A POLYNOMIAL MULTIGRID SMOOTHER FOR THE ITERATIVE SOLUTION OF THE HETEROGENEOUS HELMHOLTZ PROBLEM

WIM VANROOSE∗, BRAM REPS†, AND HISHAM BIN ZUBAIR‡

Abstract. In this paper we develop a robust multigrid preconditioned Krylov subspace method for the solution of heterogeneous indefinite Helmholtz problems. The preconditioning operator is constructed by discretizing the original Helmholtz equation on a complex stretched grid. As this preconditioning operator has the same wavenumber as the original problem, and the only difference stems from the complex stretching of the discretization grid, its spectrum closely approximates the spectrum of the original Helmholtz operator, resulting in a fast converging Krylov subspace method. We have analyzed a multigrid cycle based on polynomial smoothers and have found a condition on the parameters used in the complex stretching of the discretization grid such that the existence of a stable third order polynomial smoother is guaranteed. In practice we use three iterations of GMRES as a smoother, and have found this to be a viable smoother for the multigrid preconditioning process. We apply the method to various test problems and report on the observed convergence rate.

1. Introduction. The efficient numerical solution of the Helmholtz equation

\[ Hu \equiv -\Delta + k^2 u = f \text{ in } \Omega \]  

with a space dependent wave number \( k \) is important for many areas of science and engineering. Examples are seismic exploration \[2\], imaging with tomography \[12\] or photo lithography where the propagation of an optical wave through a photo resist determines the exposed pattern \[18\]. Even the Schrödinger equation that describes the dynamics of electrons in molecules can be rewritten as a Helmholtz equation with a space dependent wave number \[3\].

After discretization of \( H \) on a grid with grid distance \( h \), the discrete negative Laplacian, \( -\Delta_h \), in (1.1) leads to a spectrum that is spread between 0 and a point on the real axis whose magnitude is of order \( 1/h^2 \). However, the wave number will shift this spectrum in the negative direction. This leads to an indefinite matrix for wave numbers \( k \) larger than a certain threshold. This means that the spectrum is spread over both the positive real part and the negative real part of the complex plane, not necessarily excluding zero as an eigenvalue.

This indefiniteness prevents the efficient solution through a preconditioned Krylov subspace method. Typically, in these methods an unfavorable condition number caused by the Laplacian is improved by an efficient preconditioner. For positive definite problems the method of choice for preconditioning is multigrid which is linear in time. However, its nice convergence properties are destroyed when it is applied to the indefinite Helmholtz equation.

Alternative preconditioners for the Helmholtz equation have been proposed by Haber and MacLachlan \[11\] that transforms the problem into a complex valued reaction-diffusion equation. Bollhöfer, Grote and Schenk developed a multilevel strategy based on incomplete factorizations \[4\]. In his PhD thesis Pinel looked at two-level preconditioners \[13\]. Gander and Nataf looked at a preconditioner which had a analytic incomplete factorization \[10\] and Plessix and Mulder at separation of
variables [13]. A preconditioner based on multigrid was analyzed by Elman, Ernst and O’Leary [7], while Erlangga, Vuik and Oosterlee [9] used multigrid applied to a Helmholtz equation with a complex wave number. This paper is based on the work of the latter two papers.

Two difficulties emerge when multigrid is applied to the Helmholtz problem. First, typical smoothers like weighted Jacobi or Gauss-Seidel are unstable for indefinite problems. The modes with a negative eigenvalue grow under the action of the smoother. These unstable modes are the smoothest modes and for slightly indefinite problems this instability can be compensated by coarse grid correction [5, 17]. However, for substantially indefinite problems the coarse grid operator itself becomes divergent and has been analyzed in detail by Elman, Ernst and O’Leary [7]. They found that during the coarse grid correction certain modes are amplified when an eigenvalue of the coarse grid is close to zero. This gives rise to peaks in the convergence plots as a function of the wave number $k$, which can be considered as wave number dependent resonances.

An important innovation that avoids these resonances was introduced by Erlangga, Vuik and Oosterlee [9] that extended the work that Bayliss, Goldstein and Turkel did in [1]. They define their preconditioner as a complex shifted Laplacian (CSL)

$$M_{CSL} u \equiv - (\Delta + \beta^2 k^2) u \text{ in } \Omega,$$

where the wave number is multiplied by a complex number $\beta \in \mathbb{C}$. Note in particular that the symbol used for this complex number in [9] is $\beta$, whereas in this paper we write $\beta^2$, which is more compliant with our development. For problems having a constant wavenumber $k$, the spectrum of the discretized complex shifted Laplacian preconditioner can be seen as a translation of the spectrum of the Helmholtz matrix $H_h$ in the complex plane. The real part of the shift defines the horizontal displacement while the imaginary part defines the vertical displacement. The spectrum can therefore be moved as far from the origin as necessary. This makes the preconditioning operator feasible for multigrid inversion, since the shift mitigates the coarse grid correction by keeping the spectrum of the coarse grid operator away from the origin. The resonances are now broadened and washed out. However, the shift $\beta$ is a parameter in the method. From an iterative viewpoint the preconditioner and the original problem are inversely related. Measures to enhance the multigrid inversion (by increasing the shift magnitude) deteriorates the Krylov convergence, and vice versa. The optimal shift is therefore a compromise between the multigrid and the Krylov parts of the solver.

The eigenvalues of the resulting discrete preconditioned system, $(M_{CSL}^h)^{-1} H_h$, lie inside a small circle in the complex plane, away from zero, when Sommerfeld radiation boundary conditions are applied. The same complex shift idea can be used for other absorbing boundary conditions such as exterior complex stretching (ECS), where the Helmholtz operator in (1.1) is defined on a partially complex domain [15]. Similar to Sommerfeld conditions the spectrum of the preconditioner is then shifted away from the origin, while the preconditioned system is ideally clustered for the outer Krylov subspace method. In [15] the alternative complex stretched grid (CSG) preconditioner

$$M_{CSG} u \equiv - (\Delta + k^2) u \text{ in } \Omega$$

is defined, where the Helmholtz operator is retained but the domain is altered so that $\Delta$ is discretized with a complex valued grid distance. A proper choice of the domain $\Omega$, typically a complex rotation over an angle $\theta_\beta$, introduces a favorable rotation in the spectrum of the Helmholtz operator, away from the origin.
The introduction of the complex shifts, either in (1.2) or (1.3), avoids the appearance of resonances but it does not prevent the smoother from becoming unstable. In addition, both preconditioners leave the user with choosing a proper shift \( \beta \) or domain rotation \( \theta_\beta \), respectively. This paper focuses on finding a suitable smoother for complex shifted or stretched Laplacians with ECS absorbing boundary layers. We focus on polynomial smoothers that can be viewed as products of multiple \( \omega \)-Jacobi steps with a different choice of \( \omega \) in each step. Requiring that this smoother is stable leads us to conditions on the parameters used in the preconditioner.

In the numerical results section we report also the convergence rates when the polynomial smoother is replaced by GMRES(\( m \)). And we find that using GMRES(3) on all levels gives a satisfactory convergence. This builds on the work of Elman et al. [7] which analyzed and optimized a smoother schedule that combines Jacobi smoothing with GMRES. However, this gives rise to complicated multilevel methods, where many GMRES iterations are required on some levels while on others a Jacobi sweep suffices.

In this paper the wave number is denoted by \( k \). \( M^{CSG}_h \) denotes the discretized complex stretched grid preconditioning matrix, while \( M^{CSG} \) denotes the continuous preconditioning operator. Furthermore we use the following notations, see also Figure 1.1: \( h \) for the original interior real grid distance of the ECS grid, \( \theta_\gamma \) for the rotation angle of the exterior absorbing ECS layer, \( h_\gamma \) the exterior complex grid distance of the ECS layer, \( h_\gamma = h e^{i \theta_\gamma} \) and \( \theta_\beta \) for the rotation angle of the interior complex stretched domain for \( M^{CSG} \). In the same way we use \( h_\beta \) the interior complex grid distance for \( M^{CSG}_h \), \( h_\beta = h e^{i \theta_\beta} \). We also use \( \lambda^{(k)}_\beta \) for the eigenvalue corresponding to the eigenmode with the highest energy, or most oscillatory, on the interior region, \( \lambda^{(k)}_\gamma \) for the eigenvalue corresponding to the eigenmode with the highest energy, or most oscillatory, on the ECS layers and \( \lambda_0 \approx -k^2 \) the lowest energy eigenvalue, also referred to as the smoothest eigenvalue.

