WAVE-RAY ALGORITHMS FOR HELMHOLTZ EQUATIONS WITH VARIABLE WAVE NUMBERS: A ONE-DIMENSIONAL IMPLEMENTATION OF TWO-DIMENSIONAL IDEAS

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Abstract. The subject of this paper is multigrid solvers for Helmholtz operators with large wave numbers. Algorithms presented here are variations of the wave-ray solver which is modified to allow efficient solutions for operators with constant, continuous, and discontinuous wave numbers. Both geometric and algebraic multigrid frameworks are employed, all yielding efficient and scalable solvers at very little additional costs, compared to standard multigrid techniques. The algorithms are implemented in one dimension, but with a clear extension to higher dimensions.

1. Introduction. We consider a one-dimensional Helmholtz equation

\[ Lu(x) = \Delta u(x) + k^2(x)u(x) = f(x), \quad x \in \Omega, \]

accompanied by the first order Sommerfeld boundary conditions. For \( \Omega = [a, b] \) they read as

\[ \left( \frac{du(x)}{dx} + ik(x)u(x) \right)_{|x=a} = 0, \]
\[ \left( \frac{du(x)}{dx} - ik(x)u(x) \right)_{|x=b} = 0. \]  

When discretized on a sufficiently fine grid with mesh-size \( h \) (see e.g. [6] for what sufficient means) the differential problem is reduced to a system of linear equations

\[ A^h u^h = f^h, \quad A^h \in \mathbb{C}^{n \times n}, \quad f^h \in \mathbb{C}^n. \]  

Finding \( u^h \in \mathbb{C}^n \) is the goal of our numerical solvers.

Remark 1.1. Solving a one-dimensional Helmholtz equation is generally a significant simplification compared to the application-driven higher dimensional problems. Indeed, almost always, one-dimensional solvers for the Helmholtz operator do not translate well, and/or their results are not good predictors for two- or three dimensional solvers because the different level of difficulty in higher dimensions. The main challenge there is a richness and a high oscillatory character of the near-kernel of the Helmholtz operator, the problem that only very modestly presents itself in one dimension.

Our position is very different: the existing wave-ray algorithm successfully deals (in two dimensions) with the near-kernel components. Its weakness is its limited applicability: to this date, it has been developed only for constant wave numbers. Therefore, our goal is not to overcome the main challenge that is not fully present in 1D, but rather to extend the approach to variable, including discontinuous numbers, dealing with phenomenon that appear in all dimensions.

The Helmholtz operator \([1.1]\), especially with constant \( k(x) \equiv k \), is expected to be as easily solvable as the Laplace operator, a poster child for a successful application of multigrid ideas. To the contrary, Helmholtz equations is a completely different story. The main, though not the only

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one, challenge in solving the Helmholtz equation iteratively, in particular using multigrid, is the set of its near-kernel components \( nkc \), the ones that satisfy
\[
Lv \approx 0 \tag{1.4}
\]
or, in a discrete formulation,
\[
A^hv^h \approx 0^h. \tag{1.5}
\]
They play a significant role in any multigrid solver, including the ones described here. In one dimension, for instance, components \( \omega \) in the interior of \( \Omega \) are of the form \( v(x) = e^{i\omega x} \), \( |\omega| \approx k \). They are too oscillatory to be accurately approximated on the coarse (the coarsest, for an adequate multigrid efficiency) scale, and they have too small \( \text{relative residuals} \) to be efficiently treated on fine grids (details can be found e.g., in [1]). Thus, these components is a liability for most multigrid solvers as they are virtually untreatable by standard multigrid techniques that involve using directly the Helmholtz operator, e.g., [2] or its shifted complex modification [3, 4]. Such solvers therefore can be used only as preconditioners for Krylov methods, leaving to the latter the task of eliminating \( ?? \). This strategy leaves no chances for a scalability – independence of the algorithm’s performance on the parameters of the problem and of the solver. The lack of scalability is especially pronounced in higher (than one) dimensions where the number of near kernel components increases for larger \( k \) and smaller \( kh \): such algorithms can be only used for a limited range of wave numbers and using discretization with a mediocre resolution.

Another challenges include divergence of \( \text{linear} \) relaxation routines, such as the Gauss-Seidel, the Jacobi, and the SOR schemes, when applied to (1.3) and large phase discretization errors for components (1.5). The latter can be improved, as often used in one-grid algorithms, by employing high-order discretization schemes.

