# An optimal 25-point finite difference scheme for the Helmholtz equation with PML 

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#### Abstract

In this paper, we present an optimal 25 -point finite difference scheme for solving the Helmholtz equation with perfectly matched layer (PML) in two dimensional domain. Based on minimizing the numerical dispersion, we propose the refined choice strategy for choosing optimal parameters of the 25 -point finite difference scheme. Numerical experiments are given to illustrate the improvement of the accuracy and the reduction of the numerical dispersion.


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## 1. Introduction

In a Cartesian coordinate system, the 2-D scalar wave equation with no damping in the frequency domain is given by

$$
\begin{equation*}
\Delta u+k^{2} u=g \tag{1.1}
\end{equation*}
$$

where $u$ is the Fourier component of the wavefield pressure, $k \in \mathbb{R}$, called wavenumber, is a positive number, and $g$ is the Fourier transformation of the source function. The above equation, which is the well-known Helmholtz equation, appears directly or indirectly in almost all wave-related problems arisen from many science, engineering, and industry applications. Therefore, solving the Helmholtz equation, in various forms, has always been a hot topic in wave computation (cf. [1,2] and the reference therein).

To compute the solution of the above problem, due to finite memory and speed limitation of the computer, we first need to formulate the problem as a finite domain problem. Thanks to absorbing boundary conditions, we are able to truncate the infinite domain into a finite domain with less or almost no reflection; see one-way approximation (cf. [3-5]), PML (perfectly matched layer, cf. [6-12]), and so on. In this paper, PML is used to truncate the domain and absorb the outgoing waves. The PML was proposed by Bérenger in 1994 in [6], and it has the astonishing property of generating almost no reflection in theory at the interface between the interior medium (the interested domain) and the artificial absorbing medium.

Specifically, applying the PML technique to truncate the infinite domain into a bounded rectangular domain and taking the same notations as in [13] lead to the equation

$$
\begin{equation*}
\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+C k^{2} u=f \tag{1.2}
\end{equation*}
$$

where

$$
f:= \begin{cases}0, & \text { inside PML } \\ g, & \text { outside PML }\end{cases}
$$

[^0]and
$$
A:=\frac{e_{y}}{e_{x}}, \quad B:=\frac{e_{x}}{e_{y}}, \quad C:=e_{x} e_{y}
$$
in which $e_{x}:=1-i \frac{\sigma_{x}}{\omega}, e_{y}:=1-i \frac{\sigma_{y}}{\omega}$, $\omega$ is the angular frequency, $\sigma_{x}$ is a function only of $x$ defined as
\[

\sigma_{x}:= $$
\begin{cases}2 \pi a_{0} f_{0}\left(\frac{l_{x}}{L_{\mathrm{PML}}}\right)^{2}, & \text { inside PML }  \tag{1.3}\\ 0, & \text { outside PML }\end{cases}
$$
\]

with the dominant frequency $f_{0}$ of the source, the thickness $L_{\text {PML }}$ of PML, the distance $l_{x}$ from the interface between the interior region and PML region, and a constant $a_{0}$, and $\sigma_{y}$ is defined similarly. Eq. (1.2) can be seen as a general form of the Helmholtz equation (1.1) with the corresponding PML equation, since in the interior domain, $A=B=C=1$. We call it the Helmholtz-PML equation. Moreover, Eq. (1.2) is also valid for variable $k(x, y)$ (see, [14,15]).

For many years, finite difference methods (cf. [16-22,9,23,24] and the reference therein) and finite element methods (cf. [25-29]) have been widely used to discrete the Helmholtz equation (1.1) with various boundaries. As is known to all, the solution of the Helmholtz equation oscillates severely for large wavenumbers, and the quality of the numerical results usually deteriorates as the wavenumber $k$ increases (cf. [25-29]). Hence, there is a growing interest in discretization methods where the computational complexity increases only moderately with increasing wavenumber (cf. [25,28,30,20,22]). Compared with finite difference methods, discontinuous Galerkin (DG) methods can naturally handle inhomogeneous boundary conditions and curved boundaries, and they also allow the use of highly nonuniform and unstructured meshes. Moreover, DG methods also possess the property of higher accuracy. However, the finite difference method is more popular and useful in the numerical seismic wave propagation modeling (cf. [17,19]), because of its easier implementation and less computational complexity. Furthermore, we can easily extend finite difference methods to the three dimensional cases, and improve the accuracy of the solution of the Helmholtz equation by choosing optimal parameters in finite difference formulas $[20,22]$.

In this paper, we are interested in the finite difference method because of its easy implementation, although its accuracy is usually lower than that of the finite element method. For accurate modeling, the conventional 5-point finite difference scheme requires 10 gridpoints per wavelength. Therefore, for the Helmholtz equation with large wavenumbers, the resulting matrix is very large and ill-conditioned. Usually, direct methods do not perform well, and iterative methods with preconditioners are alternative [31,17,24]. In 1996, the rotated 9-point finite difference scheme for the Helmholtz equation was proposed in [20] and one group of optimal parameters were also given. This optimal 9-point scheme reduces the number of gridpoints per wavelength to 5 while preserving the accuracy of the conventional 5 -point scheme with 10 gridpoints per wavelength. Therefore, computer memory and CPU time are much saved. Shin and Sohn extended the idea of the rotated 9-point scheme to the 25-point formula in [22], which was called the extended 25-point finite difference scheme. The extended 25 -point formula reduces the number of gridpoints per wavelength to 2 , and its numerical dispersion is much less as compared with that of the rotated 9 -point scheme.

Although it is good for the Helmholtz equation, the rotated 9-point scheme is not pointwise consistent with the Helmholtz-PML equation, which was proved in [13]. To overcome this difficulty, we presented a consistent 9-point finite difference scheme following the approach in [9]. Additionally, based on minimizing the numerical dispersion (see, [29,32]), global and refined choice strategies for choosing optimal parameters of the 9-point finite difference scheme were proposed. The improvement of the accuracy and the reduction of the numerical dispersion are significant. Moreover, to solve large scale problems, in [33] we proposed a new multigrid based preconditioned Krylov subspace method for the Helmholtz equation with PML, which was discretized by the optimal 9-point finite difference scheme proposed in [13]. The applications ranged from constant wavenumbers to irregular heterogeneity structures in a medium. The new multigrid based preconditioned BiCGSTAB method for the Helmholtz-PML equation was proved to be an efficient and robust iterative method. However, due to the existence of numerical dispersion, the numerical solution still deteriorates as the wavenumber $k$ increases, although it has much improvement as compared with the rotated 9-point finite difference scheme. As the extended 25 -point scheme has better properties than the rotated 9 -point scheme (see, [22]), the goal of this paper is to propose an optimal 25-point scheme for the Helmholtz-PML equation, based on further minimizing the numerical dispersion. Moreover, we will find that, though the extended 25-point difference scheme is a popular solver for the Helmholtz equation, it is not a good choice for the Helmholtz equation with PML. We shall address this issue in detail in this paper.

