11, 31, 43], have also received renewed attention in recent years and it is this type of method we shall consider. A successful approach is to design additive Schwarz methods based on including absorption (a complex shift $k^2 \rightarrow k^2 + i\varepsilon$), with absorption parameter $\varepsilon$; see [36, 44]. Theoretical work to understand the effectiveness of this approach can be found in [35, 37] and for the heterogeneous problem in [34]; see also [33]. To be scalable, such additive Schwarz methods require a second level, known as a coarse space (though see [9] for a novel analysis for the absorptive problem). For the two-level methods in [35, 36] this is provided through a coarse grid; an approach which is effective also for the time-harmonic Maxwell problem [4].

As well as to provide scalability, coarse spaces have been devised to provide robustness to heterogeneity. This is exemplified by the “Generalised Eigenproblems in the Overlap” (GenEO) approach for symmetric positive definite (SPD) problems [52]. This approach provides a spectral coarse space, where appropriate local eigenvalue problems are solved to provide a two-level method. Another spectral coarse space is the DtN coarse space [50], which has been extended and investigated for the Helmholtz problem in [5, 16]. While the standard GenEO theory applies only in the SPD case (though see [7]), in this work we develop and explore a GenEO-type method for the Helmholtz problem and show numerically that, for a 2D model problem of a
wave guide, it provides a scalable approach that is robust to heterogeneity and increasing wave number in terms of the iteration count of a preconditioned GMRES method. Companion results for large benchmark problems arising in applications, with comparison to other methods, are found in [8].

The primary aim of this work is to explore the utility of a GenEO-type method for the heterogeneous Helmholtz problem (1.1); we call this approach H-GenEO. In particular, we highlight the following contributions:

- We present a range of numerical tests, on pollution-free meshes, comparing our proposed H-GenEO approach with another spectral coarse space applicable to the Helmholtz problem, namely the DtN method.
- We investigate the use of appropriate thresholding for the required generalised eigenproblems in both the DtN and H-GenEO coarse spaces.
- We consider robustness to non-uniform decomposition, heterogeneity, and increasing wave number as well as the scalability of the methods. We find that only the H-GenEO approach is scalable and robust to all of these factors for a 2D model problem.
- We provide scalability and timing results for H-GenEO applied to a high wave number problem.

The remainder of this work is structured as follows. We begin by considering a finite element discretisation of the Helmholtz problem in Section 2.1, before outlining the underlying domain decomposition methodology we use in Section 2.2. The main topic of interest, that of suitable spectral coarse spaces for the heterogeneous Helmholtz problem, is then detailed in Section 2.3. Extensive numerical results on a 2D model problem are provided in Section 3, along with a discussion of our findings. Finally, we draw together our conclusions in Section 4.

2. Materials and Methods.

2.1. Finite element discretisation. The problem we consider in this work is the interior Helmholtz problem (1.1), for which we must prescribe appropriate boundary conditions. In practical applications, the computational domain Ω is often truncated and the physically relevant condition, namely the far field Sommerfeld radiation condition, must be approximated on the non-physical boundary of Ω. This allows for appropriate wave behaviour to be modelled in a bounded domain. This simplest approximation which is widely used is that of a Robin (or impedance) condition and this is what we shall consider; other approaches include ABCs [55] or perfectly matched layers (PML) [3, 39]. We also suppose that Dirichlet conditions may be imposed on a boundary Γ_D ⊂ ∂Ω, with the Robin condition on the remaining boundary Γ_R = ∂Ω \ Γ_D. Thus, in general, we seek the solution of the boundary value problem

\begin{align}
-\Delta u - k^2 u &= f & \text{in } \Omega, \\
u &= u_{\Gamma_D} & \text{on } \Gamma_D, \\
\frac{\partial u}{\partial n} + ik u &= 0 & \text{on } \Gamma_R,
\end{align}

where the forcing function f(x) incorporates any sources in the domain. Note that if Γ_R ≠ ∅ the problem is well posed but if Γ_R = ∅ the problem is ill-posed for certain choices of k related to eigenfunctions of the Laplacian.

To discretise (2.1) we use standard Lagrange finite elements; the details can be found in, for example, [8] and so we provide only an outline here. Defining the relevant trial and test spaces \( V = \{ u \in H^1(\Omega): u = u_{\Gamma_D} \text{ on } \Gamma_D \} \) and \( V_0 = \)
\{u \in H^1(\Omega): u = 0 \text{ on } \Gamma_D\}, the weak formulation of (2.1) is to find \( u \in V \) such that

\begin{align*}
(2.2) \quad a(u, v) &= F(v) \quad \forall \ v \in V, \\
\end{align*}

where

\begin{align*}
(2.3) \quad a(u, v) &= \int_\Omega (\nabla u \cdot \nabla \bar{v} - k^2 u \bar{v}) \, dx + \int_{\Gamma_R} iku \bar{v} \, ds \quad \text{and} \quad F(v) = \int_\Omega f \bar{v} \, dx.
\end{align*}

Assuming a simplicial mesh \( T^h \) of \( \Omega \) with characteristic element diameter \( h \), piecewise polynomial finite element approximation reduces the problem to solving the complex linear system

\begin{align*}
(2.4) \quad Au &= f,
\end{align*}

with coefficient matrix \( A \in \mathbb{C}^{n \times n} \) and right-hand side vector \( f \in \mathbb{C}^n \) stemming from \( a(\cdot, \cdot) \) and \( F(\cdot) \) respectively; see [8]. For accurate discretisation of the Helmholtz problem, the number of degrees of freedom \( n \) is required to be large, especially for large \( k \). Indeed, to maintain the same level of accuracy of discrete solutions as \( k \) increases then the number of mesh points must increase faster than \( k \), due to the pollution effect [2]. This depends on the polynomial order of the approximation used: for instance, using piecewise linear (P1) finite elements \( k^3 h^2 \) must be bounded and so \( h \) must shrink as \( O(k^{-3/2}) \). Higher order finite elements can reduces this restriction on \( h \) but ultimately the interpolation properties of such methods degrade. Here we will utilise standard P1 elements and maintain a discretisation such that \( k^3 h^2 \) is fixed to avoid the pollution effect.

### 2.2. Underlying domain decomposition method.

To solve the discrete Helmholtz problem (2.4) we will use GMRES accelerated via a two-level overlapping domain decomposition preconditioner. For the underlying one-level method we consider the optimised restricted additive Schwarz (ORAS) method [19] (sometimes known as WRASH [43]; see discussions in [33, 34] and [35, 36] for a related IMPHRAS1 method). They key difference in ORAS compared with standard additive Schwarz methods such as RAS is that the local Dirichlet problems on subdomains are replaced by appropriate Robin problems.

To formulate the domain decomposition preconditioner, we first suppose that \( \Omega \) is decomposed into non-overlapping subdomains \( \{\Omega^\prime_s\}_{s=1}^N \), assumed to be resolved by the mesh \( T^h \). To give an overlapping decomposition, a layer of adjoining mesh elements is added to give overlapping subdomains \( \{\Omega_s\}_{s=1}^N \) by way of the extension

\begin{align*}
(2.5) \quad \Omega_s &= \text{Int} \left( \bigcup_{\text{supp}(\phi_j) \cap \Omega^\prime_s \neq \emptyset} \text{supp}(\phi_j) \right),
\end{align*}

where \( \{\phi_j\}_{j=1}^n \) are the nodal basis functions of the finite element space, \( \text{Int}(\cdot) \) denotes the interior of a domain and \( \text{supp}(\cdot) \) the support of a function. Further layers of elements can be added in a recursive manner in order to obtain subdomains with larger overlap, if desired.