The wave-ray \( \text{(wr)} \) approach, starting with the original [5], is based on a different philosophy on every one of these issues. First, at each multigrid iteration, it employs a special treatment for the \( nkc \) that efficiently reduces all of them, independently on their number and variety, serving as an actual solver rather than a preconditioner. Second, the algorithm considers the original Helmholtz equation and employs standard relaxation schemes. Finally, since the algorithm shows a (nearly) optimal, aka linear, dependence on the problem’s size, i.e., there is no need keep the size very small (for instance small enough for direct methods) and to employ high-order discretization schemes. (The costs for using such schemes in the multigrid framework is not limited to the increased costs on the finest grid – to benefit from a high-order discretization, one must also use expensive high-order (larger stencils) interpolation and coarse-grid operators. In case of Algebraic multigrid, for example, this leads to increasingly dense coarse grid operators, prohibiting using a fully efficient MG.)

The \( \text{wr} \) algorithm showed to be efficient for the most difficult, numerically, Helmholtz operator – the one with constant wave numbers, both in one [5] and two dimensions, [1, 6]. Our goal is to extend its applicability to problems with variable wave numbers, both continuous and discontinuous, while preserving all special features regarding the near-kernel treatment. Here we propose strategies, albeit implemented in one dimension, of how to achieve that, but with higher dimensions in mind – all strategies are clearly expendable to higher dimensions.

The rest of the paper is organized as follows. In Section 2 a brief explanation of the wave-ray idea is given, followed by description of the wave-ray algorithm, its parameters and numerical results for the original solver, Section 3. In Section 4 a new algebraic multigrid (AMG) version is
introduced, accompanied with numerical results for constant wave numbers. Modifications needed to apply the \( wr \) approach, both geometric and algebraic, for continuous \( k(x) \), resulting in numerical experiments presented in Section 5; versions used for discontinuous wave numbers and the corresponding numerics, appear in Section 6. A brief discussion of higher dimensions is given in Section 7.

2. Geometric Multigrid (GMG). The \( wr \) approach is based on two observations. First, a standard multigrid applied to the Helmholtz equation efficiently reduces all but the near-kernel error components. Second, the dominant part of unreduced components can be represented in the form

\[
e(x) = \hat{e}_-(x)e^{-ikx} + \hat{e}_+(x)e^{ikx}, \tag{2.1}
\]

where each function \( \hat{e}_\pm(x) \) is smooth, compared to the exponents.

Remark 2.1. It is important to note that (2.1) is not used to represent a solution, generated by some right-hand-side, but rather an unreduced error which mostly depends on \( L \) (and \( A_h \)) as it largely consists of its low energy modes. Representation (2.1) is rich: It includes, for example, all exponents with frequencies \( \omega \), \( 0 < |\omega| < 2k \), and many other functions, for instance the Hankel functions away from the origin. As analysis shows and numerical experiments confirm, in practice, the actual range is much smaller: \( (1 - \alpha_1)k \leq |\omega| \leq (1 + \alpha_2)k \), with \( \alpha_1 \approx \alpha_2 \approx 0.3 \), depending on the relaxation regiment employed.

In the \( wr \) approach, the task of computing the oscillatory \( e(x) \) is reduced to approximating two smooth functions \( \hat{e}_\pm(x) \). Given (2.1), the residual corresponding to \( e \): \( r = f - Ae \), has a similar approximate representation:

\[
r(x) = \hat{r}_-(x)e^{-ikx} + \hat{r}_+e^{ikx}, \tag{2.2}
\]

with smooth residual functions \( \hat{r}_\pm \). (Representation (2.2) is less accurate than (2.1) as higher energy (oscillatory) components with small amplitudes in \( e(x) \) have larger amplitudes in \( r(x) \).)

Approximation of \( \hat{e}_\pm \) numerically requires two main ingredients:

- Discrete coarse-grid, operators;
- Residuals \( \hat{r}_\pm \) defined on the same coarse grid.

Remark 2.2. As a nod to geometric optics terminology, all smooth hat functions are called ray functions, the equations that describe them – ray equations, and the grids on which they are represented in the discrete formulation, ray grids. Similarly, everything that is related to the Helmholtz part of the solver is called wave functions, wave operators and wave grids.

2.1. Ray operators and ray residuals. In geometric multigrid each discrete operator is a discretization of an underlined differential operator that describes the unknown function in continuum. Ray differential equations are discovered by applying differential (1.1) to (2.1), yielding

\[
Le(x) = e^{-ikx}\hat{L}_-\hat{e}_-(x) + e^{ikx}\hat{L}_+\hat{e}_+(x) = r = e^{-ikx}\hat{r}_-(x) + e^{ikx}\hat{r}_+(x), \tag{2.3}
\]

where

\[
\hat{L}_-\hat{e}_- = \hat{e}_-'' - 2ik\hat{e}_- \quad \text{and} \quad \hat{L}_+\hat{e}_+ = \hat{e}_+'' + 2ik\hat{e}_+'. \tag{2.4}
\]