This paper is organized as follows. In Section 2, we investigate the extended 25-point finite difference scheme and show that this scheme with the optimal parameters given in [22] is not pointwise consistent with the Helmholtz equation with PML. In Section 3, we present a 25-point difference scheme by using the approach suggested in paper [9], and prove that it is consistent with the Helmholtz equation with PML and is a second order scheme. We then propose the refined choice strategy for choosing optimal parameters of the 25 -point finite difference scheme based on minimizing the numerical dispersion. In Section 4, numerical experiments are given to demonstrate the efficiency of the scheme. These numerical results show that the newly proposed schemes not only improve the accuracy, but also reduce the numerical dispersion significantly. Finally, Section 5 contains the conclusion of this paper.


Fig. 1. Five-point Laplacian operators.

## 2. The extended 25-point finite difference scheme for the Helmholtz-PML equation

In this section, we investigate the extended 25 -point finite difference scheme for the Helmholtz equation with PML.
To construct finite difference schemes, we consider the network of grid points ( $x_{m}, y_{n}$ ), where $x_{m}:=x_{0}+(m-1) h$ and $y_{n}:=y_{0}+(n-1) h$. Notice that the same step size $h:=\Delta x=\Delta y$ is used for both variables $x$ and $y$. Let $u_{m, n}$ $:=\left.u\right|_{x=x_{m}, y=y_{n}}$ represent the pressure of the wave field at the location ( $x_{m}, y_{n}$ ), and similarly, let $k_{m, n}:=\left.k\right|_{x=x_{m}, y=y_{n}}$ and $f_{m, n}:=\left.f\right|_{x=x_{m}, y=y_{n}}$. The key idea of the extended 25-point finite difference scheme is to approximate $\Delta u$ by a second order centered difference using two 5-point $0^{\circ}$ stars, two $45^{\circ}$ rotated stars, the $\theta_{1}$ rotated star and the $\theta_{2}$ rotated star (see, Fig. 1), where $\theta_{1}:=\frac{180^{\circ}}{\pi} \arcsin \frac{\sqrt{5}}{5}$ and $\theta_{2}:=\frac{180^{\circ}}{\pi} \arcsin \frac{2 \sqrt{5}}{5}$.

To develop the extended 25-point difference scheme for solving the Helmholtz-PML equation (1.2), we let

$$
\begin{aligned}
& A_{m+\frac{i}{2}, n+\frac{j}{2}}:=A\left(x_{0}+\left(m-1+\frac{i}{2}\right) \Delta x, y_{0}+\left(n-1+\frac{j}{2}\right) \Delta y\right), \\
& B_{m+\frac{i}{2}, n+\frac{j}{2}}:=B\left(x_{0}+\left(m-1+\frac{i}{2}\right) \Delta x, y_{0}+\left(n-1+\frac{j}{2}\right) \Delta y\right), \\
& C_{m, n}:=C\left(x_{0}+(m-1) \Delta x, y_{0}+(n-1) \Delta y\right),
\end{aligned}
$$

for $i, j \in \mathbb{Z}_{3}:=\{-2,-1,0,1,2\}$. According to the construction of the extended 25-point difference method, we define

$$
\begin{align*}
\left.\mathcal{L}_{h} u\right|_{x=x_{m}, y=y_{n}}:= & \left.a_{1} \mathcal{L}_{h, 0}{ }^{\circ} u\right|_{x=x_{m}, y=y_{n}}+a_{2} \mathcal{L}_{2 h,\left.0^{\circ} u\right|_{x=x_{m}, y=y_{n}}+\left.a_{3} \mathcal{L}_{h, 45^{\circ} u} u\right|_{x=x_{m}, y=y_{n}}+a_{4} \mathcal{L}_{2 h,\left.45^{\circ} u\right|_{x=x_{m}, y=y_{n}}}} \\
& +\left.a_{5} \mathcal{L}_{2 h, \theta_{1}} u\right|_{x=x_{m}, y=y_{n}}+\left.a_{6} \mathcal{L}_{2 h, \theta_{2}} u\right|_{x=x_{m}, y=y_{n}}, \tag{2.1}
\end{align*}
$$

where $\sum_{j=1}^{6} a_{j}=1$,

$$
\begin{align*}
\left.\mathcal{L}_{2 h, \theta_{2}} u\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{\sqrt{5} h}\left\{\left(A_{m+\frac{1}{2}, n-1} \frac{u_{m+1, n-2}-u_{m, n}}{\sqrt{5} h}-A_{m-\frac{1}{2}, n+1} \frac{u_{m, n}-u_{m-1, n+2}}{\sqrt{5} h}\right)\right. \\
& \left.+\left(B_{m+1, n+\frac{1}{2}} \frac{u_{m+2, n+1}-u_{m, n}}{\sqrt{5} h}-B_{m-1, n-\frac{1}{2}} \frac{u_{m, n}-u_{m-2, n-1}}{\sqrt{5} h}\right)\right\}, \tag{2.2}
\end{align*}
$$

and the former five terms on the left side of the Eq. (2.1) are constructed similarly based on the second order centered difference schemes for the point $\left(x_{m}, y_{n}\right)$. We then approximate the first two terms of the left hand side of (1.2) as

$$
\left.\left[\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)\right]_{x=x_{m}, y=y_{n}} \approx \mathscr{L}_{h} u\right|_{x=x_{m}, y=y_{n}} .
$$