![Fig. 1.1: A one-dimensional illustration of the computational grids, the extension to multiple dimension is straightforward with Kronecker products. The original ECS grid (o) for the Helmholtz operator \( H \) has a real grid distance \( h \) in the interior region, for \( 0 \leq x \leq 1 \), and a complex grid distance \( h_\gamma \) on the ECS layer, for \( x > 1 \). The CSG domain (+) for the complex stretched grid preconditioner \( M^{CSG} \) has a complex grid distance \( h_\beta \) in the interior region, for \( 0 \leq x \leq 1 \), and the same complex grid distance \( h_\gamma \) on the ECS layer, for \( x > 1 \).](image)

2. Background on the spectrum. In this section we will briefly summarize the results from [15] for a D-dimensional model Helmholtz problem. In the next section a lower bound for the CSG-parameter \( \theta_\beta \) is found in order to have a stable
multigrid method for the preconditioner resulting in a good overall convergence of the
preconditioned Krylov subspace method.

Suppose we have a one dimensional complex grid

\[(z_j)_{0 \leq j \leq n+m} = \begin{cases} jh_\beta & (0 \leq j \leq n), \\ 1 + (j - n)h_\gamma & (n + 1 \leq j \leq n + m), \end{cases} \tag{2.1} \]

that consists of \(n\) intervals of complex grid distance \(h_\beta\) followed by \(m\) intervals of
complex grid distance \(h_\gamma\) as illustrated in Figure 1.1.

This particular kind of grid is used to create a CSG preconditioner \(1.3\) by
discretizing the Helmholtz equation on it. It originates from an ECS grid for the
original Helmholtz matrix \(H_h\) by replacing its interior real grid distance \(h\) by \(h_\beta = e^{i\theta_\beta}\)
for complex rotation or \(h_\beta = h(1 + i \tan(\theta_\beta))\) for complex shifting \[15\]. The exterior
grid distance \(h_\gamma = e^{i\theta_\gamma}\) or \(h_\gamma = h(1 + i \tan(\theta_\gamma))\) is the same for \(H_h\) and \(M_h^{CSG}\) and
forms the absorbing ECS layer.

We discretize the Laplacian operator \(\Delta\) in Equation \(1.1\) on \(2.1\) with the
Shortley-Weller finite difference scheme for non-uniform grids in one dimension

\[
\frac{d^2u}{dz^2}(z_j) \approx \frac{2}{h_{j-1} + h_j} \left( \frac{1}{h_{j-1}} u_{j-1} - \left( \frac{1}{h_{j-1}} + \frac{1}{h_j} \right) u_j + \frac{1}{h_j} u_{j+1} \right) \tag{2.2}
\]

in grid point \(j\), where \(h_{j-1}\) and \(h_j\) are the left and right mesh widths respectively, and
may belong either to the \(h_\beta\) category or to the \(h_\gamma\) category. The discretization leads
to a linear system

\[
M_h^{CSG} u_h \equiv -(L_h + k^2 I_h) u_h = g_h, \tag{2.3}
\]

where \(L_h\) represents the discretized Laplacian, \(I_h\) is the identity matrix and \(g_h\) is a
vector containing source function values sampled at the grid points. The discretization
matrix for the higher dimensional problem is created by Kronecker products of the
one-dimensional matrices.

**Lemma 2.1.** The spectrum of the \(D\)-dimensional Helmholtz operator in Equation \(1.1\)
discretized with the Shortley-Weller formula \(2.2\) on the CSG-grid defined in \(2.1\), is bounded in the complex plane by a triangle \(z_0 z_1 z_2\) described by the complex
points \(z_0 = -k^2\), \(z_1 = -k^2 + 4D/h_\beta^2\) and \(z_2 = -k^2 + 4D/h_\gamma^2\).

**Proof.** This easily follows from the results in \[15\] for the discretized Helmholtz
equation on an ECS-grid. \(\square\)

The eigenvalues of the Helmholtz discretization matrix on the CSG-grid are not
randomly distributed inside the triangle \(z_0 z_1 z_2\), defined in Lemma 2.1, their exact
location is related to a physical interpretation. The eigenvalues that are close to the
vertex \(z_0 = -k^2\) are aligned and correspond to the smoothest or low frequency
eigenvectors on the entire CSG-grid. We will refer to them as the smoothest eigenvalues.
There are oscillatory or high frequency eigenvectors localized on the interior part of the
CSG-grid with eigenvalues in the neighborhood of the second vertex \(z_1 = -k^2 + 4D/h_\beta^2\).
The region around the third vertex \(z_2 = -k^2 + 4D/h_\gamma^2\) contains the eigenvalues with
high frequency eigenvectors localized on the absorbing ECS layer. We will refer to them
as the high frequency eigenvalues on the interior part of the domain and the
ECS layer respectively.

**Remark 1.** We will denote the three eigenvalues that are closest to the vertices by
\(\lambda_0 \approx z_0\), \(\lambda_\beta^{(k)} \approx z_1\) and \(\lambda_\gamma^{(k)} \approx z_2\). They move closer to the three vertices of the triangle
with finer discretization, so for simplicity we will no longer make the distinction between the vertices $z_0$, $z_1$ and $z_2$ and the actual extreme eigenvalues $\lambda_0$, $\lambda_\beta^{(k)}$ and $\lambda_\gamma^{(k)}$ in the remainder of the paper.

3. A Polynomial smoother. Building a multigrid method involves designing a hierarchy of grids of different resolutions together with the proper restriction and prolongation operators to translate information from one grid to another. Another important ingredient of the multigrid method is the smoother. This is the relaxation method that is used on each level to eliminate the high frequency modes of the error. Multigrid methods can be very efficient when smoothing and coarse grid correction complement each other and perform poorly (if at all) when this complementarity cannot be put together. Due to indefiniteness the discretized Helmholtz problem poses this difficulty for multigrid built on standard relaxation methods such as $\omega$-Jacobi or Gauss-Seidel. Even if the discretization matrix has all nonzero eigenvalues on the finest multigrid level, one or more coarser representations can have eigenvalues undesirably close to zero that can destroy the smoothing of the relaxation method on that level and therefore the entire multigrid performance. One workaround is to invest computational effort in more robust smoothers. In [7] classical smoothers were replaced by the GMRES method on problematic levels when multigrid is applied to the Helmholtz problem. Instead of running a few iterates of a relaxation method, GMRES is applied to the error equation. When this is applied to the original Helmholtz problem it can take a large number of expensive iterations on every troublesome level. In the end this GMRES accelerated multigrid method is used as a preconditioner for an outer GMRES method on the Helmholtz problem.

In this paper we explore the idea of the GMRES accelerated multigrid method but applied to an altered Helmholtz operator such as the preconditioner $M_{CSG}$, instead of to the original $H$. The advantage is that it needs at most three GMRES iterations to cope with potentially indefinite multigrid levels. In this section we defend this statement with theoretical results for the $M_{CSG}$ preconditioning matrix by introducing an idealized polynomial smoother.

3.1. Construction. We will construct a third order polynomial smoother $f(t) \in P_3(\mathbb{C})$ with complex coefficients. It is intended to work for the Helmholtz problem discretized on a complex stretched grid as in (2.1), which defines the preconditioning matrix $M_{CSG}$. This polynomial should have the following properties to fit the multigrid philosophy.

- First, it should be stable: $\forall \lambda \in \sigma(M_{CSG}): |f(\lambda)| < 1$.
- Next, it should smooth the most oscillatory modes efficiently. The mode with the highest frequency in the interior region has an eigenvalue $\lambda_\beta^{(k)} = D_4 h_\beta^2 - k^2$, for a $D$-dimensional problem. The highest frequency mode on the complex absorbing layer has an eigenvalue $\lambda_\gamma^{(k)} = D_4 h_\gamma^2 - k^2$. So we should demand that $f(t)$ maps these eigenvalues as $f(\lambda_\beta^{(k)}) = 0$ and $f(\lambda_\gamma^{(k)}) = 0$.
- In contrast the smoother should leave the smoothest mode, the eigenvector that has an eigenvalue $\lambda = -k^2$, untouched. So it is required that this mode is mapped by the polynomial to the unit circle, i.e. $f(-k^2) = e^{i \phi}$.
- Finally, it is natural that the solution of the linear system is a fixed point of the smoother, so $f(0) = 1$.