Similarly, Sommerfeld boundary conditions are translated in terms of \( \hat{e}_\pm \), resulting in, at \( x = a \)

\[
e^{-ikx}\hat{e}_-'' = 0, \quad e^{ikx}[\hat{e}_+'' + 2ik\hat{e}_+] = 0. \tag{2.5}
\]
and, at $x = b$, 
\[ e^{-ikx}[(\hat{e}_-') - 2ik\hat{e}_-] = 0, \quad e^{ikx}\hat{e}_+ = 0. \] (2.6)

Advantage of using exponential basic functions $\exp(\pm ikx)$ here is clear: the high oscillations in (2.1) are completely removed from the ray description, and the two ray equations can be separated into two individual systems:
\[
\begin{cases}
  \hat{L}_-\hat{e}_- = \hat{r}_- - 2ik\hat{e}_-, \quad (a) = 0, \\
  \hat{L}_+\hat{e}_+ = \hat{r}_+ + 2ik\hat{e}_+, \quad (b) = 0;
\end{cases}
\] (2.7)

The ray operators are discretized on the ray grid with the mesh-size that satisfies $kH \approx \pi$, using a four-point stencil defined on staggered grids (details and motivation can be found in [5 1]). Ray residuals are also approximated on scale $H$, using a separation procedure that relies on the following properties. For a smooth function $g^h$ and exponential functions $e^{\pm 2ikx}$, both defined on fine scale, $h$, holds
\[
||g^h - P_h^hR_H^h g^h|| \ll ||g^h|| \quad \text{and} \quad R_H^h(e^{2ikx}g^h) \approx 0^H,
\] (2.8)

where $P_h^h$ and $R_H^h$ are a linear interpolation and a full weighting acting from $H$ to $h$ and from $h$ to $H$, respectively. In other words, $R_H^h$ preserves smooth functions and nearly eliminates functions close, in the frequency space, to $e^{\pm 2ikx}$. These considerations lead approximation procedure for $\hat{r}_H^\pm$.

Given the finest-grid wave residual, $r^h$, ray residuals can be computed as
\[
R_H^h(e^{ikx}r^h) \approx R_h^H(r^h_{-} + e^{2ikx}r^h_{+}) \approx \hat{r}_H^H.
\]

and
\[
R_H^h(e^{-ikx}r^h) \approx R_h^H(e^{-2ikx}r^h_{-} + r^h_{+}) \approx \hat{r}_H^H.
\]

3. WR algorithm. The wave-ray algorithm consists of two parts: a standard V-cycle applied to the Helmholtz equation and the additional correction by the two coarse-grid ray systems, as described in the following Pseudocode.

Wave Cycle: $\text{WaveCycle}(\ell, r^\ell)$

The input: Current grid $\ell$, the residual $r^\ell$

The output: New finest grid correction $e^1$ for $\ell = 1$

The MG framework: Correction Scheme

if $\ell == L$
  % On the coarsest grid $L$
  $e^\ell = \text{Relaxation}(A^\ell, r^\ell)$ (or $e^\ell = (A^\ell)^{-1}r^\ell$) \quad $A^\ell$ is a finite difference approximation on scale $\ell$
  $e^{\ell-1} = r^{\ell-1} + P_{\ell}^{\ell-1}e^{\ell}$ \quad ($P_{\ell}^{\ell-1}$ is a linear interpolation from grid $\ell$ to grid $\ell - 1$)
else
  % On grids $\ell = 1, \ldots, L - 1$
  $e^\ell = \text{Relaxation}(r^\ell)$
  $r^{\ell+1} = R_{\ell+1}^{\ell+1}(r^\ell - A^\ell e^\ell)$ \quad ($R_{\ell+1}^{\ell+1}$ is a full weighting from grid $\ell$ to grid $\ell + 1$)
  $e^\ell = e^\ell + \text{WaveCycle}(\ell + 1, e^{\ell+1})$
\[ e^\ell = e^\ell + \text{Relaxation}(r^\ell - A^\ell e^\ell) \]
if \( \ell > 1 \)
\[ e^{\ell-1} = e^{\ell-1} + P^{\ell-1}e^\ell \]
end if
end if

Ray Cycle: \( RayCycle(r) \)

The input: Finest grid wave residual \( r \equiv r^1 \)
The output: New finest grid correction \( e \equiv e^1 \)
The MG framework: Correction Scheme
\[ [\hat{r}_H^-, \hat{r}_H^+] = \text{Separation}(r) \]
Solve \( \hat{L}_- \hat{e}_- = \hat{r}_- \) and \( \hat{L}_+ \hat{e}_+ = \hat{r}_+ \) (by Gauss-Seidel relaxation in the propagation (negative and positive) direction);
\[ e = e^{-ikx} (P_H^- \hat{e}_H^-) + e^{ikx} (P_H^+ \hat{e}_H^+) \]

Wave Ray Cycle: \( WaveRayCycle(A, b, \hat{x}) \)