Moreover, in order to approximate the term of zeroth order with 25 points, we let

$$
\begin{aligned}
\left.\ell_{h, 0}{ }^{\circ}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m-1, n} k_{m-1, n}^{2} u_{m-1, n}+C_{m+1, n} k_{m+1, n}^{2} u_{m+1, n}\right. \\
& \left.+C_{m, n-1} k_{m, n-1}^{2} u_{m, n-1}+C_{m, n+1} k_{m, n+1}^{2} u_{m, n+1}\right), \\
\left.\ell_{2 h, 0}{ }^{\circ}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m-2, n} k_{m-2, n}^{2} u_{m-2, n}+C_{m, n-2} k_{m, n-2}^{2} u_{m, n-2}\right. \\
& \left.+C_{m+2, n} k_{m+2, n}^{2} u_{m+2, n}+C_{m, n+2} k_{m, n+2}^{2} u_{m, n+2}\right), \\
\left.l_{h, 45}{ }^{\circ}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m-1, n+1} k_{m-1, n+1}^{2} u_{m-1, n+1}+C_{m+1, n-1} k_{m+1, n-1}^{2} u_{m+1, n-1}\right. \\
& \left.+C_{m-1, n-1} k_{m-1, n-1}^{2} u_{m-1, n-1}+C_{m+1, n+1} k_{m+1, n+1}^{2} u_{m+1, n+1}\right), \\
\left.\ell_{2 h, 45}{ }^{\circ}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m-2, n-2} k_{m-2, n-2}^{2} u_{m-2, n-2}+C_{m+2, n-2} k_{m+2, n-2}^{2} u_{m+2, n-2}\right. \\
& \left.+C_{m+2, n+2} k_{m+2, n+2}^{2} u_{m+2, n+2}+C_{m-2, n+2} k_{m-2, n+2}^{2} u_{m-2, n+2}\right), \\
\left.\ell_{2 h, \theta_{1}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m+2, n-1} k_{m+2, n-1}^{2} u_{m+2, n-1}+C_{m+1, n+2} k_{m+1, n+2}^{2} u_{m+1, n+2}\right. \\
& \left.+C_{m-2, n+1} k_{m-2, n+1}^{2} u_{m-2, n+1}+C_{m-1, n-2} k_{m-1, n-2}^{2} u_{m-1, n-2}\right), \\
\left.l_{2 h, \theta_{2}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & \frac{1}{4}\left(C_{m+1, n-2} k_{m+1, n-2}^{2} u_{m+1, n-2}+C_{m+2, n+1} k_{m+2, n+1}^{2} u_{m+2, n+1}\right. \\
& \left.+C_{m-1, n+2} k_{m-1, n+2}^{2} u_{m-1, n+2}+C_{m-2, n-1} k_{m-2, n-1}^{2} u_{m-2, n-1}\right),
\end{aligned}
$$

and approximate $\left.C k^{2} u\right|_{x=x_{m}, y=y_{n}}$ by a weighted average:

$$
\left.\left.C k^{2} u\right|_{x=x_{m}, y=y_{n}} \approx \ell_{h}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}
$$

where

$$
\begin{align*}
\left.\ell_{h}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}:= & b_{1} C_{m, n} k_{m, n}^{2} u_{m, n}+\left.b_{2} \ell_{h, 0}{ }^{\circ}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}+\left.b_{3} \ell_{2 h, 0^{\circ}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}} \\
& +\left.b_{4} \ell_{h, 45^{\circ}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}+\left.b_{5} \ell_{2 h, 45^{\circ}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}} \\
& +\left.b_{6} \ell_{2 h, \theta_{1}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}+\left.b_{7} \ell_{2 h, \theta_{2}}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}, \tag{2.3}
\end{align*}
$$

in which $b_{j}(j=1,2 \ldots, 7)$ are parameters satisfying $\sum_{j=1}^{7} b_{j}=1$. These yield the extended 25-point difference approximation for the Helmholtz-PML equation (1.2) as

$$
\begin{equation*}
\left.\mathscr{L}_{h} u\right|_{x=x_{m}, y=y_{n}}+\left.\ell_{h}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}=f_{m, n} \tag{2.4}
\end{equation*}
$$

In [22], a group of optimal parameters were given for the Helmholtz equation, that is,

$$
\begin{aligned}
& a_{1}=0.0949098, \quad a_{2}=0.280677, \quad a_{3}=0.247253, \\
& a_{4}=0.0297441, \quad a_{5}=0.173708, \quad a_{6}=0.173708, \\
& b_{1}=0.363276, \quad b_{2}=0.434392, \quad b_{3}=0.0165948, \\
& b_{4}=0.1699204, \quad b_{5}=0.000825248, \quad b_{6}=0.0075106, \\
& b_{7}=0.00753368 .
\end{aligned}
$$

To analyze the relationship between the difference approximation (2.4) and the Helmholtz-PML equation (1.2), we recall the concept of consistency (cf. [34]).

Definition 2.1. Suppose that, the partial differential equation under consideration is $\mathcal{L} u=f$ and the corresponding finite difference approximation is $L_{m, n} U_{m, n}=F_{m, n}$, where $F_{m, n}$ denotes whatever approximation which has been made of the source term $f$. Let $\left(x_{m}, y_{n}\right):=\left(x_{0}+(m-1) \Delta x, y_{0}+(n-1) \Delta y\right)$. The finite difference scheme $L_{m, n} U_{m, n}=F_{m, n}$ is pointwise consistent with the partial differential equation $\mathcal{L} u=f$ at $(x, y)$, if for any smooth function $\phi=\phi(x, y)$,

$$
\begin{equation*}
\left.(\mathscr{L} \phi-f)\right|_{x=x_{m}, y=y_{n}}-\left[L_{m, n} \phi\left(x_{m}, y_{n}\right)-F_{m, n}\right] \rightarrow 0 \tag{2.6}
\end{equation*}
$$

as $\Delta x, \Delta y \rightarrow 0$ and $\left(x_{m}, y_{n}\right) \rightarrow(x, y)$.

For the extended 25-point finite difference approximation (2.4), we have the following proposition.
Proposition 2.2. The extended 25-point finite difference approximation (2.4) with optimal parameters (2.5) is not pointwise consistent with the Helmholtz-PML equation (1.2).