Once we have an overlapping decomposition into subdomains \( \{\Omega_s\}_{s=1}^N \), we define the required operators for the Schwarz preconditioner. We let \( R_s \in \mathbb{R}^{n_s \times n} \) be the discrete form of the restriction operator, restricting functions to the subdomain \( \Omega_s \),
where \( n_s \) is the number of degrees of freedom in \( \Omega_s \). The corresponding extension operator, \( R^T_s \), then acts as an extension by zero outside of \( \Omega_s \). We also utilise a partition of unity, having the discrete form of a diagonal matrix \( D_s \in \mathbb{R}^{n_s \times n_s} \) satisfying \( \sum_{s=1}^{N} R^T_s D_s R_s = I \), which appropriately scales the multiple subdomain contributions in the overlapping regions. Finally, within ORAS we require the solution of local Robin problems given by

\[
\begin{align*}
(2.6a) & \quad -\Delta w_s - k^2 w_s = f \quad \text{in } \Omega_s, \\
(2.6b) & \quad \frac{\partial w_s}{\partial n_s} + ikw_s = 0 \quad \text{on } \partial \Omega_s \setminus \partial \Omega, \\
(2.6c) & \quad C(w_s) = 0 \quad \text{on } \partial \Omega_s \cap \partial \Omega,
\end{align*}
\]

with \( C \) representing the underlying problem boundary conditions on \( \partial \Omega \), namely (2.1b)–(2.1c). Note the use of the Robin condition (2.6b) ensures the solvability of these local problems. Defining the equivalent finite element discretisation of (2.6) to be given by the stiffness matrix \( \hat{A}_s \in \mathbb{R}^{n_s \times n_s} \), the construction of the one-level ORAS preconditioner is given by the sum

\[
M^{-1}_{\text{ORAS}} = \sum_{s=1}^{N} R^T_s D_s \hat{A}_s^{-1} R_s.
\]

Note that the local solutions on each subdomain given by \( \hat{A}_s^{-1} \) can be carried out in parallel.

In order to provide robustness and scalability, the ORAS method above must be augmented by use of a coarse space to provide a two-level method. A coarse space can be thought of as a collection of linearly independent column vectors \( Z \). The vectors that are incorporated into \( Z \) are key to providing scalability, especially for indefinite problems, such as the Helmholtz problems we solve here, where the addition of a coarse space need not improve performance of the underlying one-level method [28]. There are several ways to incorporate the coarse space; here we consider an effective approach that is based on deflation. For this, a coarse space operator \( E = Z^\dagger A Z \) is constructed as well as the coarse correction operator \( Q = Z E^{-1} Z^\dagger \), which we incorporate to give a two-level ORAS method

\[
M^{-1}_{\text{ORAS},2} = M^{-1}_{\text{ORAS}} (I - AQ) + Q.
\]

We now turn our attention the choice of coarse space.

**2.3. Spectral coarse spaces.** In this work we consider and explore spectral coarse spaces for the discrete Helmholtz problem (2.4). These utilise local eigenvalue problems on subdomains in order to build a global coarse space. We will review the DtN coarse space [16] before detailing a new coarse space for Helmholtz problems based on GenEO technology [52]. We will then show a link between these two approaches.

**Remark 2.1 (Notation).** We utilise the following notation for local Dirichlet, Robin, and Neumann matrices: For a variational problem which gives rise to a system matrix \( B \), we denote by \( B_s \) the corresponding local Dirichlet matrix on \( \Omega_s \). In the case that Robin conditions are used on internal subdomain interfaces the local problem matrix is denoted by \( \hat{B}_s \). On the other hand, if Neumann conditions are used on such interfaces we denote the local matrix by \( \tilde{B}_s \).
2.3.1. The DtN coarse space. The Dirichlet-to-Neumann (DtN) coarse space, first studied in [49, 50] for elliptic problems, is based on solving local eigenvalue problems on subdomain boundaries related to a DtN map. Harmonic extensions of low-frequency modes on subdomains are then used to provide a coarse space. In order to define this approach for the Helmholtz problem, as explored in [16], we first require the Helmholtz extension operator from the subdomain boundary $\partial \Omega_s$.

On each subdomain, let $\Gamma_s = \partial \Omega_s \setminus \partial \Omega$ and suppose we have Dirichlet data $v_{\Gamma_s}$ on $\Gamma_s$. The Helmholtz extension $v$ into $\Omega_s$ is given by solving

\begin{align}
-\Delta v - k^2 v &= 0 \quad \text{in } \Omega_s, \\
v &= v_{\Gamma_s} \quad \text{on } \Gamma_s, \\
C(v) &= 0 \quad \text{on } \partial \Omega_s \cap \partial \Omega,
\end{align}

where $C(v) = 0$ represents the original problem boundary conditions, as in (2.6c). The DtN map takes Dirichlet data $v_{\Gamma_s}$ to the corresponding Neumann data on $\Gamma_s$, namely

$$\text{DtN}_{\Omega_s}(v_{\Gamma_s}) = \frac{\partial v}{\partial n} \bigg|_{\Gamma_s}$$

where $v$ is the Helmholtz extension defined by (2.9). The associated local DtN eigenproblem on subdomain $\Omega_s$ is given by

$$\text{DtN}_{\Omega_s}(u_{\Gamma_s}) = \lambda u_{\Gamma_s},$$

for eigenfunctions $u_{\Gamma_s}$ and eigenvalues $\lambda \in \mathbb{C}$. In order to build the coarse space we take the Helmholtz extension of $u_{\Gamma_s}$ in $\Omega_s$ and extend by zero into the whole domain $\Omega$ using the partition of unity; see [16].

To formulate the discrete version of the eigenproblems to be solved we require the coefficient matrices $\tilde{A}_s$, corresponding to local Neumann problems on $\Omega_s$ with boundary conditions $C = 0$ on $\partial \Omega_s \cap \partial \Omega$, similar to that supplying the local Robin problems in (2.6). Furthermore, we must distinguish between degrees of freedom on the boundary and the interior of the subdomain $\Omega_s$ and so we let $\Gamma_s$ and $I_s$ be the set of indices on the boundary and interior respectively. Recalling that $\{\phi_j\}$ are our nodal basis functions, we also define

$$M_{\Gamma_s} = \left( \int_{\Gamma_s} \phi_j \phi_i \right)_{i,j \in \Gamma_s}$$

(2.12)

to be the mass matrix on the subdomain interface. Using standard block notation to denote submatrices of $A_s$ and $\tilde{A}_s$ the discrete DtN eigenproblem can be written as

$$\left( \tilde{A}_{\Gamma_s, r_s} - A_{\Gamma_s, I_s} A^{-1}_{I_s, I_s} A_{I_s, r_s} \right) u_{r_s} = \lambda M_{\Gamma_s} u_{r_s}.$$  

(2.13)

We then make use of the Helmholtz extension of $u_{\Gamma_s}$ to degrees of freedom in $I_s$ given by $u_t = -A^{-1}_{I_s, I_s} A_{I_s, r_s} u_{r_s}$. Letting $u_s$ denote the complete local vector representing the Helmholtz extension, the corresponding global vector which enters the coarse space $Z$ is $D_s u_s$. Further motivation and details on the DtN eigenproblems can be found in [16].