The input: \( A \equiv A^1, b \equiv b^1 \), the current approximation \( \hat{x} \equiv x^1 \)
The output: New finest grid approximation \( \tilde{x} \equiv x^1 \)
The MG framework: Correction Scheme
\[ \tilde{x} = \hat{x} + \text{WaveCycle}(b - A\hat{x}) \]
\[ \tilde{x} = \hat{x} + \text{RayCycle}(b - A\hat{x}) \]

All numerical methods in this paper are run for the wave-ray cycle (and its variation described in the upcoming Sections) with the fixed set of parameters that depend on values
\[ k_{\text{max}} = \max_{x \in \Omega} k(x), \quad k_{\text{min}} = \min_{x \in \Omega} k(x). \]

They are
- The finest mesh-size satisfies \( k_{\text{max}} h < 2\pi/10 \), typically \( k_{\text{max}} h \approx 0.3 \) or less;
- The ray mesh-size satisfies \( \pi/2 < k_{\text{min}} H \leq \pi \);
- In the wave cycle the Gauss-Seidel relaxation is used on all grids except the ones with the intermediate mesh-sizes \( \tilde{h} \): \( \pi/4 < k_{\text{max}} \tilde{h} \leq \pi/2 \);
- The number of relaxation in the wave cycle: one pre- and post relaxation if Gauss-Seidel is employed; two pre- and post sweeps for Kaczmarz relaxation;
- The ray relaxation is the Gauss-Seidel that in this case is an almost direct solver;
- The number of relaxation in the ray cycle: two per ray component.

In all Tables, computations are performed until the residual satisfies:
\[ \frac{\| r_m \|}{\| r_0 \|} < 10^{-6}, \quad (3.1) \]

where \( \| r_0 \| \) and \( \| r_m \| \) are the \( \ell_2 \) norms of the initial residual and the residual after \( m \) wave-ray cycles. The numerical results for the Helmholtz equation \( (1.1) \) with constant \( k \) are presented in Table 3.1.

The results will serve as a benchmark for all other variants of the algorithm, developed and applied to problems with different types of wave numbers.

Remark 3.1. Certain values of \( k \) have to be chosen for numerical experiments; These values
| $k$     | 40  | 80  | 160 | 320 |
|---------|-----|-----|-----|-----|
| $kh = 0.625$ | 13  | 14  | 27  | 14  |
| $kh = 0.3125$ | 12  | 12  | 13  | 14  |
| $kh = 0.15625$ | 15  | 15  | 16  | 17  |

Table 3.1: The number of gmg-WR cycles needed to satisfy (3.1). The results are computed for different choices of $k$ and the finest $h$; the number of levels varies from $L = 5$ ($k = 40, kh = 0.625$) to $L = 10$ ($k = 320, kh = 0.15625$).

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The results slightly depend values of $k$ and $kh$. The difference is due to different smoothing rates of relaxation schemes and, more importantly, to accuracy of the separation procedure. The algorithm can be tailored to accommodate the separation to a particular value of $kH$; the full weighting employed here works most accurately for $kH = \pi$ - and such values do no appear in the paper.

4. Algebraic multigrid wave-ray (amgWR) algorithm. The geometric wave-ray algorithm relies on the knowledge of analytical near-kernel components of the differential Helmholtz operator $L$. An alternative algebraic version uses numerical approximations instead of analytical functions and proceeds to directly compute discrete coarse grid operators, both in wave and ray representation, bypassing the differential ones. The advantage of the approach is its ability to numerically adjust the basic functions to better satisfy (1.5).

4.1. Wave part. The main decision in the AMG is a choice of prolongation operators, $P$. Typically, they are constructed to accurately transfer the near-kernel components of the finest-grid operator: in the Helmholtz case these are components (2.1). In the WR approach, however, the wave part is not responsible for their treatment, and, therefore, $P$ is not defined by their character.

Two remaining types of components: highly oscillatory and physically smooth are well served by a standard polynomial interpolation, similarly to processing of Laplace operator. Indeed, the former are treated on sufficiently fine grid where they remain relatively smooth, while the later are reduced to the coarsest grids from which they are accurately interpolated due to their smoothness.

All coarse-grid wave operators, $\ell = 2, \ldots, L$ are computed using (4.1), with $A^1 \equiv A^h$.

Remark 4.1. Operators $A^\ell$, $\ell = 2, \ldots, L$ are very similar to the one of the discrete geometric operators – they too are some discretizations of $L$ and can be easily substituted for one another.