Proof. Assume that, $x_{m} \leq x<x_{m+1}$ and $y_{n} \leq y<y_{n+1}$. It follows from the Taylor theorem that

$$
\begin{align*}
&\left.\mathcal{L}_{h, 0^{\circ} u} u\right|_{x=x_{m}, y=y_{n}}= \frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+\mu_{1} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{2.7}\\
&\left.\mathcal{L}_{2 h, 0} 0^{\circ} u\right|_{x=x_{m}, y=y_{n}}= \frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+4 \mu_{1} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{2.8}\\
&\left.\mathcal{L}_{h, 45^{\circ} u}\right|_{x=x_{m}, y=y_{n}}= E+\mu h_{2} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{2.9}\\
& \mathcal{L}_{2 h,\left.45^{\circ} u\right|_{x=x_{m}, y=y_{n}}=} E+4 \mu_{2} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{2.10}\\
&\left.\mathcal{L}_{2 h, \theta_{1}} u\right|_{x=x_{m}, y=y_{n}}= \frac{1}{5}\left\{\frac{\partial}{\partial x}\left((4 A+B) \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left((A+4 B) \frac{\partial u}{\partial y}\right)+2 \frac{\partial}{\partial x}\left((B-A) \frac{\partial u}{\partial y}\right)\right. \\
&\left.+2 \frac{\partial}{\partial y}\left((B-A) \frac{\partial u}{\partial x}\right)\right\}+\mu_{3} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{2.11}\\
&\left.\mathscr{L}_{2 h, \theta_{2}} u\right|_{x=x_{m}, y=y_{n}}= \frac{1}{5}\left\{\frac{\partial}{\partial x}\left((A+4 B) \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left((4 A+B) \frac{\partial u}{\partial y}\right)+2 \frac{\partial}{\partial x}\left((B-A) \frac{\partial u}{\partial y}\right)\right. \\
&\left.+2 \frac{\partial}{\partial y}\left((B-A) \frac{\partial u}{\partial x}\right)\right\}+\mu_{4} h^{2}+\mathcal{O}\left(h^{3}\right), \tag{2.12}
\end{align*}
$$

in which

$$
\begin{aligned}
\mu_{1}:= & \frac{1}{24}\left\{\frac{\partial^{3}}{\partial x^{3}}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial x}\left(A \frac{\partial^{3} u}{\partial x^{3}}\right)+\frac{\partial^{3}}{\partial y^{3}}\left(B \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial^{3} u}{\partial y^{3}}\right)\right\}, \\
E:= & \frac{1}{2}\left\{\frac{\partial}{\partial x}\left((A+B) \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left((A+B) \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial x}\left((B-A) \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial y}\left((B-A) \frac{\partial u}{\partial x}\right)\right\}, \\
\mu_{2}:= & \frac{1}{48}\left\{\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{3}\left(A\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right) u\right)+\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)\left(A\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{3} u\right)\right. \\
& \left.+\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)^{3}\left(B\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right) u\right)+\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)\left(B\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)^{3} u\right)\right\}, \\
\mu_{3}:= & \frac{1}{15}\left\{\left(\frac{\partial}{\partial x}-\frac{1}{2} \frac{\partial}{\partial y}\right)^{3}\left(A\left(2 \frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right) u\right)+\left(2 \frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)\left(A\left(\frac{\partial}{\partial x}-\frac{1}{2} \frac{\partial}{\partial y}\right)^{3} u\right)\right. \\
& \left.+\left(\frac{1}{2} \frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)^{3}\left(B\left(\frac{\partial}{\partial x}+2 \frac{\partial}{\partial y}\right) u\right)+\left(\frac{\partial}{\partial x}+2 \frac{\partial}{\partial y}\right)\left(B\left(\frac{1}{2} \frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)^{3} u\right)\right\}, \\
\mu_{4}:= & \frac{1}{15}\left\{\left(\frac{1}{2} \frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{3}\left(A\left(\frac{\partial}{\partial x}-2 \frac{\partial}{\partial y}\right) u\right)+\left(\frac{\partial}{\partial x}-2 \frac{\partial}{\partial y}\right)\left(A\left(\frac{1}{2} \frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{3} u\right)\right. \\
& \left.+\left(\frac{\partial}{\partial x}+\frac{1}{2} \frac{\partial}{\partial y}\right)^{3}\left(B\left(2 \frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right) u\right)+\left(2 \frac{\partial}{\partial x}+\frac{\partial}{\partial y}\right)\left(B\left(\frac{\partial}{\partial x}+\frac{1}{2} \frac{\partial}{\partial y}\right)^{3} u\right)\right\} .
\end{aligned}
$$

Similarly, we have

$$
\begin{equation*}
\ell_{h}\left(C k^{2} u\right)=C k^{2} u+\mu_{5} h^{2}+\mathcal{O}\left(h^{3}\right) \tag{2.13}
\end{equation*}
$$

in which

$$
\mu_{5}=\left(\frac{b_{2}}{4}+b_{3}+\frac{b_{4}}{2}+2 b_{5}+\frac{5 b_{6}}{4}+\frac{5 b_{7}}{4}\right)\left(\frac{\partial^{2}}{\partial x^{2}}\left(C k^{2} u\right)+\frac{\partial^{2}}{\partial y^{2}}\left(C k^{2} u\right)\right)
$$

It follows from equations (2.7)-(2.13) that the left hand side of the extended 25-point finite difference approximation (2.4) is equivalent to

$$
\begin{aligned}
& \left(a_{1}+a_{2}+\frac{a_{3}+a_{4}}{2}+\frac{4}{5} a_{5}+\frac{1}{5} a_{6}\right)\left\{\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)\right\} \\
& \quad+\left(\frac{a_{3}+a_{4}}{2}+\frac{2}{5} a_{5}+\frac{2}{5} a_{6}\right)\left\{\frac{\partial}{\partial x}\left((B-A) \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial y}\left((B-A) \frac{\partial u}{\partial x}\right)\right\} \\
& \quad+\left(\frac{a_{3}+a_{4}}{2}+\frac{1}{5} a_{5}+\frac{4}{5} a_{6}\right)\left\{\frac{\partial}{\partial y}\left(A \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial x}\left(B \frac{\partial u}{\partial x}\right)\right\}+\zeta_{h^{2}} h^{2}+\mathcal{O}\left(h^{3}\right),
\end{aligned}
$$

in which

$$
\zeta_{h^{2}}=\left(a_{1}+4 a_{2}\right) \mu_{1}+\left(a_{3}+4 a_{4}\right) \mu_{2}+a_{5} \mu_{3}+a_{6} \mu_{4}+\mu_{5}
$$

Since $A \neq B$ almost everywhere in PML, the necessary condition for the consistency is

$$
\left\{\begin{array}{l}
a_{1}+a_{2}+\frac{a_{3}+a_{4}}{2}+\frac{4}{5} a_{5}+\frac{1}{5} a_{6}=1, \\
\frac{a_{3}+a_{4}}{2}+\frac{2}{5} a_{5}+\frac{2}{5} a_{6}=0 \\
\frac{a_{3}+a_{4}}{2}+\frac{1}{5} a_{5}+\frac{4}{5} a_{6}=0
\end{array}\right.
$$

The above condition is not satisfied by the group of optimal parameters (2.5). Therefore, we come to the conclusion of this proposition.