It will be shown that such a polynomial smoother can be constructed for each level in the multigrid hierarchy if the complex stretched grid for $M_{CSG}$ fits certain requirements.
The third order polynomial can be written as

\[ f(t) = (1 - \omega_1 t)(1 - \omega_2 t)(1 - \omega_3 t), \]  

(3.1)

where \( \omega_1, \omega_2, \omega_3 \in \mathbb{C} \). This polynomial can be interpreted as a sequence of three \( \omega \)-Jacobi steps with different weights. The coefficients \( \omega_2 \) and \( \omega_3 \) in (3.1) are set by the requirements that the most oscillatory modes should be mapped to zero. Since the eigenvalues associated to the most oscillatory eigenvectors \( \lambda^{(k)}_{\beta} \) and \( \lambda^{(k)}_{\gamma} \) should be zeros of \( f(t) \) we have

\[ f(t) = (1 - \omega_1 t)(1 - t/\lambda^{(k)}_{\beta})(1 - t/\lambda^{(k)}_{\gamma}) \]

We now choose \( \omega_1 \) such that \( f(-k^2) = e^{\varphi} \) with \( \varphi \in [0, 2\pi) \). This ensures that the smooth modes are hardly affected by the polynomial smoother. This leads to

\[ \omega_\varphi = \omega_1(\varphi) = -\frac{1}{k^2} \left( 1 - \frac{e^{i\varphi}}{(1 + k^2/\lambda^{(k)}_{\beta})(1 + k^2/\lambda^{(k)}_{\gamma})} \right) \]  

(3.2)

So the choice of the point on the unit circle to which the smoothest eigenvalue \( \lambda = -k^2 \) is mapped by \( f(t) \) defines the coefficient \( \omega_\varphi \). However, as we will discuss next, not all choices of \( \varphi \) lead to a stable smoother. We now treat \( \varphi \) as parameter of the smoother.

**Example 1.** To illustrate how the spectrum is mapped by the third order polynomial for various choices of \( \varphi \) we discuss the example that is shown in Figure 3.1 for a wave number \( k = 100 \). The operator is discretized, as discussed in section 3.1, with 192 finite difference points in the interior and 64 points on the exterior in each dimension. This gives a grid distance \( h = 0.7812 \cdot 10^{-2} \) that is rotated in the interior by 8 degrees to \( h_\beta = e^{i0.08}\pi h \) and in the exterior by 30 degrees to \( h_\gamma e^{i30\cdot\pi/180} h \).

The largest eigenvalues of \( M^{CS}_G \) are \( \lambda^{(k)}_{\beta} = (11.5 - i3.61) \cdot 10^4 \) and \( \lambda^{(k)}_{\gamma} = (5.55 - i11.35) \cdot 10^4 \). The spectrum lies in the third and the fourth quadrant of the complex plane and is bounded by the three line segments that connect \(-k^2\) and these two eigenvalues. This is shown in Figure 3.1 a).

In Figure 3.1 c), we show the results for \( \varphi = 0.015, 0.016, 0.017, 0.018, 0.019, 0.020, 0.021 \) radians. For each of these angles we have different function \( f \), only for larger \( \varphi \) the map is stable.

**Remark 2.** We have made the choice to map \( \lambda^{(k)}_{\beta} \) and \( \lambda^{(k)}_{\gamma} \) to zero. This does not necessarily lead to the most efficient smoother. It might be better to choose eigenvalues that are slight inside the triangle to map to zero. In a similar way for \( \omega \)-Jacobi a choice of \( \omega = 2/3 \) leads to a better smoother than a choice of \( \omega = 1/2 \) for the Poisson problem with Dirichlet conditions 5.

3.1.1. **Explicit choice for \( \varphi \)**. This section shows that on all levels of the multi-grid hierarchy a choice for \( \varphi \) in (3.2) can be made such that the smooth modes are mapped inside the unit circle. We represent the polynomial in (3.1) in the general form,

\[ f(t) = a + b(k^2 + t) + c(k^2 + t)^2 + d(k^2 + t)^3, \]  

(3.3)

but the coefficients are, at this moment, unspecified. The polynomial can be viewed as a Taylor expansion around \(-k^2\) and so we have a simple relation between the
coefficients and the derivatives

\[ a = f(-k^2), \]
\[ b = f'(-k^2), \]
\[ c = f''(-k^2)/2, \]
\[ d = f'''(-k^2)/6. \]

We will find \( a, b, c \) and \( d \in \mathbb{C} \) so that the following requirements are met:

\[ f(0) \equiv 1, \quad \text{(fixed point property)} \tag{3.4} \]
\[ f(-k^2) \equiv e^{i\varphi}, \quad \text{(map \(-k^2 \text{ to the unit circle})} \tag{3.5} \]
\[ \arg(f'(-k^2)/h^2) \equiv \varphi - \pi/2, \quad \text{(map of top edge is tangent to the circle)} \tag{3.6} \]
\[ f(\lambda^{(k)}_{\beta}) \equiv 0, \quad \text{(high energy eigenvalues mapped to zero)} \tag{3.7} \]
\[ f(\lambda^{(k)}_{\gamma}) \equiv 0, \quad \text{(high energy eigenvalues mapped to zero).} \tag{3.8} \]

These conditions rule that the exact solution should be a fixed point (3.4), and that the smoothest modes should be mapped to the unit circle (3.5). In (3.6) we make the choice to select \( \varphi \) such that the top edge of the bounding triangle, that can be parameterized by \(-k^2 + s/h^2 \) with \( s \in [0,8] \), is mapped tangent to the unit circle in \( e^{i\varphi} \) by \( f(t) \). Equations (3.7) and (3.8) rule that the most oscillatory modes should be mapped to zero. This elaborates upon the idea of an ideal smoother: stability for all eigenmodes and the most error reduction in the range of the most oscillatory modes.

We immediately see that \( a = e^{i\varphi} \). An alternative way to express that the first order term of \( f \) in \(-k^2 \) should touch the circle is to impose that \( a \) and \( b s/h^2 \in \mathbb{C} \) should be orthogonal when we translate to \( \mathbb{R}^2 \). This leads to

\[ \Re (b/h^2) \cos(\varphi) + \Im (b/h^2) \sin(\varphi) = 0. \tag{3.9} \]

Since both \( b \) and \( \varphi \) are unknowns this is a non-linear equation. The solution will give bounds on \( \varphi \).

**Lemma 3.1.** Let \( k \) be the wave number of the \( D \)-dimensional Helmholtz equation and \( h_\beta \) and \( h_\gamma \) be the mesh widths on the interior and the exterior region, respectively. Let \((b_1, c_1, d_1)^T \) and \((b_2, c_2, d_2)^T \) be the solution the linear system

\[
\begin{pmatrix}
  k^2 & k^4 & k^6 \\
  4d/h^2_\beta & (4d)^2/h^4_\beta & (4d)^3/h^6_\beta \\
  4d/h^2_\gamma & (4d)^2/h^4_\gamma & (4d)^3/h^6_\gamma
\end{pmatrix} \begin{pmatrix}
  x \\
  1 \\
  1
\end{pmatrix} = \begin{pmatrix}
  y \\
  1 \\
  1
\end{pmatrix}
\]

with right hand sides \( y = (1,0,0)^T \) and \( y = (1,1,1)^T \), respectively. If

\[ |\Re (b_2/h^2_\beta)| \leq |b_1/h^2_\beta| \tag{3.11} \]

then there are two solutions for \( \varphi \),

\[ \varphi = \arg(b_1/h^2_\beta) \pm \arccos \left( \frac{\Re (b_2/h^2_\beta)}{|b_1|} \right). \tag{3.12} \]
Proof. The system of equations represented by Equations (3.4)-(3.8) has five equations for the unknown coefficients $a, b, c, d$ and $\varphi$. Equation (3.5) immediately implies $a = e^{i\varphi}$, where the parameter $\varphi \in [0, 2\pi)$ is still to be determined. The following strategy solves for the remaining coefficients. We take the first and the last two equations and solve the resulting linear system

$$
\begin{pmatrix}
  k^2 & k^4 & k^6 \\
  k^2 + \lambda^{(k)}_\beta & (k^2 + \lambda^{(k)}_\beta)^2 & (k^2 + \lambda^{(k)}_\beta)^3 \\
  k^2 + \lambda^{(k)}_\gamma & (k^2 + \lambda^{(k)}_\gamma)^2 & (k^2 + \lambda^{(k)}_\gamma)^3
\end{pmatrix}
\begin{pmatrix}
b \\
c \\
d
\end{pmatrix}
= \begin{pmatrix}
1 - e^{i\varphi} \\
-e^{i\varphi} \\
-e^{i\varphi}
\end{pmatrix}.
(3.13)
$$

Note that $k^2 + \lambda^{(k)}_\beta = 4D/h^2$ and $k^2 + \lambda^{(k)}_\gamma = 4D/h^2\rho$. For every angle $\varphi$ this system has a unique solution if $\lambda^{(k)}_\beta \neq \lambda^{(k)}_\gamma \neq 0$. It is a Vandermonde matrix that appears typically in interpolation problems. The solution can be written as a linear combination of the solutions $(b_1, c_1, d_1)^T$ and $(b_2, c_2, d_2)^T$ of the same linear system with $(1, 0, 0)^T$ and $(1, 1, 1)^T$ as right hand side. The solution for $b$, the first derivative of $f(t)$ in $-k^2$, is then $b_1 - e^{i\varphi}b_2$.