4.2. Ray part. Construction of coarse grid ray operators starts on the finest grid, using the Helmholtz discrete operator, $A^h$. Using $e^{-ikz}$ and $e^{ikz}$, substitution of error in the form (2.1) into the wave residual equation $A^h e^h = r^h$, produces finest-grid ray operators $A_{-}^h$ and $A_{+}^h$:

\[
A^h e^h = e^{-ikz} A_{-}^h e^h + e^{ikz} A_{+}^h e^h,
\]
with their stencils given by

\[ \hat{S}^-_h = \frac{1}{h^2} \left[ e^{ikh} \left( -2 + k^2 h^2 \right) e^{-ikh} \right] \]

and

\[ \hat{S}^+_h = \frac{1}{h^2} \left[ e^{-ikh} \left( -2 + k^2 h^2 \right) e^{ikh} \right] \]

Ray operator \( \hat{A}^H_\pm \) on scale \( H \) are then computed as

\[ \hat{A}^H_\pm = (P^h_H)^t (\hat{A}^h_\pm) (P^h_H). \] (4.3)

A linear interpolation again is sufficiently accurate for smooth \( \hat{e}_\pm \).

Ray residuals are approximated by

\[ \hat{r}^H_- = (P^h_H)^t (e^{ikx} \hat{r}^h_\pm) \]

and

\[ \hat{r}^H_+ = (P^h_H)^t (e^{-ikx} \hat{r}^h_\pm). \]

The amgWR algorithm is applied to (1.3) with constant \( k \), Table 4.1, with parameters as in Table 3.1. Again, the results clearly improve or at least stabilize when the algorithm is applied for small \( kh \). This effect becomes more pronounced for larger wave numbers, they are similar to the ones of the gmgWR.

| \( k \) | 40 | 80 | 160 | 320 |
|---|---|---|---|---|
| \( kh = 0.625 \) | 16 | 34 | > 50 | > 50 |
| \( kh = 0.3125 \) | 11 | 13 | 18 | 43 |
| \( kh = 0.15625 \) | 11 | 10 | 12 | 18 |
| \( kh = 0.078125 \) | 11 | 10 | 12 | 14 |

**Table 4.1**

Presented here is the number of the AMG wave-ray cycles needed to satisfy (3.1). The results are obtained both for different values of \( k \) and \( kh \) where \( h \) is the finest scale mesh-size.

5. Continuous wave numbers: amgWR and amgWR(c). As an example of a variable wave number here

\[ k(x) = k_0 \sqrt{1 + m(x)}, \text{ with } |m(x)| < 1, \] (5.1)

is considered, and in the numerics

\[ m(x) = \alpha \cos(\beta x) \] (5.2)

is used. Such form allows to investigate how amplitude and oscillations in \( m(x) \) affect algorithmic performance. First, the amgWR with exponential basic functions \( u_\pm(x) = e^{\pm ik_0 x} \) is tested, Tables
Table 5.1
The number of the AMG WR cycles needed to satisfy (3.1); β = 1.

| α  | 0.1 | 0.2 | 0.4 | 0.8 |
|----|-----|-----|-----|-----|
| k₀ = 40 | 10  | 10  | 11  | 13  |
| k₀ = 160 | 11  | 11  | 12  | 14  |

Table 5.2
The number of the AMG WR cycles needed to satisfy (3.1); β is proportional to k₀, with k₀/β varying from 0.1 to 1, α = 0.5; "D" stands for divergence.

| β  | 0.1k₀ | 0.25k₀ | 0.5k₀ | 0.75k₀ | k₀ |
|----|-------|--------|-------|--------|----|
| k₀ = 25 | 12   | 11    | 11    | 30    | 41 |
| k₀ = 50 | 12   | 11    | 11    | D     | D  |
| k₀ = 100 | 13   | 13    | 13    | D     | D  |
| k₀ = 200 | 15   | 21    | 19    | D     | D  |

5.1-5.2 Table 5.1 presents the results for smooth k(x) with β fixed at 1, computed for two different values of k₀.

In Table 5.2, wave numbers are considered for a variety of k₀ and β values and α = 0.5. The results suggest that α value does not impact convergence, at least when it remains bounded by one. Increase in β leads to slowdown and divergence.

The next variation amgWR(c) improves convergence by modifying the basis functions, while still maintaining directions as defined by the exponents. The new basis functions are sought in the ray form

\[ u_±(x) = \hat{u}_±(x)e^{±ik₀x}, \]  

where \( \hat{u}_± \) satisfy

\[ \Delta \hat{u}_±(x) ± 2ik₀\hat{u}_± + k₀²m(x)\hat{u}_±(x) = 0, \]  

with boundary conditions derived from (1.2),

\[
\begin{cases} 
\hat{u}_±'(a) + i(k(a) ± k₀)\hat{u}_±(a) = 0, \\
\hat{u}_±'(b) - i(k(b) ± k₀)\hat{u}_±(b) = 0.
\end{cases}
\]

Discrete equations for \( \hat{u}_± \) on scale \( H \) can be obtained either geometrically or algebraically, and functions \( \hat{u}_± \) are computed, as discussed in Section 2.1 using \( \hat{r}_± = 0 \). After \( \hat{u}_±^H \) are approximated and interpolated to the finest scale, \( h \), the modified basis functions (5.3) are reconstructed and employed in the wave-ray algorithm. The numerical results are given in Table 5.3 using parameters identical to the ones in Table 5.2.