From this proposition we conclude that, the extended 25-point scheme with optimal parameters (2.5) is not a good choice for the Helmholtz-PML equation, thus we need to adapt the difference scheme to our problem.

## 3. An optimal 25-point finite difference scheme for the Helmholtz equation with PML

In this section, we propose a 25 -point finite difference scheme which is pointwise consistent with the Helmholtz-PML equation, and then present a refined optimization rule for choosing the parameters of the finite difference scheme such that the numerical dispersion is minimized well. Finally, we generalize the scheme to a case with non-equidistant grid.

### 3.1. A consistent 25-point difference scheme

First, we propose a consistent 25 -point finite difference scheme for the Helmholtz-PML equation. The approach of constructing this kind of difference schemes was proposed in [9] and further developed in [13].

We denote

$$
\begin{equation*}
\left.\tilde{\mathcal{L}}_{h, x} u\right|_{(m, n+j)}:=\frac{A_{m+\frac{1}{2}, n+j}\left(u_{m+1, n+j}-u_{m, n+j}\right)-A_{m-\frac{1}{2}, n+j}\left(u_{m, n+j}-u_{m-1, n+j}\right)}{h^{2}} \tag{3.1}
\end{equation*}
$$

for $j \in \mathbb{Z}_{2}:=\{-1,0,1\}$,

$$
\begin{equation*}
\left.\tilde{\mathcal{L}}_{2 h, x} u\right|_{(m, n+j)}:=\frac{A_{m+1, n+j}\left(u_{m+2, n+j}-u_{m, n+j}\right)-A_{m-1, n+j}\left(u_{m, n+j}-u_{m-2, n+j}\right)}{(2 h)^{2}}, \tag{3.2}
\end{equation*}
$$

for $j \in \mathbb{Z}_{3}$, and let

$$
\begin{aligned}
\left.\tilde{\mathscr{L}}_{h, x} u\right|_{x=x_{m}, y=y_{n}}:= & \left.\gamma_{1} \tilde{\mathscr{L}}_{h, x} u\right|_{(m, n)}+\frac{\gamma_{2}}{2}\left(\left.\tilde{\mathscr{L}}_{h, x} u\right|_{(m, n-1)}+\left.\tilde{\mathscr{L}}_{h, x} u\right|_{(m, n+1)}\right), \\
\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{x=x_{m}, y=y_{n}}:= & \left.\gamma_{3} \tilde{\mathscr{L}}_{2 h, x} u\right|_{(m, n)}+\frac{\gamma_{4}}{2}\left(\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{(m, n-2)}+\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{(m, n+2)}\right) \\
& +\frac{\gamma_{5}}{2}\left(\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{(m, n-1)}+\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{(m, n+1)}\right),
\end{aligned}
$$

where $\sum_{j=1}^{5} \gamma_{j}=1$. Then we approximate the first term of the left hand side of (1.2) as

$$
\left.\left.\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)\right|_{x=x_{m}, y=y_{n}} \approx \tilde{\mathscr{L}}_{h, x} u\right|_{x=x_{m}, y=y_{n}}+\left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{x=x_{m}, y=y_{n}}
$$

We deal with the approximation of the second term in a similar way, that is,

$$
\left.\left.\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)\right|_{x=x_{m}, y=y_{n}} \approx \tilde{\mathscr{L}}_{h, y} u\right|_{x=x_{m}, y=y_{n}}+\left.\tilde{\mathscr{L}}_{2 h, y} u\right|_{x=x_{m}, y=y_{n}}
$$

Let $\tilde{\mathscr{L}}_{h}:=\tilde{\mathscr{L}}_{h, x}+\tilde{\mathscr{L}}_{h, y}+\tilde{\mathscr{L}}_{2 h, x}+\tilde{\mathscr{L}}_{2 h, y}$. We obtain the following 25 -point finite difference approximation for the HelmholtzPML equation (1.2)

$$
\begin{equation*}
\left.\tilde{\mathcal{L}}_{h} u\right|_{x=x_{m}, y=y_{n}}+\left.\ell_{h}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}=f_{m, n} . \tag{3.3}
\end{equation*}
$$

The above finite difference scheme tells us how to discrete the interior points. Next, we give some remarks on how to deal with boundary points.

Remark 3.1. As the PML has a good property of absorbing outgoing waves, we assume that there are no waves outside the interior domain and PML. Computationally, we deal with the boundary points ( $x_{m}, y_{n}$ ) in the same way as interior points except that, we simply set $u_{m+i, n+j}=0$ if the point ( $x_{m+i}, y_{n+j}$ ) lies outside PML.

The next proposition presents the error analysis for the 25-point difference scheme (3.3).
Proposition 3.2. If $\sum_{j=1}^{5} \gamma_{j}=1$ and $\sum_{j=1}^{7} b_{j}=1$, then 25-point finite difference approximation (3.3) is pointwise consistent with the Helmholtz-PML equation (1.2) and is a second order scheme.