With this solution we can find an angle $\varphi$ that satisfies the remaining condition (3.6).

$$
\Re(b/h^2_\beta) \cos(\varphi) + \Im(b/h^2_\beta) \sin(\varphi) = 0, \quad (3.14)
$$

$$
\Leftrightarrow \Re((b_1 - e^{i\varphi}b_2)/h^2_\beta) \cos(\varphi) + \Im((b_1 - e^{i\varphi}b_2)/h^2_\beta) \sin(\varphi) = 0,
$$

$$
\Leftrightarrow \Re(b_1/h^2_\beta) \cos(\varphi) + \Im(b_1/h^2_\beta) \sin(\varphi) - \Re(b_2/h^2_\beta) = 0.
(3.15)
$$

If $|\Re(b_2/h^2_\beta)| \leq |b_1/h^2_\beta|$ then this last equation for $\varphi$ has solutions

$$
\varphi = \arctan(\Re(b_1/h^2_\beta)/|b_1|) = \arctan(\Im(b_1/h^2_\beta)).
$$

Lemma 3.1 gives two possible values for $\varphi$ in (3.2) such that the top line segment of the bounding triangle of the spectrum of the preconditioner is mapped tangent to the unit circle. However, one choice of $\varphi$ gives a stable spectrum while the other does not.

**Corollary 3.2.** If $\lambda^{(k)}_\beta \neq \lambda^{(k)}_\gamma \neq k^2$ and $|\Re(b_2/h^2_\beta)| < |b_1/h^2_\beta|$ then only one of the two choices of $\varphi$ guarantees that $f(t)$ is stable for the smooth modes.

**Proof.** Since $\lambda^{(k)}_\beta \neq \lambda^{(k)}_\gamma \neq k^2$, the system (3.4)-(3.8) has a nonzero solution. The respective maps of the two line segments, $-k^2 + s/h^2_\beta$ and $-k^2 + s/h^2_\gamma$ with $s \in [0, 8]$, of the bounding triangle that meet in $-k^2$ also meet in $f(-k^2) = e^{i\varphi}$. The two choices for $\varphi$ given by Lemma 3.1 map the line segment that connects $-k^2$ and $\lambda^{(k)}_\beta$, which is closest to the real axis, such that it is tangent to the unit circle in $e^{i\varphi}$. Since the angle between this line and the line segment that connects $-k^2$ and $\lambda^{(k)}_\gamma$ is preserved by the holomorphic polynomial map $f$, this second line is either mapped outside the unit circle or inside the unit circle. The low energy eigenvalues near $-k^2$ are bounded by these two lines and so these eigenvalues are mapped inside the unit circle if this
second line is also mapped inside the circle. □

Remark 3. Note that if the system \((3.4), (3.8)\) has no solution, i.e. \(|\Re(b_2/h_3^2)| > |b_1/h_3^2|\), then the inner product of the first order term \(f(-k^2)\) and the second order term \(f'(k^2)s/h_3^2\), \((3.15)\) in the proof of Lemma 3.1, is either positive or negative. This corresponds to mapping the top line of the bounding triangle outside or inside the unit circle respectively, instead of having it as a tangent. However for all physical choices of the ECS-layer, and thus \(\lambda^{(k)}_{\beta}\) and \(\lambda^{(k)}_{\gamma}\), we have \(\Re(b_2/h_3^2) > 0\) and so the inner product will be negative for all possible choices of \(\varphi\), which will always result in an inward mapping of the top line of the triangle. In this case we pick \(\varphi = 0\) and \(\omega_1\) is then

\[
\omega_1 = -\frac{1}{k^2} \left( 1 - \frac{1}{(1 + k^2/\lambda^{(k)}_{\beta})(1 + k^2/\lambda^{(k)}_{\gamma})} \right).
\]

Example 2. It is useful to check the condition in \((3.11)\) of Lemma 3.1 in a real multigrid context. In this example we look at a hierarchy of a two-dimensional problem where the mesh widths in each dimension are \(h_\beta = 2^{-l}e^{i\theta_\beta}\) in the inner region and \(h_\gamma = 2^{-l}e^{i\theta_\gamma}\) on the absorbing layer. On each multigrid level \(l = 1, 2, \ldots, 7\) we need to construct a stable smoother.

For the fine levels, \(h_\beta\) and \(h_\gamma\) are small and \(\lambda^{(k)}_{\beta} = -k^2 + 8/h_\beta^2\) and \(\lambda^{(k)}_{\gamma} = -k^2 + 8/h_\gamma^2\) are dominated by the second term. We then have that \(\lambda^{(k)}_{\beta} \approx 2^{2l+3}e^{-i\theta_\beta}\) and \(\lambda^{(k)}_{\gamma} \approx 2^{2l+3}e^{-i\theta_\gamma}\) and both lie in the fourth quadrant of the complex plane. Since the smooth modes lie near \(-k^2\) in the third quadrant, the spectrum of the preconditioner matrix \(M^{\text{CSG}}_k\) on the finest levels extends from the third to the fourth quadrant.

On the coarsest levels, however, the first terms in \(\lambda^{(k)}_{\beta} = -k^2 + 8/h_\beta^2\) and \(\lambda^{(k)}_{\gamma} = -k^2 + 8/h_\gamma^2\) are small and the shift over \(-k^2\) dominates. So for the lowest levels it is possible that both \(\lambda^{(k)}_{\beta}\) and \(\lambda^{(k)}_{\gamma}\) lie in the third quadrant of the complex plane. The spectrum will then be negative definite as it fits completely inside the third quadrant.

Since \(h_\beta\) and \(h_\gamma\) change over the levels the solutions \(b_1\) and \(b_2\) of the linear system in Lemma 3.1 will change as well on each level. Consequently, \(\varphi_1\) along with \(\omega_1\) will also change from level to level. Note that these are the coefficients of the smoother in Equation 3.2.

In Figure 3.2 we check the condition in \((3.11)\) for each of the levels. The dashed line marks where \(|\Re(b_2/h_3^2)| = |b_1/h_3^2|\) as a function of \(k\) and \(\theta_\beta\), the rotation angle of the mesh width \(h_\beta\). The dashed lines to the left come from the coarsest levels, while the lines to the right come from the finer levels. For a particular level \(l\) and for the wave numbers \(k\) on the right of the corresponding dashed line we can choose any \(\varphi\) and get a stable smoother. For wave numbers on the left of the dashed line, we have to solve for \(\varphi\) as discussed earlier in order to achieve a stable smoother.

The other way round, for a given wave number, the \(\varphi\) of the coarsest levels can be chosen arbitrarily since the condition of Remark 3 is fulfilled. For those levels we pick \(\varphi = 0\) and \(\omega_1\) accordingly. This example is continued in Example 3.

3.1.2. Stability for all eigenvalues. The condition that the image of the line between \(-k^2\) and \(\lambda^{(k)}_{\beta}\) is tangent to the unit circle is not sufficient to guarantee stability. In Figure 3.3 we illustrate that, although, the image is tangent to the unit circle, it
can lead to an unstably mapped spectrum. In this section we want to extend the region in the spectrum of smoothest eigenvalues that are mapped inside the circle. Again, we look at the line
\[ -k^2 + s/h_\beta^2, \quad \text{with } s \in [0, 8], \]
where \( h_\beta^2 \) is the mesh width of the inner part of the domain. It is mapped by the polynomial to
\[ f(-k^2 + s/h_\beta^2) = a + \frac{b}{h_\beta^2} s + \frac{c}{h_\beta^4} s^2 + \mathcal{O}(s^3). \]
We want this to stay inside the unit circle so we have that
\[ |f(-k^2 + s/h_\beta^2)|^2 \leq 1 \quad \text{for } s \ll 1. \]

**Lemma 3.3.** Let \( k \) be the wave number of the Helmholtz problem and \( h_\beta \) and \( h_\gamma \) the mesh widths of the CSG-preconditioner such that there is a stable solution of the tangent equation for \( \varphi \). Let \( b \) and \( c \) be the coefficients of the corresponding polynomial of the form (3.3). If
\[ \Re(\frac{c}{h_\beta^4} e^{-ı\varphi}) < -\frac{1}{2} \left| \frac{b}{h_\beta^2} \right|, \] (3.16)
then an extended part of the spectrum is mapped inside the unit circle.