What remains is to determine which eigenvectors of (2.13) should be incorporated into the coarse space. A variety of selection criteria were investigated in [16] which
made it clear that the best choice was to select eigenvectors corresponding to eigenvalues with the smallest real part. That is, a threshold on the abscissa $\eta = \text{Re}(\lambda)$ should be used, namely

$$\eta < \eta_{\text{max}},$$

(2.14)

where $\eta_{\text{max}}$ depends on $k_s = \max_{x \in \Omega_s} k(\vec{x})$. The choice $\eta_{\text{max}} = k_s$ is advocated in [16], however, we recently showed that taking a slightly larger threshold $\eta_{\text{max}} = k_s^{4/3}$ can be beneficial in certain cases in order to gain robustness to the wave number [5]. Unfortunately, this only occurs for the homogeneous problem with sufficiently uniform subdomains. To construct a more robust coarse space we will build upon the GenEO approach.

**2.3.2. The GenEO coarse space.** The Generalised Eigenproblems in the Overlap (GenEO) coarse space was derived in [52] to provide a rigorously robust approach for symmetric positive definite problems even in the presence of heterogeneities. In recent years, this approach have been extended and used within various settings and applications, for example [7, 19, 38, 48]; see also the discussion on developments for other spectral coarse spaces in [51].

Within the original derivation [52], the generalised eigenproblems are defined in a variational framework on the assumption that $a(\cdot, \cdot)$ is a symmetric and coercive bilinear form. On a subdomain $\Omega_s$, an overlapping zone $\Omega_s^o$ is defined as the parts of $\Omega_s$ which overlap with another subdomain and the local eigenproblem

$$a_{\Omega_s}(u, v) = \lambda a_{\Omega_s^o}(\Xi_s(u), \Xi_s(v)) \quad \forall \ v \in V(\Omega_s),$$

(2.15)

is solved for small $\lambda$, where $\Xi_s$ represents the action of the partition of unity operator on $\Omega_s$. To be clear, $a_D(\cdot, \cdot)$ represents the underlying variational problem on the domain $D$ with problem boundary conditions on $\partial \Omega$ and natural (“do nothing”) conditions on $\partial D \setminus \partial \Omega$. The eigenproblem (2.15) provides an appropriate link in order to bound the condition number of the preconditioned operator independently of the heterogeneity and number of subdomains. This bound depends on the smallest eigenvalue $\lambda$ whose corresponding eigenfunction is not incorporated into the GenEO coarse space. Hence, to achieve a desired rate of convergence, all eigenfunctions corresponding to eigenvalues smaller than a threshold (say, $\lambda < \lambda_{\text{max}}$) must be computed. Alternatively, one may opt in practice to compute a fixed number of eigenfunctions per subdomain and use these in order to accelerate convergence.

The restriction within the right-hand side of (2.15) to the overlapping zone is not an essential requirement and alternative formulations can be used. In order to remove the need to track overlap regions, one possibility is to replace $\Omega_s^o$ with the whole of $\Omega_s$, as in [19, 38]. When formulating the discrete eigenproblem, this requires only the local Neumann matrix $\tilde{A}_s$ to be constructed. In this case we must solve

$$\tilde{A}_s u = \lambda D_s A_s D_s u,$$

(2.16)

where $A_s = R_s A R_s^T$ is the local Dirichlet matrix, a sub-matrix of $A$. As with the DtN method, the vectors which then go into the coarse space $Z$ are $R_s^T D_s u$. It is this form of the GenEO eigenproblem in (2.16) that we shall build upon to develop an approach tailored to the heterogeneous Helmholtz problem.

**2.3.3. H-GenEO: a GenEO-type coarse space for Helmholtz problems.** In consideration of GenEO approaches for the Helmholtz problem, a key hurdle is the
loss of operators being definite or self-adjoint. While some progress has been made at the theoretical level for closely related problems \([6, 7]\), currently available analysis has yet to overcome all the challenges present for the Helmholtz problem and rigorous justification for a choice spectral coarse space remains out of reach. The approach taken in \([6, 7]\) is to formulate the GenEO eigenproblem for a nearby symmetric positive definite problem, here corresponding to a Laplace problem and hence given the name \(\Delta\text{-GenEO}\). This problem can be given by setting \(k = 0\) in (2.1) and (2.3). Letting \(L_s\) be the local Dirichlet matrix for this problem in \(\Omega_s\), and \(\tilde{L}_s\) the equivalent Neumann matrix, the \(\Delta\text{-GenEO}\) eigenproblem is given by

\[
\tilde{L}_s u = \lambda D_s L_s D_s u.
\]

(2.17)

This is a positive (semi-)definite eigenproblem with real non-negative eigenvalues \(\lambda\) and, as such, eigenvectors can be chosen in the standard way using a threshold \(\lambda < \lambda_{\text{max}}\). Unfortunately, for the Helmholtz problem the \(\Delta\text{-GenEO}\) approach can perform rather poorly when \(k\) becomes large (see Table 3.1 in Section 3), as might be anticipated from the fact that solutions to the Laplace problem differ considerably to those of the Helmholtz problem in this range.

In order to provide an appropriate spectral coarse space for the Helmholtz problem it stands to reason that a Helmholtz operator must be included. If we try to apply the GenEO eigenproblem (2.16) as is, with matrices stemming from the Helmholtz bilinear form in (2.3), we must first note that the problem is non-self-adjoint and, as such, eigenvalues \(\lambda\) are no longer real in general. As a threshold criterion, as with the DtN approach, we can consider the abscissa \(\eta = \text{Re}(\lambda)\) instead and seek eigenvectors corresponding to \(\eta < \eta_{\text{max}}\). Unfortunately, this formulation fails to be robust and numerically we have found that the eigensolver we use can often break down. Given that, without any relevant theory, it is no longer clear (2.16) provides an appropriate eigenproblem, we develop a different approach which yields a robust method in our numerical experiments.

While the above approaches consider only Helmholtz, or only Laplace, operators in their formulation, we instead link the underlying Helmholtz problem to the positive definite Laplace problem. Since this GenEO-type method targets the Helmholtz problem we call it “H-GenEO”. The local eigenproblem utilised is given by

\[
\tilde{A}_s u = \lambda D_s L_s D_s u.
\]

(2.18)

Since eigenvalues are complex (though, in our experience, tend to cluster close to the real line) we threshold based on the abscissa \(\eta < \eta_{\text{max}}\). We will see the effectiveness of the H-GenEO coarse space for a 2D model problem in Section 3. When used with a threshold (typically we use \(\eta_{\text{max}} = \frac{1}{2}\)), we observe that the number of GMRES iterations for the H-GenEO approach is independent of the wave number \(k\), which is not true of the DtN method in general. Before continuing to our numerical results, we first show a link between the DtN and GenEO eigenproblems and how the H-GenEO method is related.

2.3.4. A link between DtN and GenEO. While the DtN and GenEO eigenproblems look rather different, here we show a link between the two approaches. In particular, consider the GenEO method when we remove the partition of unity matrices \(D_s\) from (2.16), so that we are left with the Neumann matrix on the left and the Dirichlet matrix on the right, namely \(\tilde{A}_s u = \lambda A_s u\). Further, let us use subscripts \(O_s\) and \(I_s\) to denote overlap and interior degrees of freedom in \(\Omega_s\) respectively. Then,
moving all terms to the left-hand side, the GenEO eigenproblem can be written as

\[(2.19) \quad \begin{pmatrix} \tilde{A}_{O_s,O_s} - \lambda A_{O_s,O_s} & (1 - \lambda)A_{O_s,I_s} \\ (1 - \lambda)A_{I_s,O_s} & (1 - \lambda)A_{I_s,I_s} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{O_s} \\ \mathbf{u}_{I_s} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \]

where we have used the fact that the Neumann matrix is equal to Dirichlet matrix except in the block associated with the overlap degrees of freedom. Forming the Schur complement of (2.19) with respect to the \(A_{I_s,I_s}\) block and dividing by \(1 - \lambda\) we obtain

\[(2.20) \quad \left( \tilde{A}_{O_s,O_s} - A_{O_s,I_s}A_{I_s,I_s}^{-1}A_{I_s,O_s} \right) \mathbf{u}_{O_s} = \frac{\lambda}{1 - \lambda} \left( A_{O_s,O_s} - \tilde{A}_{O_s,O_s} \right) \mathbf{u}_{O_s}. \]