The amgWR(c) modified approach compliments amgWR: it diverges when the former converges well and shows good results when the other diverges. The combined Table 5.4 gives the best of the two approaches’ results. Clearly, these are just the first steps in understanding what are the best strategies in dealing with oscillatory wave numbers – but the results are quite encouraging.
The number of the amgWR(c) cycles needed to satisfy (3.1); beta is proportional to $k_0$, with $k_0/\beta$ varying from 0.1 to 1, $\alpha = 0.5$; "D" stands for divergence.

| $\beta$ | 0.1$k_0$ | 0.25$k_0$ | 0.5$k_0$ | 0.75$k_0$ | $k_0$ |
|---------|----------|-----------|----------|-----------|------|
| $k_0 = 25$ | D | D | 13 | 13 | 18 |
| $k_0 = 50$ | D | D | 13 | 14 | 16 |
| $k_0 = 100$ | D | D | 13 | 14 | 21 |
| $k_0 = 200$ | D | D | 17 | 14 | 20 |

Table 5.3

The number of the amgWR or amgWR(c) cycles, whichever is the smallest, needed to satisfy (3.1); beta is proportional to $k_0$, with $k_0/\beta$ varying from 0.1 to 1, $\alpha = 0.5$.

| $\beta$ | 0.1$k_0$ | 0.25$k_0$ | 0.5$k_0$ | 0.75$k_0$ | $k_0$ |
|---------|----------|-----------|----------|-----------|------|
| $k_0 = 25$ | 12 | 11 | 11 | 13 | 18 |
| $k_0 = 50$ | 12 | 11 | 11 | 14 | 16 |
| $k_0 = 100$ | 13 | 13 | 13 | 14 | 21 |
| $k_0 = 200$ | 15 | 21 | 17 | 14 | 20 |

Table 5.4

6. Discontinuous Wave Numbers: amgWR(d) and amgWR(c). Considered here is a discontinuous wave number in the form

$$k(x) = \begin{cases} 
k_1, & \text{if } x \leq \bar{x}, \\
k_2, & \text{if } x > \bar{x},
\end{cases}$$

(6.1)

with $k_1 \geq k_2$ for definiteness. First, the amgWR is applied using basic functions

$$u_\pm(x) = \begin{cases} 
e^{\pm ik_1 x}, & \text{if } x \leq \bar{x}, \\
e^{\pm ik_2 x}, & \text{if } x > \bar{x}.
\end{cases}$$

(6.2)

The results for $k_1 = k$ and $k_2 = \gamma k$, $0 < \gamma < 1$ are given in Table 6.1, they are restricted to cases when both $k_1$ and $k_2$ are large enough to benefit from ray representation. The algorithm can be easily adjusted to accommodate small values of $k$ but it is not in the scope of this paper.

| $k$ | 40 | 80 | 160 | 320 |
|-----|----|----|-----|-----|
| $\gamma = 0.8$ | 18 (13) | 31(14) | 36(19) | $>50\ (20)$ |
| $\gamma = 0.5$ | 18(13) | 33(15) | 37(21) | $>50\ (23)$ |
| $\gamma = 0.25$ | 18(13) | 33(15) | 37(21) | $>50\ (23)$ |

Table 6.1

The number of the amgWR cycles needed to satisfy (3.1); with basis functions (6.9) and (in parenthesis) with each of (6.8) functions pre-smoothed by one wave cycle.

There is a clear benefit of pre-smoothing of the basis functions which are discontinuous at $\bar{x}$; it is very likely that a local processing near $x = \bar{x}$ would be sufficient, optimization of the pre-smoothing
strategy is a subject of future investigation. Overall, the algorithm loses efficiency compared to constant $k$.

6.1. Residual Separation for Discontinuous Wave Numbers. Ray residuals $\tilde{r}_\pm$ are approximated on scale that satisfies $\pi/2 \leq kH \leq \pi$. Wave numbers (6.1) yield two different scales: $H_1$, with $\pi/2 \leq k_1 H_1 \leq \pi$, and $H_2$, with $\pi/2 \leq k_2 H_2 \leq \pi$. If $\gamma > 1/2$ then $H_1 = H_2 = H$, and the standard separation procedure described in Section 4 works perfectly well. However, if $\gamma \leq 1/2$ then $H_2 \geq 2H_1$ and the separation and possibly the approximation of $\tilde{e}_\pm$ is better done on different scales for $x \leq \bar{x}$ and $x > \bar{x}$.