Proof. Assume that $x_{m} \leq x<x_{m+1}$ and $y_{n} \leq y<y_{n+1}$. It follows from the Taylor theorem that

$$
\begin{align*}
& \left.\tilde{\mathcal{L}}_{h, x} u\right|_{x=x_{m}, y=y_{n}}=\left(\gamma_{1}+\gamma_{2}\right) \frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+v_{1} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{3.4}\\
& \left.\tilde{\mathscr{L}}_{h, y} u\right|_{x=x_{m}, y=y_{n}}=\left(\gamma_{1}+\gamma_{2}\right) \frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+v_{2} h^{2}+\mathcal{O}\left(h^{3}\right), \tag{3.5}
\end{align*}
$$

in which

$$
\begin{aligned}
& \nu_{1}:=\frac{1}{24}\left(\gamma_{1}+\gamma_{2}\right)\left\{\frac{\partial^{3}}{\partial x^{3}}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial x}\left(A \frac{\partial^{3} u}{\partial x^{3}}\right)\right\}+\frac{\gamma_{2}}{2} \frac{\partial^{3}}{\partial y^{2} \partial x}\left(A \frac{\partial u}{\partial x}\right), \\
& \nu_{2}:=\frac{1}{24}\left(\gamma_{1}+\gamma_{2}\right)\left\{\frac{\partial^{3}}{\partial y^{3}}\left(B \frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial^{3} u}{\partial y^{3}}\right)\right\}+\frac{\gamma_{2}}{2} \frac{\partial^{3}}{\partial x^{2} \partial y}\left(B \frac{\partial u}{\partial y}\right) .
\end{aligned}
$$

Similarly, we have

$$
\begin{align*}
& \left.\tilde{\mathscr{L}}_{2 h, x} u\right|_{x=x_{m}, y=y_{n}}=\left(\gamma_{3}+\gamma_{4}+\gamma_{5}\right) \frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+v_{3} h^{2}+\mathcal{O}\left(h^{3}\right),  \tag{3.6}\\
& \left.\tilde{\mathscr{L}}_{2 h, y} u\right|_{x=x_{m}, y=y_{n}}=\left(\gamma_{3}+\gamma_{4}+\gamma_{5}\right) \frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+v_{4} h^{2}+\mathcal{O}\left(h^{3}\right), \tag{3.7}
\end{align*}
$$

where

$$
\begin{aligned}
\nu_{3}:= & \gamma_{3}\left\{\frac{1}{12} \frac{\partial^{3}}{\partial x^{3}}\left(A \frac{\partial u}{\partial x}\right)+\frac{1}{3} \frac{\partial}{\partial x}\left(A \frac{\partial^{3} u}{\partial x^{3}}\right)\right\}+\frac{\gamma_{4}}{2}\left\{4 \frac{\partial^{3}}{\partial y^{2} \partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{1}{6} \frac{\partial^{3}}{\partial x^{3}}\left(A \frac{\partial u}{\partial x}\right)+\frac{2}{3} \frac{\partial}{\partial x}\left(A \frac{\partial^{3} u}{\partial x^{3}}\right)\right\} \\
& +\frac{\gamma_{5}}{2}\left\{\frac{\partial^{3}}{\partial y^{2} \partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{1}{6} \frac{\partial^{3}}{\partial x^{3}}\left(A \frac{\partial u}{\partial x}\right)+\frac{2}{3} \frac{\partial}{\partial x}\left(A \frac{\partial^{3} u}{\partial x^{3}}\right)\right\}, \\
v_{4}:= & \gamma_{3}\left\{\frac{1}{12} \frac{\partial^{3}}{\partial y^{3}}\left(B \frac{\partial u}{\partial y}\right)+\frac{1}{3} \frac{\partial}{\partial y}\left(B \frac{\partial^{3} u}{\partial y^{3}}\right)\right\}+\frac{\gamma_{4}}{2}\left\{4 \frac{\partial^{3}}{\partial x^{2} \partial y}\left(B \frac{\partial u}{\partial y}\right)+\frac{1}{6} \frac{\partial^{3}}{\partial y^{3}}\left(B \frac{\partial u}{\partial y}\right)+\frac{2}{3} \frac{\partial}{\partial y}\left(B \frac{\partial^{3} u}{\partial y^{3}}\right)\right\} \\
& +\frac{\gamma_{5}}{2}\left\{\frac{\partial^{3}}{\partial x^{2} \partial y}\left(B \frac{\partial u}{\partial y}\right)+\frac{1}{6} \frac{\partial^{3}}{\partial y^{3}}\left(B \frac{\partial u}{\partial y}\right)+\frac{2}{3} \frac{\partial}{\partial y}\left(B \frac{\partial^{3} u}{\partial y^{3}}\right)\right\} .
\end{aligned}
$$

It follows from (3.4)-(3.7) and (2.13) that the left hand side of the 25-point finite difference approximation (3.3) is equivalent to

$$
\begin{equation*}
\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)+C k^{2} u+\theta_{h^{2}} h^{2}+\mathcal{O}\left(h^{3}\right) \tag{3.8}
\end{equation*}
$$

where $\theta_{h^{2}}=\sum_{j=1}^{4} v_{j}+\mu_{5}$. From (1.2) and (3.8) we conclude the results of this proposition.
From the proposition above, we see that the 25 -point finite difference scheme (3.3) is a second order scheme for arbitrary constants $\gamma_{j}\left(j \in \mathbb{N}_{5}:=\{1,2, \ldots, 5\}\right)$ and $b_{j}\left(j \in \mathbb{N}_{7}:=\{1,2, \ldots, 7\}\right)$ provided $\sum_{j=1}^{5} \gamma_{j}=1$ and $\sum_{j=1}^{7} b_{j}=1$. A further observation yields the following proposition.

Proposition 3.3. The 25 -point difference schemes (2.4) and (3.3) are equivalent in the interior area if

$$
\begin{align*}
& a_{5}=a_{6}, \quad \gamma_{5}=\frac{8}{5} a_{5}, \quad \gamma_{4}=\frac{a_{4}}{2}, \\
& \gamma_{3}=a_{2}+\frac{a_{4}}{2}, \quad \gamma_{2}=\frac{a_{3}}{2}, \quad \gamma_{1}=a_{1}+\frac{1}{2} a_{3}+\frac{2}{5} a_{5} . \tag{3.9}
\end{align*}
$$

Proof. For brevity, we only give the proof under the condition that $k$ is a positive constant. When $k$ is a variable, the same conclusion can be obtained similarly.