Now if the overlap degrees of freedom \(O_s\) are precisely those used as boundary degrees of freedom \(\Gamma_s\) in the DtN method we see that (2.20) resembles the DtN eigenproblem (2.13). The primary difference stems from the right-hand side where we now have the difference between the Dirichlet and Neumann matrices on the boundary degrees of freedom as opposed to a mass matrix, though we note that these can coincide for certain choices of discretisation, for example a simple finite difference scheme on a Cartesian grid where forward or backward differences are used to approximate the Neumann condition. The other difference, aside from the partition of unity in the true GenEO approach, stems from a transformation of the eigenvalues, namely the comparative eigenvalues for the DtN method are

\[\mu = \frac{1}{\lambda^2}.\]

Now consider the H-GenEO eigenproblem (2.18) without the partition of unity matrices. Splitting for the moment \(A = L - k^2 M\) we have

\[(2.21) \quad \begin{pmatrix} \tilde{L}_{O_s,O_s} - \lambda L_{O_s,O_s} - k^2 M_{O_s,O_s} & (1 - \lambda)L_{O_s,I_s} - k^2 M_{O_s,I_s} \\ (1 - \lambda)L_{I_s,O_s} - k^2 M_{I_s,O_s} & (1 - \lambda)L_{I_s,I_s} - k^2 M_{I_s,I_s} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{O_s} \\ \mathbf{u}_{I_s} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \]

Now dividing by \(1 - \lambda\) and defining \(\kappa^2 = \frac{k^2}{1 - \lambda}\) and the corresponding Helmholtz matrices with wave number \(\kappa\) as \(B = L - k^2 M\) we have

\[(2.22) \quad \begin{pmatrix} \tilde{B}_{O_s,O_s} + \frac{\lambda}{1 - \lambda} (L_{O_s,O_s} - L_{O_s,I_s}) & B_{O_s,I_s} \\ B_{I_s,O_s} & B_{I_s,I_s} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{O_s} \\ \mathbf{u}_{I_s} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \]

Using the fact that \(\tilde{L}_{O_s,O_s} - L_{O_s,O_s} = \tilde{B}_{O_s,O_s} - B_{O_s,O_s}\), the resulting Schur complement system is then given as

\[(2.23) \quad \left( \tilde{B}_{O_s,O_s} - B_{O_s,I_s}B_{I_s,I_s}^{-1}B_{I_s,O_s} \right) \mathbf{u}_{O_s} = \frac{\lambda}{1 - \lambda} \left( B_{O_s,O_s} - \tilde{B}_{O_s,O_s} \right) \mathbf{u}_{O_s}. \]

Thus we see that H-GenEO corresponds to solving GenEO problems based on a wave number which varies with the eigenvalue. In particular, since we will ultimately be interested in the eigenvalues \(\lambda\) close to zero, we solve Helmholtz problems at different wave numbers close to \(k\).

To further exhibit the link between these spectral coarse spaces for the Helmholtz problem, we consider example eigenfunctions for both the DtN (2.13) and H-GenEO (2.18) eigenproblems on the central subdomain of a \(5 \times 5\) decomposition into square subdomains for a homogeneous model problem with \(k = 46.5\) (see Section 3 for details). Figure 2.1 displays a selection of eigenfunctions and in the top two rows we plot DtN (top row) and H-GenEO (middle row) eigenfunctions which show the same
features, visually being very similar. Note that, since the central subdomain does not touch the Robin boundary $\Gamma_R$, both eigenproblems are real and symmetric, albeit indefinite, and so all eigenvalues $\lambda$ are real. With DtN, as $\lambda$ increases, variation in the eigenfunctions tends to be restricted to the boundary, as can be seen in Figures 2.1c–2.1e. Such behaviour is observed for many H-GenEO eigenfunction too, however, we also obtain distinct eigenfunctions which are not found amongst DtN eigenfunctions: examples are given in the bottom row of Figure 2.1 and we note that they tend to exhibit large variation in the interior of the subdomain. Nonetheless, there is a clear link between many of the DtN and H-GenEO eigenfunctions.

$$
\begin{align*}
\text{DtN} & \quad \lambda = -225.2 \\
& \quad \lambda = -1.6 \\
& \quad \lambda = 4.6 \\
& \quad \lambda = 32.0 \\
& \quad \lambda = 107.5 \\
\text{H-GenEO} & \quad \lambda = -0.258 \\
& \quad \lambda = -0.006 \\
& \quad \lambda = 0.019 \\
& \quad \lambda = 0.149 \\
& \quad \lambda = 0.466 \\
\text{H-GenEO} & \quad \lambda = -0.431 \\
& \quad \lambda = -0.233 \\
& \quad \lambda = 0.315 \\
& \quad \lambda = 0.315 \\
& \quad \lambda = 0.438 
\end{align*}
$$

Fig. 2.1: Local eigenfunctions for $k = 46.5$. Top row: Examples using DtN (2.13). Middle row: Equivalent examples using H-GenEO (2.18). Bottom row: Examples using H-GenEO which are not found amongst the DtN eigenfunctions.

3. Results and Discussion. In this section we present and discuss numerical results computed using FreeFEM [40], in particular through the functionality of ffddm, which handles the underlying domain decomposition data structures. As a model problem we consider the case of a wave guide in 2D, defined on the unit square $\Omega = (0,1)^2$. We impose homogeneous Dirichlet conditions on two opposite sides, namely (2.1b) with $u_{\Gamma_D} = 0$ on $\Gamma_D = \{0,1\} \times [0,1]$, and Robin conditions on the two remaining sides, that is (2.1c) on $\Gamma_R = [0,1] \times \{0,1\}$. A point source is located in the centre of the domain at $(\frac{1}{2}, \frac{1}{2})$ and provides the forcing function $f$. A schematic of this model problem is found in Figure 3.1.
To discretise the problem we triangulate $\Omega$ using a Cartesian grid with spacing $h$ and alternating diagonals to form a simplicial mesh (see Figure 3.1 where $h = \frac{1}{4}$). The discrete problem (2.4) is then built from using P1 finite element approximation on this mesh. In order to avoid the pollution effect we choose $k$ and $h$ simultaneously so that $k^3 h^2 = \frac{2\pi}{10}$ is fixed. The large sparse linear system (2.4) is solved using right-preconditioned GMRES, with the preconditioner given by the two-level ORAS method (2.8) and choice of coarse space as stated. We terminate the GMRES iteration once a relative residual tolerance of $10^{-6}$ is reached. Unless otherwise stated, within the domain decomposition preconditioner we use minimal overlap: that is, one layer of adjoining mesh elements are added to the non-overlapping subdomains via the extension in (2.5). To solve the local eigenvalue problems in the two-level methods we make use of ARPACK [46], while both the subdomain solves and coarse space operator solves are given by MUMPS [1].

We will first compare coarse spaces in the simplest case of a homogeneous problem, investigating the choice of eigenvalue threshold used. We then show results on how the methods perform in a variety of settings, for instance with non-uniform subdomains, heterogeneity and additional overlap. Finally, a high wave number scalability test is performed for H-GenEO with timings reported.