**Proof.** The condition \( |f(-k^2 + s/h_\beta^2)|^2 \leq 1 \) becomes
\[ aa^* + \left( \frac{b}{h_\beta^2} a^* + \left( \frac{b}{h_\beta^2} \right)^* a \right) s + \left( \frac{c}{h_\beta^4} a^* + \left( \frac{c}{h_\beta^4} \right)^* a + \left( \frac{b}{h_\beta^2} \right)^* \frac{b}{h_\beta^2} \right) s^2 + \mathcal{O}(s^3) < 1. \] (3.17)
for \( s \ll 1 \). Since \( a = e^{ı\varphi} \) we have that \( aa^* = 1 \). Because \( \varphi \) is such that \( \frac{b}{h_\beta^2} a^* + \left( \frac{b}{h_\beta^2} \right)^* a = 0 \) and the line segment that connects \(-k^2\) and \( \Lambda^{(k)}_\gamma \) is mapped inside the circle, it is clear that
\[ \frac{c}{h_\beta^4} a^* + \left( \frac{c}{h_\beta^4} \right)^* a + \left( \frac{b}{h_\beta^2} \right)^* \frac{b}{h_\beta^2} < 0 \]
\[ 2\Re(\frac{c}{h_\beta^4} a^*) + \left| \frac{b}{h_\beta^2} \right| < 0 \]
is required to ensure a stable map. \( \Box \)

**Remark 4.** If the condition in (3.16) is fulfilled, the set of eigenvalues that is mapped inside the unit circle is extended. However, to guarantee that the complete spectrum is mapped inside the unit circle, we would need to check the higher order term in (3.17). Since \( f(-k^2 + s/h_\beta^2) \) is zero for \( s = 8 \) and \( f(t) \) is a low order polynomial, it is likely that the condition in (3.16) is sufficient to make the map of the complex spectrum stable. Numerical experiments confirm this conjecture.

**Example 3.** This example is a continuation of Example 2 and it uses the same multigrid hierarchy to illustrate how we can use the extra condition in (3.16). We extend
the plot of Figure 3.2 and add the condition of Lemma 3.3. The solid line in the figure shows where \( 2 \Re \left( \frac{\beta}{\pi} e^{-i\varphi} \right) + \left| \frac{h}{\pi} \right| = 0 \), as a function of \( k \) and the rotation angle \( \theta_\beta \) of \( h_\beta \) for each level in the multigrid hierarchy. In red we have added the condition of Lemma 3.3. We see that for a given \( k \) the smoother is only fully stable for a rotation angle \( \theta_\beta \) above the red line. In principle we can adjust \( h_\beta \) of the CSG until this condition is met.

For example at \( k = 4 \) we see that the three coarsest levels have their bounding line to the left. That means that we can pick any angle \( \varphi \) for these levels. For the fourth level the bounding region is on the right. This means that we have to solve Equation 3.12, however, if the rotation angle \( \theta_\beta \) is smaller than 5 degrees, we are not sure that the spectrum is completely mapped inside the unit circle. We therefore pick the rotation angle of \( h_\beta \) to be larger than 5 degrees. For the finer levels we are still inside the region where we need to solve for \( \varphi \), but the angle of \( h_\beta \) can be taken very small here.

This example also illustrates how multigrid on the original Helmholtz matrix will behave badly. Indeed, we see that the extra condition on \( \theta_\beta \) for the preconditioner is necessary to ensure stability. The drawback is that we need to choose the same \( h_\beta \) for the complete multigrid hierarchy. So in this example \( \theta_3 \), and thus \( h_\beta \), is determined by the fourth coarsest level.

**Remark 5.** Figure 3.2 illustrates that for particular choices of \( k \) of the Helmholtz problem the rotation angle \( \theta_\beta \) of the complex stretched grid preconditioner can be very small. For these cases \( M_h^{CSG} \) and \( H_h \) will be very close to each other and the Krylov iteration will be efficient. However, for realistic problems when the wave number is space dependent it is very hard to identify these wave numbers in a robust way. For robustness it is therefore a good strategy not to choose the smallest possible \( \theta_\beta \), since small variations in the wave number will turn the smoother unstable.

### 3.2. Strategy to determine the parameters of the smoothers for all levels.

From the examples it is clear that a stable third order polynomial smoother is easy to construct for all the levels except one. Indeed, let us assume that we have to solve a problem with \( k = 75 \) and that we use the multigrid hierarchy of Example 2 and 3. For the four coarsest levels this \( k \) is on the right of the dashed line, which means that for these levels \( \varphi = 0 \) is a stable choice. For these levels the spectrum of the CSG-preconditioner lies almost entirely in the third quadrant. In a similar way the smoother of the finest levels is easily constructed since for those levels the solid line leads to negative angles. However, for level \( l = 5 \) we can only guarantee a stable smoother if \( \theta_\beta > 5.5 \). So once we have determined \( h_\beta \) we need to calculate \( \varphi \) and the corresponding \( \omega_\phi \) in (3.2) for each level. For the coarsest level we can pick any \( \varphi \) but we prefer \( \varphi = 0 \).

While this strategy leads to a stable smoother for the homogeneous Helmholtz problem, a more robust smoother is preferred for heterogeneous problems, where the spectrum of the discretization matrix could slightly deviate from the describing triangle. Since our manually tuned third order polynomial is a particular polynomial with \( p(0) = 1 \) it gives an upper bound for the convergence of GMRES(3) as a stand alone relaxation method. As a consequence a multigrid method for a preconditioner such as \( M_h^{CSG} \) only needs three iterations of GMRES when it is used as a smoother. This is in contrast to a much higher and undetermined number of iterations for the original Helmholtz matrix \( H_h \) as is shown in [7].

To justify the smoothing property of GMRES(3) consider again the bounding
triangle in Lemma 4.2. The lowest energy eigenvalues in the top of the triangle, around $-k^2 = O(1)$, are relatively close to the origin compared to the high energy eigenvalues $\lambda_{\beta}^{(k)} = -k^2 + 4d/h^2 = O(1/h^2)$ and $\lambda_{\gamma}^{(k)} = -k^2 + 4d/h^2 = O(1/h^2)$, especially when a high accuracy condition $h = O(k^{-3/2})$ is used. So whenever the minimal third order polynomial $p(t)$ is constructed for the spectrum with the constraint $p(0) = 1$, then the region of the smoothest modes will be pulled towards 1 by this polynomial map whereas the high energy region is more freely minimized.

4. GMRES as smoother.

4.1. Two-grid analysis. We focus our initial numerical experiments on solving the preconditioning problem $M_h^{CSG} u_h = b_h$ efficiently with multigrid. First, we collect the convergence rates of the two grid operator

$$TG = S^\nu (I - I_H^h (M_H^{CSG})^{-1} I_h^H M_h^{CSG}) S^\nu,$$

(4.1)

where $S$ denotes the polynomial smoother, $I_H^h$ and $I_h^H$ the restriction and interpolation operators, respectively. The coarse grid operators $M_h^{CSG}$ is a discretization of the problem with grid distance $H$, as discussed in the previous sections.

In the numerical experiments we solve $M_h^{CSG} u_h = b_h$ with zero right hand side and a random initial guess $u_h^{(0)}$. The reported convergence rates are the asymptotic rates measured by the ratio $\|e^{(k)}\|/\|e^{(k-1)}\|$. We compare the convergence rate of the polynomial smoother, with the parameters chosen as in the previous section, with GMRES(1), GMRES(2) and GMRES(3). The measured convergence rates for various levels in the multigrid hierarchy are shown in the Figure 4.1.

Note that the explicit constructed third order polynomial forms an worst case bound for the convergence of GMRES(3).

4.2. Performance of a V-cycle. After the two grid analysis multigrid with GMRES as smoother is tested on the preconditioner $M_h^{CSG}$ for the homogeneous Helmholtz problem (1.1) in a square domain $\Omega = (0,1)^2$ with a point source

$$\delta(x,y) = \begin{cases} 1, & \text{if } x = 1/2 = y, \\ 0, & \text{elsewhere}. \end{cases}$$

(4.2)

All boundaries are extended with an ECS-layer with an angle $\theta_\gamma = \frac{\pi}{6}$ to absorb outgoing waves. Although a more stringent relation between $k$ and the mesh width $h$ might be desirable for physical accuracy, we only wish to observe iterative behavior for which 10 points per wavelength suffices, which translates into the requirement $kh \leq 0.625$. The preconditioning matrix $M_h^{CSG}$ is constructed by discretizing the problem on a complex stretched grid with a small inner angle $\theta_\beta = 0.18 \approx \frac{\pi}{18} > \theta_0$ where $\theta_0$ is the critical angle for stability of the polynomial smoother. The angle for the ECS-layers is kept at $\theta_\gamma = \frac{\pi}{6}$ as in the original Helmholtz problem.