Current implementation is a compromise: ray functions are approximated on the same scale $H = \min \{H_1, H_2\} = H_1$ throughout $\Omega$, meaning that both residuals $\tilde{r}_\pm$ are eventually assembled there. However, scale $H_2$ is used in the separation routine in the following way.

- Residuals $\tilde{r}_\pm^H$ are approximated as discussed in Section 4;
- For $x > \bar{x}$ the averaging continuous to scale $H_2$:

$$\left(\tilde{r}_\pm^{H_2}\right)_{x > \bar{x}} = \left(\tilde{r}_\pm^{H_1}\right)_{x > \bar{x}}$$

Thus, the residuals are properly separated on $x > \bar{x}$;

- Ray residuals are reconstructed on the ray grid

$$\tilde{r}_\pm^H = \begin{cases} \tilde{r}_\pm^{H_1}, & \text{if } x \leq \bar{x}, \\ P_{H_2}^{H_1} \tilde{r}_\pm^{H_1}, & \text{if } x > \bar{x}, \end{cases} \quad (6.3)$$

where $P_{H_2}^{H_1}$ is a linear interpolation from scale $H_2$ to scale $H$; it works because $\tilde{r}_\pm^{H_2}$ are smooth.

6.2. AMG and Geometric Optics. The next modification is based the laws of geometric optics. If an incident wave is given by $e^{-ik_2 x}$, propagating in the negative direction and entering $\Omega$ from the right, solution $Lu = 0$ is of the form

$$\pi_-(x) = \begin{cases} C_r^- e^{-ik_1 x}, & \text{if } x \leq \bar{x}, \\ e^{-ik_2 x} + C_t^- e^{ik_2 x}, & \text{if } x > \bar{x}, \end{cases} \quad (6.4)$$

with reflection and transmission coefficients $C_r^-$ and $C_t^-$ given by:

$$C_r^- = \frac{k_1 - k_2}{k_1 + k_2} e^{-2ik_2 \bar{x}}, \quad C_t^- = \frac{2k_2}{k_1 + k_2} e^{i(k_1 - k_2) \bar{x}}. \quad (6.5)$$

For $\pi_+(x)$, with an incident wave $e^{ik_1 x}$, entering $\Omega$ from the left, the solution is given by

$$\pi_+(x) = \begin{cases} e^{ik_1 x} + C_r^+ e^{-ik_1 x}, & \text{if } x \leq \bar{x}, \\ C_t^+ e^{ik_2 x}, & \text{if } x > \bar{x}. \end{cases} \quad (6.6)$$

with coefficients $C_r^+$ and $C_t^+$ given by:

$$C_r^+ = \frac{k_1 - k_2}{k_1 + k_2} e^{2ik_1 \bar{x}}, \quad C_t^+ = \frac{2k_1}{k_1 + k_2} e^{i(k_1 - k_2) \bar{x}}. \quad (6.7)$$
The new basic functions are composed of components of (6.4)-(6.6) that propagate in the same direction:

\[ u^-(x) = \begin{cases} 
Cte^{-ik_1x}, & \text{if } x \leq \bar{x}, \\
e^{-ik_2x}, & \text{if } x > \bar{x}, 
\end{cases} \quad (6.8) \]

and

\[ u^+(x) = \begin{cases} 
\hat{e}e^{ik_1x}, & \text{if } x \leq \bar{x}, \\
Cte^{ik_2x}, & \text{if } x > \bar{x}. 
\end{cases} \quad (6.9) \]

Table 6.2 presents numerical results for different values and ratios of \( k_1 \) and \( k_2 \). Once more, the results significantly improve when the basic functions are preprocessed and the efficiency becomes similar to the one obtained for constant wave numbers.

| \( k \) | \( \gamma = 0.8, (p = 0) \) | \( \gamma = 0.5, (p = 1) \) | \( \gamma = 0.25, (p = 2) \) |
|---|---|---|---|
| 40 | 30 (11) | 45 (11) | 23 (12) |
| 80 | 27 (21) | 44 (11) | 23 (12) |
| 160 | 18 (12) | 31 (13) | 33 (13) |
| 320 | 13 (12) | 36 (15) | 27 (14) |

Table 6.2: The number of the amgWR(d) cycles needed to satisfy (3.1), with the basic functions defined by (6.8)-(6.9) without and with (in parenthesis) pre-smoothing by one AMG wave cycle; parameter \( p \) describes the ratio between the ray scales \( H_2 = 2^pH_1 \) in Section 6.1.

6.3. \textit{gmgWR(d): Adaptation of Ray Operators.} The original \textit{gmgWR} has a limited application for Helmholtz operators with discontinuous wave numbers. As shown in Table 6.2, its performance deteriorates even for \( \gamma \approx 1 \), and it completely falls apart as \( \gamma \) becomes smaller.

| \( k \) | \( \gamma = 0.95 \) | \( \gamma = 0.8 \) | \( \gamma = 0.4 \) | \( \gamma = 0.25 \) |
|---|---|---|---|---|
| 40 | 21 | 52 | 24 | D |
| 80 | 55 | 45 | 62 | D |
| 160 | 51 | 80 | D | D |
| 320 | 43 | 68 | D | D |

Table 6.3: The number of the GMG WR cycles needed to satisfy (3.1); \( D \) stands for divergence.