3.1. A comparison of methods for the homogeneous problem with uniform partitioning. In Table 3.1 we give some benchmark results for the simplest problem of a homogeneous wave guide using a uniform decomposition into 25 square subdomains. We see that the one-level ORAS method (2.7) performs relatively poorly as the wave number $k$ increases. The standard DtN coarse space (2.13) (with $\eta_{\text{max}} = k$) is able to reduce iteration counts with a relatively small coarse space size, however, there is still a clear increase in iterations as $k$ increases. The $\Delta$-GenEO method (2.17), with $\lambda_{\text{max}} = \frac{1}{2}$, performs poorly here, often doing worse than the one-level method despite a larger coarse space than the DtN approach; this may be because the impedance conditions from the wave guide problem are not included in the definition of the $\Delta$-GenEO coarse space and so the eigenfunctions are not appropriate here. Finally, the standard H-GenEO method (2.18) (with $\eta_{\text{max}} = \frac{1}{2}$) performs well and significantly reduces the iteration counts, by a factor of 10 for the largest wave number, and provides robustness to increasing wave number $k$ (in fact iteration counts tend to decrease with $k$). We note that the size of the H-GenEO coarse space is larger than the DtN coarse space and we now explore this further.

![Fig. 3.1: Schematic of the 2D wave guide model problem with example triangular mesh.](image)

To discretise the problem we triangulate $\Omega$ using a Cartesian grid with spacing $h$ and alternating diagonals to form a simplicial mesh (see Figure 3.1 where $h = \frac{1}{4}$). The discrete problem (2.4) is then built from using P1 finite element approximation on this mesh. In order to avoid the pollution effect we choose $k$ and $h$ simultaneously so that $k^3 h^2 = \frac{2\pi}{10}$ is fixed. The large sparse linear system (2.4) is solved using right-preconditioned GMRES, with the preconditioner given by the two-level ORAS method (2.8) and choice of coarse space as stated. We terminate the GMRES iteration once a relative residual tolerance of $10^{-6}$ is reached. Unless otherwise stated, within the domain decomposition preconditioner we use minimal overlap: that is, one layer of adjoining mesh elements are added to the non-overlapping subdomains via the extension in (2.5). To solve the local eigenvalue problems in the two-level methods we make use of ARPACK [46], while both the subdomain solves and coarse space operator solves are given by MUMPS [1].

We will first compare coarse spaces in the simplest case of a homogeneous problem, investigating the choice of eigenvalue threshold used. We then show results on how the methods perform in a variety of settings, for instance with non-uniform subdomains, heterogeneity and additional overlap. Finally, a high wave number scalability test is performed for H-GenEO with timings reported.

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Table 3.1: Preconditioned GMRES iteration counts and size of coarse space (in parentheses) for the homogeneous problem when using ORAS and various coarse spaces. A uniform decomposition into 5 × 5 square subdomains is used, giving 25 subdomains in total.

| k  | h⁻¹ | one-level | DtN   | Δ-GenEO | H-GenEO |
|----|-----|----------|-------|---------|---------|
| 18.5 | 100 | 73       | 19 (147) | 53 (135) | 21 (164) |
| 29.3 | 200 | 97       | 26 (218) | 100 (271) | 18 (370) |
| 46.5 | 400 | 125      | 35 (303) | 148 (560) | 17 (779) |
| 73.8 | 800 | 156      | 42 (502) | 220 (1120) | 15 (1712) |

In Table 3.2 we provide results for both the DtN and H-GenEO methods with differing eigenvalue thresholds $\eta_{\text{max}}$. For DtN we use the standard threshold $\eta_{\text{max}} = k$, the suggested threshold from [5] $\eta_{\text{max}} = k^{4/3}$, and the larger threshold of $\eta_{\text{max}} = k^{3/2}$. For H-GenEO we use the standard threshold $\eta_{\text{max}} = \frac{1}{2}$ as well as the weaker thresholds of $\frac{1}{4}$ and $\frac{1}{8}$, the latter giving coarse space sizes more comparable to the standard DtN approach. To differentiate between these methods we use the notation DtN($\eta_{\text{max}}$) and H-GenEO($\eta_{\text{max}}$) where $\eta_{\text{max}}$ is as specified. We notice in Table 3.2 that increasing the DtN threshold to $\eta_{\text{max}} = k^{4/3}$ significantly improves the iteration counts for this problem so that they are almost independent of $k$, albeit very slightly growing. Increasing the threshold further only marginally improves the iteration counts, which still grow slightly with $k$, but at the expense of a coarse space almost twice the size. On the other hand, if we relax the H-GenEO threshold we start to see higher iteration counts and lose some robustness but generally iteration counts do not increase with $k$ as they do for the standard DtN method. We note that, for this homogeneous problem, roughly comparable coarse space sizes give approximately similar iteration counts and so it is primarily the thresholds used in DtN and H-GenEO that dictate the different growth behaviour we observe.

Table 3.2: Preconditioned GMRES iteration counts and size of coarse space (in parentheses) for the homogeneous problem when using ORAS and the DtN and H-GenEO coarse spaces with varying eigenvalue thresholds. A uniform decomposition into 5 × 5 square subdomains is used, giving 25 subdomains in total.

| k  | h⁻¹ | DtN($k$) | DtN($k^{4/3}$) | DtN($k^{3/2}$) | H-GenEO($\frac{1}{8}$) | H-GenEO($\frac{1}{4}$) | H-GenEO($\frac{1}{2}$) |
|----|-----|----------|----------------|----------------|----------------------|----------------------|----------------------|
| 18.5 | 100 | 19 (147) | 13 (260) | 11 (403) | 46 (80)              | 31 (105)              | 21 (164)              |
| 29.3 | 200 | 26 (218) | 14 (483) | 13 (759) | 53 (139)              | 33 (189)              | 18 (370)              |
| 46.5 | 400 | 35 (303) | 14 (868) | 12 (1479) | 56 (245)              | 35 (378)              | 17 (779)              |
| 73.8 | 800 | 42 (502) | 16 (1588) | 15 (2925) | 40 (546)              | 25 (800)              | 15 (1712)              |

To explore the growth in the size of the coarse space further, in Figure 3.2a we plot coarse space size against the wave number $k$. From this we can see that growth for DtN($k^{4/3}$) is approximately proportional to $k^{4/3}$, while for H-GenEO($\frac{1}{2}$) it is around $k^{5/3}$ for our model problem. When the thresholds are relaxed it becomes less clear.
on the precise relationship but we note that the coarse space sizes grow more slowly with a weaker threshold, especially for the DtN approach. The faster growth seen for DtN\((k^{4/3})\) and H-GenEO\((\frac{1}{2})\) may help accommodate the stronger robustness to \(k\) observed in the iteration counts of Table 3.2. These two approaches appear to provide the best trade-off for obtaining a well-behaved method and so we will focus primarily on these approaches, but first we consider the question of scalability.

3.2. Scalability of DtN and H-GenEO for the homogeneous problem with uniform partitioning. We now investigate the scalability of the DtN and H-GenEO methods. This will depend on the threshold used and so we compare results for DtN\((k)\) and H-GenEO\((\frac{1}{2})\) as well as DtN\((k^{4/3})\) and H-GenEO\((\frac{1}{2})\), with each pair of approaches giving broadly similar iteration counts. Results for the homogeneous problem with \(k = 73.8\) and \(h^{-1} = 800\) are given in Table 3.3 for an increasing number of uniform square subdomains \(N\). We see that the DtN\((k)\) approach does not exhibit scalability here, with iteration counts that noticeably increase with \(N\). Similarly, with the weaker threshold, H-GenEO\((\frac{1}{2})\) also fails to be scalable. On the other hand, both DtN\((k^{4/3})\) and H-GenEO\((\frac{1}{2})\) are scalable here, with low iteration counts that vary little with \(N\).