The preconditioning matrix $M_h^{CSG}$ is inverted by applying subsequent $V(\nu_1,\nu_2)$-cycles where the standard smoother, e.g. $\omega$-Jacobi, is replaced by the GMRES method, where $\nu_1$ and $\nu_2$ indicate the number of pre and post smoothing steps, respectively. One smoothing step consists of a GMRES solve on the error which is stopped after $s$ iterations, simply denoted as GMRES$(s)$. It constructs a minimal polynomial of order $s$ and so will cost $s$ matrix vector products. The number of cycles needed to converge to a relative residual of order $10^{-7}$ are presented in Table 4.1 for different configurations and wave numbers. In the experiments with the $V(1,0)$-cycle we see that
s = 4 does not improve the method much more than s = 3. Earlier we showed that a third order polynomial is sufficient to guarantee a stable smoother. The experiments with s = 2 also converge, but only after a substantially larger number of V-cycles. Increasing the number of smoothing steps \((\nu_1, \nu_2)\) to more than (1,1) does not pay off in the eventual number of V-cycles needed to reach the tolerance. The table also shows the timings for \(k = 80\). The V(1,0) with 2, 3 and 4 and V(1,1) with s = 2 and s = 3 perform similarly.

Based on these observations we prefer V(1,0) and V(1,1)-cycles with GMRES(3) smoothing for the numerical experiments presented in the next section. Figure 4.2 shows that the averaged convergence rate of these V-cycles do not grow larger than 40\% (+) and 25\% (*) for V(1,0) and V(1,1), respectively. Note that there is, however, a slightly variation as a function of the wave number \(k\). The convergence rate of the first V(1,0) or V(1,1)-cycle alone is below 35\% and 8\% respectively. In the numerical experiments only one V-cycle will be used to approximately invert the preconditioning matrix \(M_{CSG}^h\). The convergence rate of the V(2,1)-cycles is relatively close to that of the V(1,1)-cycles as could be expected after considering Table 4.1.

5. Numerical experiments. In this section we test the \(M_{CSG}^h\) preconditioner on three two-dimensional benchmark problems. The experiments cover both homogeneous media with constant wave numbers \(k\) and heterogeneous media where the wave number is space-dependent. The discretized problem is solved with a Krylov subspace method that we will call the outer Krylov method. The complex stretched grid matrix \(M_{CSG}^h\) is constructed from the same original Helmholtz equation but on a different grid with the inner part slightly rotated in the complex plane over an angle \(\theta_\beta\). It is used as a preconditioner and approximately inverted with one V-cycle with GMRES(3) smoothing. As a consequence of this non-standard smoother the actual preconditioner is not the same in every outer Krylov step. Therefore the flexible GMRES method [16] and the Bi-CGSTAB method are used as outer Krylov subspace methods. Whenever Bi-CGSTAB converged after the first matrix-vector product of the last iteration, this iteration is counted as a half. The experiments are all run in Matlab on two quad core Intel Xeon CPUs (E5462 @ 2.80GHz). The mentioned CPU times are scaled by the total number of grid points, including the ECS boundary layers, so it expresses the

| \((\nu_1, \nu_2)\) | GMRES(s) | \(k\) | CPU \((k = 80)\) |
|----------------|----------|------|----------------|
|                |          | 20   | 40   | 60   | 80   |
| (1,0)          | s = 2    | 18   | 19   | 20   | 20   | 7.23 |
|                | s = 3    | 13   | 14   | 14   | 14   | 7.88 |
|                | s = 4    | 11   | 12   | 12   | 13   | 8.58 |
| (1,1)          | s = 2    | 11   | 11   | 10   | 12   | 7.85 |
|                | s = 3    | 8    | 9    | 9    | 9    | 8.53 |
|                | s = 4    | 7    | 7    | 7    | 7    | 10.33|
| (2,1)          | s = 2    | 9    | 9    | 8    | 10   | 17.46|
|                | s = 3    | 7    | 7    | 7    | 8    | 44.35|
|                | s = 4    | 6    | 6    | 6    | 6    | 94.13|

Table 4.1: Number of multigrid V-cycles with different number of GMRES smoothing steps to solve the preconditioner for a constant \(k\).
computational cost per grid point.

Case 1: Constant $k$. In the first experiment we continue with the homogeneous Helmholtz problem with the point source in (4.2) from section 4.2. The complex shifted Laplacian preconditioner was tested on this model problem for Sommerfeld boundary conditions in [8]. The idea was also compared with the complex stretched grid preconditioner when applied with ECS boundary conditions in [15]. For the latter boundary conditions both strategies result in a good preconditioning matrix for a Krylov subspace method but still need to be (approximately) inverted by a cheap method. A multigrid method is preferred for this purpose as it is easily extended to higher dimensions where other standard methods, such as ILU, suffer from severe memory problems. Automatic configurations of multigrid (in this context) are often less efficient than manually tuned ones. In this paper we improve the multigrid performance on the complex stretched grid preconditioner in order to achieve a better overall convergence and to develop a robust and efficient solver for indefinite Helmholtz problems.

$$k^2 = 20 40 60 80 100$$

$$\text{interior grid}$$

| $k$  | $20^2$ | $40^2$ | $60^2$ | $80^2$ | $100^2$ |
|------|--------|--------|--------|--------|---------|
| MG(V(1,0)) FGMRES | 26(0.08) | 46(0.7) | 54(1.65) | 77(2.78) | 84(4.03) |
| Bi-CGSTAB | 19.5(0.10) | 35.5(0.61) | 50.5(1.64) | 82(2.69) | 99(3.39) |
| MG(V(1,1)) FGMRES | 17(0.08) | 26(0.48) | 34(1.27) | 44(1.79) | 47(2.27) |
| Bi-CGSTAB | 9.5(0.09) | 17.5(0.52) | 22(1.29) | 35(2.04) | 32.5(1.97) |
| MG(V(2,1)) FGMRES | 14(0.15) | 21(2.34) | 28(6.17) | 37(8.34) | 39(5.89) |
| Bi-CGSTAB | 8.5(0.17) | 15(1.86) | 19(5.04) | 27(2.33) | 26(6.03) |
| ILU(0) GMRES | 66(0.18) | 147(3.7) | 266(20) | 294(24.1) | 490(96.1) |
| ILU(0.1) GMRES | 77(0.20) | 160(4.2) | 274(22.3) | 317(30.8) | 1722(1309) |

Table 5.1: Number of FGMRES, Bi-CGSTAB and GMRES iterations (and CPU time per grid point $\times 10^3$) for different preconditioning strategies for Case 1.

Table 5.1 displays the number of iterations and the CPU time per grid point $\times 10^3$ for FGMRES and Bi-CGSTAB for different values of the wave number $k$. The number of outer Krylov iterations with MG(V(1,1)) is significantly smaller than with MG(V(1,0)) for all values of $k$ and results in a faster CPU time. Although a MG(V(2,1)) inversion of the preconditioner requires even less outer Krylov iterations, the total CPU time is again higher than for the MG(V(1,1)) case. This confirms what was observed in Table 4.1 and Figure 4.2 that extra smoothing steps do not pay off because it does not quite improve the approximate preconditioner inversion. Figure 5.1 visualizes the typical relation between the wave number $k$ and the convergence speed, which is obviously influenced by the increasing number of grid points for growing $k$.

As a reference the same problem is solved with ILU(0) and ILU(0.1) inversion of the preconditioner and GMRES as the outer Krylov method. Both iteration numbers and CPU times are not competitive to multigrid inversion of the preconditioner.