In the interior area, $A=B=C=1$, thus replacing $u_{m+i, n+j}$ with $U_{m+i, n+j}\left(i, j \in \mathbb{Z}_{3}\right)$ in the formula (3.3) gives

$$
\begin{align*}
& T_{1} U_{m-2, n-2}+T_{2} U_{m-1, n-2}+T_{4} U_{m, n-2}+T_{3} U_{m+1, n-2}+T_{1} U_{m+2, n-2} \\
& \quad+T_{3} U_{m-2, n-1}+T_{5} U_{m-1, n-1}+T_{6} U_{m, n-1}+T_{5} U_{m+1, n-2}+T_{2} U_{m+2, n-1} \\
& \quad+T_{4} U_{m-2, n}+T_{6} U_{m-1, n}+T_{0} U_{m, n}+T_{6} U_{m+1, n}+T_{4} U_{m+2, n} \\
& \quad+T_{2} U_{m-2, n+1}+T_{5} U_{m-1, n+1}+T_{6} U_{m, n+1}+T_{5} U_{m+1, n+1}+T_{3} U_{m+2, n+1} \\
& \quad+T_{1} U_{m-2, n+2}+T_{3} U_{m-1, n+2}+T_{4} U_{m, n+2}+T_{2} U_{m+1, n+2}+T_{1} U_{m+2, n+2} \\
& =  \tag{3.10}\\
& g_{m, n},
\end{align*}
$$

in which

$$
\begin{aligned}
& T_{0}:=-\frac{1}{h^{2}}\left(4 \gamma_{1}+\gamma_{3}\right)+b_{1} k^{2}, \quad T_{1}:=\frac{\gamma_{4}}{4 h^{2}}+\frac{b_{5}}{4} k^{2}, \quad T_{2}:=\frac{\gamma_{5}}{8 h^{2}}+\frac{b_{6}}{4} k^{2}, \\
& T_{3}:=\frac{\gamma_{5}}{8 h^{2}}+\frac{b_{7}}{4} k^{2}, \quad T_{4}:=\frac{1}{4 h^{2}}\left(\gamma_{3}-\gamma_{4}\right)+\frac{b_{3}}{4} k^{2}, \quad T_{5}:=\frac{\gamma_{2}}{h^{2}}+\frac{b_{4}}{4} k^{2}, \\
& T_{6}:=\frac{1}{h^{2}}\left(-\gamma_{2}+\gamma_{1}-\frac{\gamma_{5}}{4}\right)+\frac{b_{2}}{4} k^{2} .
\end{aligned}
$$

Then replacing $u_{m, n}$ with its finite difference approximation $U_{m, n}$ in the extended 25-point finite difference approximation, (2.4) yields

$$
\begin{align*}
& \hat{T}_{1} U_{m-2, n-2}+\hat{T}_{2} U_{m-1, n-2}+\hat{T}_{4} U_{m, n-2}+\hat{T}_{3} U_{m+1, n-2}+\hat{T}_{1} U_{m+2, n-2} \\
& \quad+\hat{T}_{3} U_{m-2, n-1}+\hat{T}_{5} U_{m-1, n-1}+\hat{T}_{6} U_{m, n-1}+\hat{T}_{5} U_{m+1, n-2}+\hat{T}_{2} U_{m+2, n-1} \\
& \quad+\hat{T}_{4} U_{m-2, n}+\hat{T}_{6} U_{m-1, n}+\hat{T}_{0} U_{m, n}+\hat{T}_{6} U_{m+1, n}+\hat{T}_{4} U_{m+2, n} \\
& \quad+\hat{T}_{2} U_{m-2, n+1}+\hat{T}_{5} U_{m-1, n+1}+\hat{T}_{6} U_{m, n+1}+\hat{T}_{5} U_{m+1, n+1}+\hat{T}_{3} U_{m+2, n+1} \\
& \quad+\hat{T}_{1} U_{m-2, n+2}+\hat{T}_{3} U_{m-1, n+2}+\hat{T}_{4} U_{m, n+2}+\hat{T}_{2} U_{m+1, n+2}+\hat{T}_{1} U_{m+2, n+2} \\
& =  \tag{3.11}\\
& g_{m, n},
\end{align*}
$$

where

$$
\begin{aligned}
& \hat{T}_{0}:=\frac{1}{h^{2}}\left(-4 a_{1}-a_{2}-2 a_{3}-\frac{a_{4}}{2}-\frac{4}{5} a_{5}-\frac{4}{5} a_{6}\right)+b_{1} k^{2}, \\
& \hat{T}_{1}:=\frac{a_{4}}{8 h^{2}}+\frac{b_{5}}{4} k^{2}, \quad \hat{T}_{2}:=\frac{a_{5}}{5 h^{2}}+\frac{b_{6}}{4} k^{2}, \quad \hat{T}_{3}:=\frac{a_{6}}{5 h^{2}}+\frac{b_{7}}{4} k^{2}, \\
& \hat{T}_{4}:=\frac{a_{2}}{4 h^{2}}+\frac{b_{3}}{4} k^{2}, \quad \hat{T}_{5}:=\frac{a_{3}}{2 h^{2}}+\frac{b_{4}}{4} k^{2}, \quad \hat{T}_{6}:=\frac{a_{1}}{h^{2}}+\frac{b_{2}}{4} k^{2} .
\end{aligned}
$$

Comparing the parameters of (3.10) and (3.11) leads to the result of this proposition.
From Proposition 3.3, in the interior area, we have the extended 25 -point finite difference scheme (2.4) with optimal parameters (2.5) equivalent to the 25 -point finite difference scheme (3.3) with the parameters below

$$
\begin{array}{llr}
\gamma_{1}=0.2880195, & \gamma_{2}=0.12362650, & \gamma_{3}=0.29554905, \\
\gamma_{4}=0.014872050, & \gamma_{5}=0.27793280, & b_{1}=0.363276, \\
b_{2}=0.434392, & b_{3}=0.0165948, & b_{4}=0.1699204,  \tag{3.12}\\
b_{5}=0.000825248, & b_{6}=0.0075106, & b_{7}=0.00753368 .
\end{array}
$$

In order to distinguish with the extended 25 -point scheme (the extended 25 p), we call the difference scheme (3.3) with parameters (3.12) as the global optimal 25 -point scheme for the Helmholtz-PML equation (or simply the global 25p).