Comparing the size of the coarse spaces employed, we see that the DtN\((k^{4/3})\) coarse space grows faster with \(N\) and becomes larger than the H-GenEO\((\frac{1}{2})\) coarse space, which may account for its particularly strong robustness to \(N\) here. From Figure 3.2b we see that for both DtN approaches the coarse space size grows approximately proportional to \(N^{0.6}\) while for the H-GenEO method it is around \(N^{0.4}\). This suggests H-GenEO may be advantageous when \(N\) becomes large due to the smaller coarse space required. We note that the size of the DtN\((k)\) or H-GenEO\((\frac{1}{2})\) coarse space sometimes shrinks as we increase \(N\) and in these cases the iteration counts tend to be particularly poor, suggesting that the thresholds of \(\eta_{\text{max}} = k\) for DtN and
Table 3.3: Preconditioned GMRES iteration counts (above) and size of coarse space (below) for the homogeneous problem when using ORAS with the DtN and H-GenEO coarse spaces and a varying number of subdomains $N$ for $k = 73.8$ and $h^{-1} = 800$. A uniform decomposition into $\sqrt{N} \times \sqrt{N}$ square subdomains is used.

| $N$ | 4  | 9  | 16 | 25 | 36 | 49 | 64 | 81 | 100 | 121 | 144 | 169 | 196 |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|
| DtN($k$) | 28 | 32 | 40 | 42 | 51 | 76 | 49 | 94 | 90 | 36 | 37 | 96 | 154 |
| DtN($k^{4/3}$) | 15 | 16 | 19 | 16 | 16 | 15 | 16 | 15 | 15 | 16 | 17 | 17 | 17 |
| H-GenEO($\frac{1}{8}$) | 26 | 31 | 36 | 40 | 71 | 127 | 81 | 116 | 247 | 194 | 138 |
| H-GenEO($\frac{1}{2}$) | 13 | 15 | 15 | 15 | 15 | 15 | 16 | 16 | 16 | 18 | 18 | 18 | 19 |
| DtN($k$) | 124 | 251 | 362 | 502 | 605 | 736 | 843 | 1000 | 946 | 1329 | 1554 | 1529 | 1327 |
| DtN($k^{4/3}$) | 392 | 790 | 1175 | 1588 | 1994 | 2366 | 2753 | 3176 | 3611 | 3976 | 4369 | 4955 | 5118 |
| H-GenEO($\frac{1}{8}$) | 200 | 305 | 408 | 546 | 536 | 600 | 788 | 733 | 936 | 927 | 780 | 974 | 1264 |
| H-GenEO($\frac{1}{2}$) | 852 | 1116 | 1428 | 1712 | 1903 | 2261 | 2444 | 2629 | 3120 | 3204 | 3482 | 3882 | 3816 |

$\eta_{\text{max}} = \frac{1}{8}$ are not doing a suitable job in capturing the eigenfunctions required for scalability. As such, we now narrow our focus to the DtN($k^{4/3}$) and H-GenEO($\frac{1}{2}$) approaches.

3.3. Robustness of DtN and H-GenEO for the homogeneous problem with METIS decomposition. We now consider utilising non-uniform subdomains, as provided through the software METIS [42]. In Table 3.4 we compare DtN($k^{4/3}$) and H-GenEO($\frac{1}{2}$) in this situation, again for the homogeneous problem. We observe that both methods retain their robustness, providing scalable and nearly $k$-independent iteration counts. We note that the coarse space sizes for each method tends to be slightly larger with the more general decompositions used by METIS but otherwise the same trends are seen. As such, we conclude that non-uniform decompositions can be well-handled by the spectral coarse spaces employed here.

3.4. The effect of heterogeneity. We now turn our attention to the key property of robustness to heterogeneities. For this we consider layered media within the wave guide. Three configurations, each having ten layers, will be used and are detailed in Figure 3.3. The heterogeneity is introduced in the wave speed $c(x)$ and in each case $c$ takes values from 1 to $\rho$, where $\rho$ is a contrast parameter determining the strength of the heterogeneity. The wave number is then given by $k = \omega/c$ where $\omega$ is the angular frequency; we will vary both $\omega$ and $\rho$ in our tests. Note that for the DtN method the eigenvalue threshold will now depend on $k_s = \max_{x \in \Omega_s} k(x)$ which may be different for different subdomains $\Omega_s$. To avoid notational clutter we omit the subscript when referring to the method, namely retaining the name DtN($k^{4/3}$).

Results for DtN($k^{4/3}$) and H-GenEO($\frac{1}{2}$) for the increasing layers problem (Figure 3.3a) are provided in Table 3.5. Unfortunately we see that the DtN($k^{4/3}$) loses robustness with the heterogeneity present in this problem. In particular, we lose any robustness to the wave number $k$ and for the largest wave number used we also see that changes in the contrast, given by $\rho$, can begin to have a sizeable impact on the iteration counts despite otherwise being relatively stable to changes in $\rho$. To a lesser
Table 3.4: Preconditioned GMRES iteration counts (above) and size of coarse space (below) for the homogeneous problem when using ORAS with DtN($k^{4/3}$) or H-GenEO($\frac{1}{2}$) and a varying number of subdomains. A non-uniform decomposition into $N$ subdomains is used, given by METIS.

| $k$    | $h^{-1}$ | Number of subdomains $N$ | DtN($k^{4/3}$) | H-GenEO($\frac{1}{2}$) |
|--------|---------|--------------------------|----------------|------------------------|
|        |         | 20 | 40 | 80 | 120 | 160 | 200 | 20 | 40 | 80 | 120 | 160 | 200 |
| 18.5   | 100     | 10 | 10 | 10 | 10 | 10 | 10 | 15 | 17 | 19 | 22 | 27 | 27 |
| 29.3   | 200     | 12 | 15 | 11 | 12 | 12 | 12 | 15 | 17 | 19 | 20 | 22 | 23 |
| 46.5   | 400     | 12 | 13 | 15 | 13 | 13 | 13 | 15 | 16 | 16 | 18 | 20 | 20 |
| 73.8   | 800     | 15 | 15 | 14 | 16 | 14 | 16 | 15 | 16 | 17 | 17 | 17 | 19 |
| 117.2  | 1600    | 14 | 15 | 16 | 17 | 15 | 16 | 14 | 15 | 15 | 16 | 16 | 16 |
| 18.5   | 100     | 281 | 422 | 652 | 843 | 1005 | 1157 | 201 | 285 | 383 | 471 | 524 | 589 |
| 29.3   | 200     | 477 | 758 | 1130 | 1410 | 1693 | 1922 | 400 | 574 | 783 | 958 | 1097 | 1245 |
| 46.5   | 400     | 959 | 1466 | 2132 | 2677 | 3151 | 3553 | 869 | 1193 | 1670 | 2008 | 2253 | 2507 |
| 73.8   | 800     | 1695 | 2563 | 3751 | 4672 | 5486 | 6199 | 1863 | 2456 | 3433 | 4147 | 4749 | 5338 |
| 117.2  | 1600    | 3049 | 4695 | 6831 | 8486 | 9896 | 11092 | 4238 | 5680 | 7575 | 9049 | 10273 | 11305 |

Fig. 3.3: Piecewise constant layer profiles for the wave speed $c(x)$. For the darkest shade $c(x) = 1$ while for the lightest shade $c(x) = \rho$, with $\rho$ being the contrast factor.

extent we also lose scalability with DtN($k^{4/3}$) as the iteration counts now slowly increase with $N$. On the other hand, H-GenEO($\frac{1}{2}$) has strong robustness throughout, both with respect to the wave number $k$, the contrast in the heterogeneity $\rho$, and scalability as $N$ increases. As such, we see a clear preference for H-GenEO($\frac{1}{2}$) as a stable and reliable method for heterogeneous problems.