Case 2: Wedge problem. In the second experiment the proposed preconditioning technique is tested on a mildly heterogeneous problem

$$Hu \equiv - (\Delta + k(x,y))u = g(x,y).$$

The rectangular domain $(0m, 600m) \times (0m, 1000m)$ is split in 3 regions where the speed of sound $c$ takes 3 different values (1500 m/s, 2000 m/s and 3000 m/s). This brings
along heterogeneity in the wave number that is defined as $k(x,y) = (2\pi f/c(x,y))^2$, with $f \in (10Hz, 50Hz)$ the frequency of the point source

$$g(x,y) = \delta(x,y) = \begin{cases} 1, & \text{if } x = 300, y = 0, \\ 0, & \text{elsewhere,} \end{cases}$$

The wedge problem was tested for Sommerfeld boundary conditions on all edges of the domain with the complex shifted Laplacian preconditioner [8]. For this paper the ECS boundary layers are used to absorb outgoing waves, with a complex stretched grid preconditioner.

|            | $f$   | 10  | 20  | 30  | 40  | 50  |
|------------|-------|-----|-----|-----|-----|-----|
|            | interior grid | 32 × 64 | 64 × 128 | 64 × 128 | 128 × 256 | 128 × 256 |
| MG(V(1,0)) | FGMRES | 38(1.03) | 68(2.57) | 108(5.43) | 128(9.31) | 153(12.74) |
| Bi-CGSTAB  |       | 29(0.98) | 64.5(2.17) | 124(4.19) | 134.5(4.64) | 259(8.60) |
| MG(V(1,1)) | FGMRES | 26(0.94) | 44(2.00) | 68(3.56) | 79(5.15) | 96(6.95) |
| Bi-CGSTAB  |       | 18(1.04) | 35(2.15) | 53.5(3.29) | 79.5(4.89) | 102(6.30) |

Table 5.2: Number of FGMRES and Bi-CGSTAB iterations (and CPU time per grid point × 10³) for different preconditioning strategies for Case 2.

In Table 5.2 we see that MG(V(1,1)) beats MG(V(1,0)) when it comes to outer Krylov iterations. The CPU time of the MG(V(1,0)) test is only slightly faster for $k = 10$ and $k = 40$ for Bi-CGSTAB. Other tests involved more smoothing steps and the use of ILU for approximate inversion as in Case 1, but were again not competitive and are therefore left out of the table.

*Case 3: Ionization problem.* The model for the last experiment is the 2D Helmholtz problem

$$Hu \equiv - (\Delta + k(x,y)) u = g(x,y),$$

on the square domain $(0, 50)^2$ with a strongly varying wave number

$$k(x,y) = \mu \left( \frac{1}{e^{x^2}} + \frac{1}{e^{y^2}} \right) + k_0^2,$$

where $0 < k_0 < 5, 0 < \mu < 10$ and a source function

$$g(x,y) = \frac{1}{e^{x^2} + e^{y^2}}.$$
Table 5.3: Number of FGMRES and Bi-CGSTAB iterations (and CPU time per grid point × 10^{2}) for different preconditioning strategies for Case 3 with $\mu = 1$.

| interior grid | FGMRES | Bi-CGSTAB |
|---------------|--------|-----------|
| $k_0$         |        |           |
| 0.5           | $64^2$ | 127(0.72) | 181(1.54) | 238(3.19) | 281(4.22) |
| 1.5           | $128^2$| 184(1.65) | 260(2.71) | 347(3.91) | 410(4.77) |
| 2.5           | $256^2$| 305(2.57) | 436(3.54) | 557(4.59) | 676(5.62) |
| 3.5           | $512^2$| 500(4.92) | 711(5.29) | 922(6.63) | 1132(7.97) |
| 4.5           |        |           |           |           |           |

Table 5.4: Number of FGMRES and Bi-CGSTAB iterations (and CPU time per grid point × 10^{2}) for different preconditioning strategies for Case 3 with $\mu = 7$.

| interior grid | FGMRES | Bi-CGSTAB |
|---------------|--------|-----------|
| $k_0$         |        |           |
| 0.5           | $64^2$ | 127(0.72) | 181(1.54) | 238(3.19) | 281(4.22) |
| 1.5           | $128^2$| 184(1.65) | 260(2.71) | 347(3.91) | 410(4.77) |
| 2.5           | $256^2$| 305(2.57) | 436(3.54) | 557(4.59) | 676(5.62) |
| 3.5           | $512^2$| 500(4.92) | 711(5.29) | 922(6.63) | 1132(7.97) |
| 4.5           |        |           |           |           |           |

eigenvalues on the real axis, left of the smoothest eigenvalues, but are less sensitive to grid changes such as complex stretching or grid coarsening. This can pollute the multigrid functionality for the preconditioning matrix.

In Table 5.3 we see that for $k_0 = 1.5$ the Bi-CGSTAB method with MG(V(1,0)) inversion of the preconditioner takes 303 iterations to converge which is high in comparison with FGMRES which only needs 127 iteration. This outlier in the convergence is even more apparent when $\mu = 7$ in Table 5.4. For $k_0 = 0.5$ the Bi-CGSTAB method with MG(V(1,0)) and MG(V(1,1)) takes 457.5 and 872 iterations respectively, in comparison to 139 and 75 for FGMRES that seems to cope better with the issues of resonances caused by the coarse grid correction.

The reason why resonances appear in this problem with a space dependent wave number that have evanescent waves, is that at the coarse level the discretization is too rough to resolve the details of the variation of the wave number. This leads to slightly different eigenvalues on subsequent levels and this gives rise to the resonances in the convergences.

The FMGRES does not suffer from these resonances because the problematic eigenmodes are resolved by the Ritz eigenvalue and the Krylov converges superlinearly as if this mode is not present. A discussion on superlinear convergence in the iterative solution of linear systems can be found in [19].

It is important to note that similar results are obtained when Galerkin is used to construct the coarse operators.

6. Conclusions and outlook. In this paper we have analyzed the iterative solution of an Helmholtz equation discretized with finite differences and an absorbing boundary condition based on complex scaling. The iterative solver is based on a Krylov subspace and it is preconditioned with multigrid that uses a polynomial smoother. The multigrid is applied to a Helmholtz problem discretized on a complex valued grid.

For each level of the multigrid hierarchy, the spectrum of the discrete preconditioning operator is bounded by a triangle that lies entirely in the lower half of the complex plane. Based on the properties of the triangle, we show that it is possible
to choose the parameters of the preconditioner such that a third order polynomial smoother is stable for all levels and all wave numbers. This smoother can be viewed as a sequence of three damped Jacobi steps with three different $\omega$’s.

The hand tuned third order polynomial forms an bound for the convergence of the GMRES(3) as a smoother. GMRES is more effective, not only because GMRES optimizes the coefficients automatically, but also selects the coefficients differently in each smoothing step. This will give a better performance than any fixed polynomial that is optimized manually.

Note that GMRES(3) does not necessarily have a smoothing behavior in the strict sense. However, the behavior of this GMRES smoother is bounded by the hand tuned polynomial that has the smoothing property. We have also found in the various tests on model problems that the method gives satisfactory results.

The numerical results are obtained for the a preconditioner based on complex shifted grids, but we expect that similar results will be obtained for a complex shifted Laplacian. In [15] we have shown that the complex shifted grid preconditioner is equivalent to the complex shifted Laplacian preconditioner and that it gives the same Krylov space convergence. In [9], the complex shifted Laplacian is also inverted with ILU. However, we have found that the inversion of the preconditioner based on the multigrid combined with the polynomial smoother, performs better, both in compute time and required memory than inversion by ILU.

Unfortunately, the number of Krylov iterations still grows linearly with the wave number $k$ and for large wave numbers the number of iterations increases significantly. This is illustrated in figure 5.1. We intend to give an analysis of the dependence in an upcoming publication.

We have found that the introduction of complex shifts is not sufficient to eliminate all the difficulties with the coarse grid correction. For problems with space dependent wave numbers that allow evanescent waves the coarse grid correction can still be problematic since the space dependence is felt differently on the various levels of the multigrid hierarchy.

When the multigrid is combined with FGMRES we observe that the convergence is not disturbed by diverging coarse grid corrections. This suggests that deflation can be effective. This is a possible subject for future research.

Another subject of future research is the efficient implementation for 3D problems. On modern hardware stencil computations are typically communication bound since there are only a few floating point operations for each read from the slow memory. For the polynomial smoother, however, there are optimizations possible that increase the number of floating points operations per load. The application of the polynomial smoother can be implemented by loading a cube of the domain into fast memory and then applying the three matrix-vector products [6]. In this way we reduce the communication with the slow memory.

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REFERENCES

[1] A. Bayliss, C.I. Goldstein, and E. Turkel. An iterative method for the Helmholtz equation. *Journal of Computational Physics*, 49(3):443–457, 1983.

[2] A. Ben-Menahem and S.J. Singh. *Seismic waves and sources*. Dover Publications, 1998.
[3] H. bin Zubair, B. Reps, and W. Vanroose. A preconditioned iterative solver for the scattering solutions of the Schrödinger equation. *accepted for publication in Communications in Computational Physics*, 2010.