The reason for such a poor performance is a non-adequate description of interfaces between different media by ray equations. To address that, ray equation(s), with stencils that are crossed by such interfaces are modified based on information from a much more detailed finest wave grid. If, for example, \( k(x - h) = k(x) = k_1 \) and \( k(x + h) = k_2 \) and assuming

\[ u(x) = \begin{cases} 
\hat{e}_x e^{\pm ik_1x} & \text{if } x \leq \bar{x}, \\
\hat{e}_x e^{\pm ik_2x} & \text{if } x > \bar{x}, 
\end{cases} \quad (6.10) \]
then substituting \(u(x)\) into a discrete Helmholtz equation, centered at \(\bar{x}\), and subsequently applying Taylor expansion, yields a modified differential ray operator centered at \(\bar{x}\):

\[
\hat{L}_\pm \hat{e}_\pm(\bar{x}) + \left[ \hat{e}_\pm(x) + h \hat{e}'_\pm(x) + \frac{h^2}{2} \hat{e}''_\pm(x) \right] \frac{V_\pm}{h^2},
\]

where

\[
V_\pm = e^{\pm ik_2 h} e^{\pm \frac{ik}{2} h} - e^{\pm \frac{ik_1 h}{2}}.
\]

Table 6.4 shows that modification of one ray discrete equation for each of \(\hat{e}_\pm\) leads to a significant improvement.

| \(k\) | 40 | 80 | 160 | 320 |
|------|----|----|-----|-----|
| \(\gamma = 0.8\) | 18 | 21 | 23 | 23 |
| \(\gamma = 0.4\) | 22 | 20 | 21 | 21 |
| \(\gamma = 0.25\) | 21 | 25 | 25 | 21 |

Table 6.4

The number of the \(gmgWR(d)\) cycles needed to satisfy (3.1)

Although the results by the \(gmgWR(d)\) are modes compared to the ones of the \(amgWR(d)\), its setup costs are smaller, and this could play a role in higher dimensions, where fast convergence might be outweighed by high setup costs. Which approach will have a better overall performance in two- and three dimensions remains to be seen.

7. Conclusions and extension to higher dimensions. In this paper, steps to extend the existing geometric wave-ray algorithm for the Helmholtz operator with constant wave numbers to problems with both continuous and discontinuous wave numbers, are outlined. The results, achieved by modification of the existing geometric and new algebraic versions of the wave ray algorithms, are comparable to the results shown by the original wave ray algorithm for constant \(k\). The summary of the results observed for different versions of the algorithm for various types of the wave numbers are shown in Table 7.1.

The extension to higher dimensions relies on an analogue of the error representation (2.1):

\[
e(x) = \sum_{k=1}^{K} a_k(x) e^{i k^2 x}, \quad x \in \Omega \subset \mathbb{R}^d, \quad k_k \in \mathbb{R}^d, \quad |k_k| = k, \quad d = 2, 3,
\]

along with the used in the original two-dimensional \(gmgWR(d)\) algorithm. The frequencies \(k_k\) are uniformly distributed along a circle (sphere) of radius \(k\). The number of the basis functions \(K = O(1)\) grows for higher dimensions; for instance, for the two-dimensional solver in [1] \(K = 8\) was sufficient.

The next step is to extend the ideas presented in Sections 4-6 to two dimensions. The first results in this direction were obtained for the two-dimensional \(amgWR\) solver, and they are promising [?]. The new algorithm along with the original two-dimensional \(gmgWR\) [1] will serve as a foundation for implementing other strategies presented in this paper.
Table 7.1  
The number of different types of WR cycles, generic or adapted to a particular type of wave numbers, needed to satisfy (3.1). For constant \( k \) for the AMG WR the number in parenthesis is the number of cycles if the problem is considered on finer grid with \( kh = 0.078125 \).

| \( k \) | 40 | 80 | 160 | 320 |
|-------|----|----|-----|-----|
| Constant \( k \): GMG | 12 | 12 | 13 | 14 |
| Constant \( k \): AMG | 11(11) | 13(10) | 18(12) | 43(14) |
| Continuous \( k \) (\( \alpha = 0.4, \beta = 20 \)): AMG | 13 | 7 | 8 | 9 |
| Discontinuous \( k \) (\( \gamma = 0.25 \)) GMG(d) | 21 | 25 | 25 | 21 |
| Discontinuous \( k \) (\( \gamma = 0.25 \)) AMG(d) | 14 | 14 | 15 | 16 |

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