We also consider the case of a diagonal layers problem (Figure 3.3c) in Table 3.6. Here the issues with DtN($k^{4/3}$) are reduced but there is still some increase in iteration counts, especially for higher wave numbers $k$ and a larger number of subdomains $N$. We note, in results not shown here, that DtN($k^{3/2}$) also suffers from the same lack of robustness. For H-GenEO($\frac{1}{2}$), however, we still have good robustness to the parameters of the problem. At this point it is worth mentioning that, with H-GenEO, for small wave numbers $k$ there can be some slight loss in scalability but this diminishes as the wave number increases. We note that for the problem instances of small $k$ and
Table 3.5: Preconditioned GMRES iteration counts (above) and size of coarse space (below) for the heterogeneous increasing layers problem when using ORAS with $\text{DtN}(k^{4/3})$ or $\text{H-GenEO}(\frac{1}{2})$ and a varying number of subdomains. A uniform decomposition into $\sqrt{N} \times \sqrt{N}$ square subdomains is used.

| Number of subdomains $N$ | $\omega$ | $h^{-1}$ | $\rho$ | $\text{DtN}(k^{4/3})$ | $\text{H-GenEO}(\frac{1}{2})$ |
|--------------------------|---------|---------|-------|----------------------|---------------------|
|                          | 10      |         | 100   | 16 36 64 100 144 196 | 16 36 64 100 144 196 |
|                          | 29.3    | 200     | 100   | 29 37 41 52 55 58   | 15 16 19 18 18 19   |
|                          |         |         | 1000  | 44 44 50 58 52 52   | 15 15 17 18 17 17   |
|                          | 46.5    | 400     | 100   | 32 38 41 66 65 73   | 15 16 16 19 18 18   |
|                          |         |         | 1000  | 60 67 75 84 73 72   | 14 15 16 18 17 17   |
|                          | 73.8    | 800     | 100   | 35 43 42 40 58 69   | 15 17 16 17 18 17   |
|                          |         |         | 1000  | 87 95 108 112 117 110| 14 15 15 16 16 16   |
|                          |         |         |       | 89 93 107 111 114 109| 14 15 15 16 16 16   |

large $N$ where iteration counts are highest, the number of eigenvectors per subdomain is small and so the achieved tolerance on the eigenvalues may be somewhat weaker than $\frac{1}{2}$, which may explain the slightly poorer performance. Since we are primarily interested in increasingly large wave numbers, where this issue diminishes, we do not worry further about this and assert that for problems of interest $\text{H-GenEO}(\frac{1}{2})$ provides a scalable method.

We further consider the heterogeneous problem when making use of METIS for more general non-uniform subdomain decompositions in order to ensure that $\text{H-GenEO}$ is able to handle both difficulties together. For this we consider the alternating layers problem (Figure 3.3b) and provide results in Table 3.7. We find that $\text{H-GenEO}(\frac{1}{2})$ performs very well and continues to provide a rather robust method, even in the presence of heterogeneity on non-uniform subdomains. This further evidences the strength of the $\text{H-GenEO}(\frac{1}{2})$ approach and we now study it more closely, dropping reference to the eigenvalue tolerance and simply denoting the method as $\text{H-GenEO}$.

### 3.5. The effect of boundary conditions within the H-GenEO eigenproblem

We now consider the choice of boundary conditions within H-GenEO in light of
Table 3.6: Preconditioned GMRES iteration counts (above) and size of coarse space (below) for the heterogeneous diagonal layers problem when using ORAS with DtN($k^{4/3}$) or H-GenEO($\frac{1}{2}$) and a varying number of subdomains. A uniform decomposition into $\sqrt{N} \times \sqrt{N}$ square subdomains is used.

| $\omega$ | $h^{-1}$ | $\rho$ | Number of subdomains $N$ | DtN($k^{4/3}$) | H-GenEO($\frac{1}{2}$) |
|---------|----------|--------|--------------------------|----------------|---------------------|
|         |          |        | 16 | 36 | 64 | 100 | 144 | 196 | 16 | 36 | 64 | 100 | 144 | 196 |
| 10      |          |        | 13 | 14 | 13 | 14 | 21 | 25 | 16 | 18 | 20 | 18 | 23 | 25 |
| 29.3    | 200      | 100    | 13 | 14 | 14 | 14 | 22 | 25 | 16 | 18 | 20 | 18 | 23 | 25 |
| 1000    |          |        | 13 | 14 | 14 | 14 | 22 | 25 | 16 | 18 | 20 | 18 | 23 | 25 |
| 10      |          |        | 15 | 14 | 14 | 16 | 25 | 31 | 16 | 17 | 17 | 26 | 21 | 22 |
| 46.5    | 400      | 100    | 15 | 14 | 15 | 16 | 25 | 34 | 16 | 17 | 18 | 27 | 22 | 22 |
| 1000    |          |        | 15 | 14 | 15 | 16 | 25 | 34 | 16 | 17 | 18 | 27 | 22 | 22 |
| 10      |          |        | 14 | 18 | 16 | 15 | 20 | 26 | 16 | 17 | 17 | 17 | 19 | 20 |
| 73.8    | 800      | 100    | 15 | 18 | 16 | 15 | 32 | 39 | 16 | 17 | 17 | 19 | 20 |
| 1000    |          |        | 15 | 18 | 16 | 15 | 32 | 39 | 16 | 17 | 17 | 19 | 20 |
| 10      |          |        | 336 | 593 | 866 | 1090 | 1376 | 1390 | 260 | 376 | 499 | 689 | 737 | 828 |
| 29.3    | 200      | 100    | 336 | 594 | 866 | 1090 | 1376 | 1389 | 259 | 375 | 499 | 687 | 737 | 826 |
| 1000    |          |        | 336 | 594 | 866 | 1090 | 1375 | 1390 | 259 | 375 | 499 | 687 | 737 | 826 |
| 10      |          |        | 621 | 1075 | 1540 | 1910 | 2370 | 2622 | 543 | 789 | 1095 | 1384 | 1599 | 1825 |
| 46.5    | 400      | 100    | 621 | 1074 | 1539 | 1908 | 2369 | 2615 | 541 | 790 | 1093 | 1381 | 1596 | 1824 |
| 1000    |          |        | 621 | 1075 | 1539 | 1907 | 2368 | 2614 | 541 | 790 | 1093 | 1381 | 1596 | 1824 |
| 10      |          |        | 1164 | 1947 | 2692 | 3592 | 4145 | 4608 | 1145 | 1636 | 2243 | 2823 | 3233 | 3681 |
| 73.8    | 800      | 100    | 1163 | 1947 | 2693 | 3592 | 4130 | 4566 | 1141 | 1633 | 2239 | 2822 | 3232 | 3671 |
| 1000    |          |        | 1163 | 1946 | 2693 | 3592 | 4131 | 4569 | 1141 | 1633 | 2239 | 2822 | 3232 | 3671 |

The fact that, for wave propagation problems, impedance conditions can often prove more practical within overlapping Schwarz methods. To this end, we consider the H-GenEO eigenproblem where the Neumann boundary condition is replaced by an impedance condition instead (i.e., the Robin condition in (2.6b)). Results for this impedance-H-GenEO method are given in Table 3.8 for the homogeneous problem with uniform square subdomains. We see that, while the use of this eigenproblem retains the $k$-independent behaviour of H-GenEO, it lacks scalability as we increase the number of subdomains $N$. This shows that the Neumann condition within the eigenproblem is an important aspect of H-GenEO.