[4] M. Bollhöfer, M.J. Grote, and O. Schenk. Algebraic multilevel preconditioner for the Helmholtz equation in heterogeneous media. *SIAM Journal on Scientific Computing*, 31(5):3781–3805, 2009.

[5] W.L. Briggs, V.E. Henson, and S.F. McCormick. *A multigrid tutorial*. SIAM, 2000.

[6] K. Datta, S. Kamil, S. Williams, L. Oliker, J. Shalf, and K. Yelick. Optimization and performance modeling of stencil computations on modern microprocessors. *SIAM review*, 51(1):129–159, 2009.

[7] H.C. Elman, O.G. Ernst, and D.P. O’Leary. A multigrid method enhanced by Krylov subspace iteration for discrete Helmholtz equations. *SIAM Journal of Scientific Computing*, 23(4):1291–1315, 2002.

[8] Y.A. Erlangga, C.W. Oosterlee, and C. Vuik. A novel multigrid based preconditioner for heterogeneous Helmholtz problems. *SIAM Journal on Scientific Computing*, 27(4):1471–1492, 2006.

[9] Y.A. Erlangga, C. Vuik, and C.W. Oosterlee. On a class of preconditioners for solving the Helmholtz equation. *Applied Numerical Mathematics*, 50(3-4):409–425, 2004.

[10] M.J. Gander and F. Nataf. ALU for Helmholtz problems: a new preconditioner based on the analytic parabolic factorization. *Journal of Computational Acoustics*, 9(4):1499–1506, 2001.

[11] E. Haber and S. MacLachlan. A fast method for the solution of the helmholtz equation. *submitted*, 2010.

[12] F. Natterer and F. Wubbeling. A propagation-backpropagation method for ultrasound tomography. *Inverse Problems*, 11:1225, 1995.

[13] X. Pinel. *A perturbed two-level preconditioner for the solution of three-dimensional heterogeneous Helmholtz problems with applications to geophysics*. PhD Thesis, Université de Toulouse, 2010.

[14] R.E. Plessix and W.A. Mulder. Separation-of-variables as a preconditioner for an iterative Helmholtz solver. *Applied Numerical Mathematics*, 44(3):385–400, 2003.

[15] B. Reps, W. Vanroose, and H. bin Zubair. On the indefinite Helmholtz equation: Complex stretched absorbing boundary layers, iterative analysis, and preconditioning. *Journal of Computational Physics*, 229(22):8384–8405, 2010.

[16] Y. Saad. A flexible inner-outer preconditioned GMRES algorithm. *SIAM Journal on Scientific Computing*, 14:461–461, 1993.

[17] Y. Shapira. *Matrix-Based Multigrid: Theory and Applications*. Kluwer Academic Publishers, 2003.

[18] H.P. Urbach and D.A. Bernard. Modeling latent-image formation in photolithography, using the Helmholtz equation. *Journal of the Optical Society of America A*, 6(9):1343–1356, 1989.

[19] H.A. Van der Vorst. *Iterative Krylov methods for large linear systems*. Cambridge University Press, 2003.

[20] W. Vanroose, F. Martin, T.N. Rescigno, and C.W. McCurdy. Complete photo-induced breakup of the H2 molecule as a probe of molecular electron correlation. *Science*, 310(5755):1787, 2005.
Fig. 3.1: This figure illustrates Example 1. a) The spectrum of the Helmholtz problem on a complex stretched grid for $k = 100$ on the domain $(0, 1)^2$. It is discretized with 192 by 192 finite difference points on the interior and ECS with 64 points as an absorbing boundary layer. The grid is rotated over 8 degrees in the interior and 30 degrees on the exterior. The spectrum is bounded by the line segments that connect $-k^2$, and $\lambda^{(k)}_\beta$ and $\lambda^{(k)}_\gamma$ that form a triangle. b) Map of the spectrum under the third order polynomial $f(t)$ which is constructed such that $f(-k^2) = e^{i\varphi}$, $f(\lambda^{(k)}_\beta) = 0$ and $f(\lambda^{(k)}_\gamma) = 0$. For this map $\varphi = 0.9167$ degrees. c) The smoothest modes are mapped near the unit circle. Depending on the angle $\varphi$, these are mapped outside or inside the unit circle.
Fig. 3.2: Illustration of the conditions in (3.11) and (3.16) in a multigrid hierarchy and as a function of the wave number $k$ and the rotation angle $\theta_\beta$ of the mesh width of the interior region. The details of the multigrid hierarchy is given in Example 2. The dashed lines are drawn where $|\Re(b_2/h_2^2)| = |b_1/h_1^2|$ for each of the levels. For each level and wave numbers on the right of the dashed line, any choice of the rotation angle $\theta_\beta$ and $\varphi$ gives a stable smoother for that particular level. On the left of the dashed line we need to solve for $\varphi$. However, only the region above the solid line gives a stable smoother. The solid lines are based on the condition in (3.16). In order to build a stable smoother on each level of the hierarchy for all possible $k$ we can choose the angle of rotation of the inner region $\theta_\beta$ around 10 degrees, which is above all solid lines.
Fig. 3.3: This figure illustrates that it is not sufficient to choose the angle $\varphi$ such that the top of the bounding triangle of the spectrum is tangent to the unit circle. Although the smoothest modes are still mapped inside the circle and the oscillatory modes are mapped near zero, an intermediate part of the spectrum goes outside the circle under the transformation, leading to unstable modes. The solution is to adjust $h_\beta$, the mesh width in the interior region, until the complete spectrum is mapped inside the circle. In Lemma 3.3 a condition is formulated that realizes this. The solid lines form the image of the bounding triangle. The 2D example is discretized with 32 grid points in the interior and 16 grid points in the ECS layer in one direction. The interior is scaled by an angle of 5 degrees, while the exterior has 30 degrees. The wave number is $k=40$. 
Fig. 3.4: The map of the spectrum under the third order polynomial smoother for each level of the multigrid hierarchy. The wave number is $k = 40$. The interior angle of the complex stretched grid is $\theta_\beta = \pi/18$, which leads to a stable smoother for all levels and all $k$. The ECS rotation is $\theta_\gamma = \pi/6$. The grid is a Kronecker product of a grid with 7, 15, 31, 63, 127 and 255 points in one dimension. One quarter of the grid points lie on the ECS contour.
Fig. 4.1: The measured two grid convergence with one pre and one post smoothing step for the Helmholtz equation on a $(0,1)^2$ domain as a function of the wave number $k$. The domain has an ECS layer on two of the boundaries. We compare the convergence of the polynomial smoother with the convergence of GMRES(1), GMRES(2) and GMRES(3) as smoother. From the top left to the bottom right we show results for $31^2$, $63^2$, $127^2$, $255^2$ and $511^2$ grid points. The rotation angle of the inner part is $\theta = \frac{\pi}{18} = 0.1745$, which is above the critical angle of the polynomial smoother. We note that for each of these two grid tests the convergence suffers when $k$ is such that $\lambda_\beta^{(k)}$ of the coarser level, crosses the imaginary axis. Since the polynomial smoother is a particular polynomial, it gives a worst case bound for the GMRES(3) smoother.
Fig. 4.2: The measured convergence rate of different V-cycles with GMRES(3)-smoothing applied to the preconditioning matrix $M_h^{CSG}$, as a function of the wave number $k$. The matrix is built by discretizing the homogeneous Helmholtz problem with ECS boundary layers on a complex stretched grid with $\theta_\beta = 0.18$ as the rotation angle for the interior domain. The dashed lines show the residual reduction after one V-cycle, while the solid lines are average rates over more subsequent cycles. Doubling the amount of smoothing from $V(1,0)$ (+) to $V(1,1)$ (*) improves the rate from under 40% to under 25%. The performance of the first V-cycle alone even decreases from under 35% to under 8%. Eventually only one such V-cycle will be used to approximately invert the preconditioner $M_h^{CSG}$. The experiment with $V(2,1)$ (×) indicates that an extra smoothing step does not seem to improve the rates in the same order, maximum 15% average and maximum 5% for the first cycle.
Fig. 5.1: Number of iterations (left) and CPU time scaled by the total number of grid points (right) for FGMRES and Bi-CGSTAB as a function of the wave number $k$. The Helmholtz matrix $H$ was preconditioned with one V(1,1) cycle with GMRES(3)-smoothing applied to the $M_h^{CSG}$ with angle $\theta_\beta = 0.18$. The number of grid points grows with $k$ according to the rule $kh \leq 0.625$. 