3.6. The effect of more overlap when using H-GenEO. So far all our results use minimal overlap. Here we consider the case of increasing the overlap between subdomains, this is done by adding on layers of adjoining elements to each subdomain in a symmetric way, so that minimal overlap is given by an overlap parameter of 2; that is the overlapping region has a width of 2 elements. In Table 3.9 we report results for increasing overlap when using H-GenEO for the homogeneous problem with $k = 46.5$ and $h^{-1} = 400$ and where a uniform decomposition is used. We see that adding on a small amount of overlap can slightly decrease the iteration counts but
Table 3.7: Preconditioned GMRES iteration counts for the heterogeneous alternating layers problem with $\rho = 10/100/1000$ when using ORAS with H-GenEO(\frac{1}{2}) and a varying number of subdomains. A non-uniform decomposition into $N$ subdomains is used, given by METIS.

| $\omega / h^{-1}$ | 20   | 40   | 80   | 120  | 160  | 200  |
|-------------------|------|------|------|------|------|------|
| 18.5 100          | 17   | 17   | 17   | 19   | 19   | 19   |
| 29.3 200          | 16   | 16   | 16   | 17   | 17   | 17   |
| 46.5 400          | 17   | 17   | 17   | 18   | 18   | 18   |
| 73.8 800          | 16   | 16   | 16   | 17   | 17   | 17   |
| 117.2 1600        | 15   | 16   | 16   | 16   | 16   | 16   |

Table 3.8: Preconditioned GMRES iteration counts for the homogeneous problem when using ORAS with impedance-H-GenEO (the eigenproblem (2.18) is altered to have impedance as opposed to Neumann boundary conditions on the left-hand side) and a varying number of subdomains. A uniform decomposition into $\sqrt{N} \times \sqrt{N}$ square subdomains is used.

| $k / h^{-1}$ | 4    | 9    | 16   | 25   | 36   | 49   | 64   | 81   | 100  | 121  | 144  | 169  | 196  |
|--------------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 18.5 100     | 17   | 19   | 23   | 27   | 30   | 36   | 42   | 45   | 43   | 58   | 61   | 61   | 67   |
| 29.3 200     | 17   | 19   | 22   | 25   | 34   | 33   | 41   | 38   | 35   | 49   | 60   | 62   | 65   |
| 46.5 400     | 15   | 18   | 19   | 22   | 26   | 25   | 26   | 39   | 43   | 47   | 52   | 51   | 54   |
| 73.8 800     | 15   | 19   | 19   | 20   | 25   | 27   | 26   | 35   | 33   | 39   | 43   | 44   | 51   |

increasing the overlap width further can give much poorer results, especially when using a large number of subdomains $N$. We note that the size of the coarse space decreases somewhat as the overlap is increased, however, the extra computational effort required to deal with the larger subdomains will hamper any gains from this, along with the increased iteration counts. From these results we determine that the H-GenEO coarse space is best suited to the case of minimal overlap, as we have used elsewhere throughout this work.

3.7. High wave number scalability and timing results for H-GenEO. To conclude our numerical results we consider the use of H-GenEO within a high wave number example and explore timings and the overall scalability of the approach. To this end we consider the homogeneous wave guide with a wave number of $k = 186.0$ and mesh width $h^{-1} = 3200$, giving a total problem size of 10,246,401 dofs. To deal with this large problem we use METIS to give a non-uniform decomposition into subdomains and assign one core per subdomain to solve using the ARCHIE-WeSt supercomputing facility on up to 400 cores (the machine uses Intel Xeon Gold 6138 processors at 2.0 GHz with 4.8 GB RAM per core).

Results are tabulated in Table 3.10 and, in addition, we detail the run time (in seconds), using this to determine the parallel efficiency based on the smallest run on $N = 80$ cores, and the percentage of time spent by the eigensolver to solve
Table 3.9: Preconditioned GMRES iteration counts (above) and size of coarse space (below) for the homogeneous problem when using ORAS with H-GenEO, varying the amount of overlap (in terms of element width, with 2 representing minimal overlap) and number of subdomains for $k = 46.5$ and $h^{-1} = 400$. A uniform decomposition into $\sqrt{N} \times \sqrt{N}$ square subdomains is used.

| Overlap | Number of subdomains $N$ |
|---------|--------------------------|
|         | 4  | 9  | 16 | 25 | 36 | 49 | 64 | 81 | 100 | 121 | 144 | 169 | 196 |
| 2       | 14 | 15 | 17 | 16 | 16 | 20 | 26 | 19 | 19 | 22 | 21 |
| 4       | 10 | 11 | 12 | 13 | 12 | 17 | 14 | 16 | 17 | 21 | 20 |
| 8       | 8  | 10 | 10 | 13 | 12 | 20 | 23 | 22 | 26 | 31 | 27 |
| 16      | 13 | 21 | 26 | 26 | 37 | 77 | 61 | 75 | 86 | 109 | 178 | 157 | 164 |

The H-GenEO eigenproblems. The timing results are also displayed graphically in Figure 3.4. We see that the iteration counts show good scalability, increasing only very mildly as we increase the number of subdomains fivefold. This is also seen in the run times, which decrease as we use more cores, and hence more subdomains, to solve the problem. In particular, we see that the parallel efficiency remains over $100\%$, showing strong scalability of the approach, in part due to the fact that as $N$ increases we have to solve smaller eigenproblems and so the percentage of time spent by the eigensolver drops significantly as we increase $N$. Overall these provide promising results that the H-GenEO method can be effective for the solution of high wave number problems in 2D.

Table 3.10: Results and timings for the homogeneous problem when using ORAS with H-GenEO($\frac{k}{4}$) and a varying number of subdomains for $k = 186.0$ and $h^{-1} = 3200$, giving a total of 10,246,401 dofs. A non-uniform decomposition into $N$ subdomains is used, given by METIS.

| $N$  | 80  | 120 | 160 | 200 | 240 | 280 | 320 | 360 | 400 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Iteration count | 14  | 16  | 15  | 16  | 17  | 17  | 18  | 19  | 19  |
| Coarse space size | 16014 | 19018 | 21348 | 23747 | 25560 | 27270 | 28793 | 30357 | 31773 |
| Run time (s) | 1214.4 | 614.6 | 404.4 | 279.3 | 217.3 | 195.0 | 159.4 | 154.0 | 147.6 |
| Parallel efficiency | —   | 132% | 150% | 174% | 186% | 178% | 190% | 175% | 165% |
| Eigensolve time | 68.6% | 70.1% | 66.8% | 62.7% | 53.7% | 52.3% | 41.6% | 39.3% | 37.3% |
4. Conclusions. In this work we have developed and explored a GenEO-type coarse space for additive Schwarz methods that is appropriate for the heterogeneous Helmholtz problem. We have conducted extensive numerical tests to show how this approach behaves on a 2D model test problem of a wave guide discretised using finite elements on a pollution-free mesh, comparing our method with the DtN coarse space. We find that only our H-GenEO approach is robust to heterogeneity and increasing wave number $k$, and further provides a scalable method such that iteration counts of right-preconditioned GMRES remain almost constant as the number of subdomains grows. Wave number independent convergence is observed, albeit at the cost of a coarse space which grows as $k$ increases, and is achieved consistently for non-uniform partitioning into subdomains and in the presence of strong heterogeneity. These results show promise that H-GenEO can be used as an effective coarse space for challenging heterogeneous problems.

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