### 3.2. Choice strategies for optimal parameters of the finite difference scheme

We now go further into the problem of the choice strategies for optimal parameters. Since the solution of the Helmholtz equation is oscillating seriously for large wavenumbers, for a finite difference scheme, only the convergence order is not
enough. In fact, the accuracy of the numerical solution deteriorates with increasing wavenumber $k$. The phenomenon is the so-called 'pollution effect'. As the result of the 'pollution', the wavenumber of the numerical solution is different from the wavenumber of the exact solution, and this is the so called 'numerical dispersion' (see, [29,32]). Therefore, in order to reduce the 'numerical dispersion', we need to minimize the error between the numerical wavenumber and the exact wavenumber. If the difference scheme has optimal convergence order, and the parameters are chosen such that the scheme has minimal numerical dispersion in the interior area, then we regard it as an optimal scheme for the Helmholtz-PML equation (see, [13,21]).

To optimize the 25-point scheme (3.3), we first assume a plane-wave solution of the form $U(x, y)=\mathrm{e}^{-\mathrm{i} k(x \cos \theta+y \sin \theta)}$, where $\theta$ is the propagation angle from the $y$-axis. Moreover, the classical dispersion analysis is generally done in the infinite domain with the source $g=0$ and the wavenumber $k$ being a positive constant (see, [20,22]). For the convenience of analysis, let $v$ be the velocity of propagation, $\lambda$ be the wavelength, and $G$ be the number of gridpoints per wavelength, that is, $G=\frac{\lambda}{h}$. Since $\lambda=\frac{2 \pi v}{\omega}$ and $k=\frac{\omega}{v}$, we have $k h=\frac{2 \pi}{G}$. Also, denote

$$
\begin{aligned}
& P_{1}:=\cos (k h \sin \theta)=\cos \left(\frac{2 \pi}{G} \sin \theta\right), \quad Q_{1}:=\cos (k h \cos \theta)=\cos \left(\frac{2 \pi}{G} \cos \theta\right), \\
& P_{2}:=\cos (2 k h \sin \theta)=\cos \left(\frac{4 \pi}{G} \sin \theta\right), \quad Q_{2}:=\cos (2 k h \cos \theta)=\cos \left(\frac{4 \pi}{G} \cos \theta\right), \\
& R_{1}:=\cos (k h(2 \sin \theta-\cos \theta))=\cos \left(\frac{2 \pi}{G}(2 \sin \theta-\cos \theta)\right), \\
& R_{2}:=\cos (k h(\sin \theta+2 \cos \theta))=\cos \left(\frac{2 \pi}{G}(\sin \theta+2 \cos \theta)\right), \\
& R_{3}:=\cos (k h(\sin \theta-2 \cos \theta))=\cos \left(\frac{2 \pi}{G}(\sin \theta-2 \cos \theta)\right), \\
& R_{4}:=\cos (k h(2 \sin \theta+\cos \theta))=\cos \left(\frac{2 \pi}{G}(2 \sin \theta+\cos \theta)\right) .
\end{aligned}
$$

By substituting $U_{m+j, n+l}:=\mathrm{e}^{-\mathrm{i} k\left(x_{m+j} \cos \theta+y_{n+l} \sin \theta\right)} \quad\left(j, l \in \mathbb{Z}_{3}\right)$ into Eq. (3.10), dividing both sides by the factor $\mathrm{e}^{-\mathrm{ik}\left(x_{m} \cos \theta+y_{n} \sin \theta\right)}$, and finally applying the Euler formula $\mathrm{e}^{\mathrm{i} x}=\cos x+\mathrm{i} \sin x$ lead to the dispersion equation

$$
\begin{equation*}
k^{2} h^{2} L=R, \tag{3.13}
\end{equation*}
$$

where

$$
\begin{aligned}
L:= & b_{1}+\frac{b_{2}}{2}\left(P_{1}+Q_{1}\right)+\frac{b_{3}}{2}\left(P_{2}+Q_{2}\right)+b_{4} P_{1} Q_{1}+b_{5} P_{2} Q_{2}+\frac{b_{6}}{2}\left(R_{1}+R_{2}\right)+\frac{b_{7}}{2}\left(R_{3}+R_{4}\right), \\
R:= & 2 \gamma_{1}\left(2-P_{1}-Q_{1}\right)+2 \gamma_{2}\left(P_{1}+Q_{1}-2 P_{1} Q_{1}\right)+\frac{\gamma_{3}}{2}\left(2-P_{2}-Q_{2}\right) \\
& +\frac{\gamma_{4}}{2}\left(P_{2}+Q_{2}-2 P_{2} Q_{2}\right)+\frac{\gamma_{5}}{2}\left(Q_{1}-P_{2} Q_{1}+P_{1}-P_{1} Q_{2}\right) .
\end{aligned}
$$

Then replacing $k$ on the left side of the Eq. (3.13) with the numerical wavenumber $k^{N}$ yields

$$
\begin{equation*}
k^{N}=\frac{1}{h} \sqrt{\frac{R}{L}} \tag{3.14}
\end{equation*}
$$

With the Taylor expansion, we have

$$
\begin{align*}
\left(k^{N}\right)^{2}= & k^{2}+\left\{-\frac{1}{12}\left[\gamma_{1}+\gamma_{2}+4\left(\gamma_{3}+\gamma_{4}+\gamma_{5}\right)\right]+\left[\frac{b_{2}}{4}+b_{3}+\frac{b_{4}}{2}+2 b_{5}+\frac{5}{4}\left(b_{6}+b_{7}\right)\right]\right. \\
& \left.+\frac{1}{24}\left(\gamma_{1}-5 \gamma_{2}+4 \gamma_{3}-20 \gamma_{4}-2 \gamma_{5}\right) \sin ^{2}(2 \theta)\right\} k^{4} h^{2}+\mathcal{O}\left(k^{5} h^{3}\right), \quad k h \rightarrow 0 \tag{3.15}
\end{align*}
$$

The above equation indicates that $\left(k^{N}\right)^{2}$ approximates $k^{2}$ in a second order. Moreover, the term associated with $k^{4} h^{2}$ presents the pollution effect, which depends on the wavenumber $k$, the parameters of the finite difference formula (3.3) and the wave's propagation angle $\theta$ from the $y$-axis. For the optimal 9-point finite difference scheme proposed in [13], a similar estimate for the relation $\left(k^{N}\right)^{2}$ and $k^{2}$ is obtained; see Remark 3.4. It is easy to see that, for both the 25 -point scheme (3.3) and the 9 -point scheme proposed in [13], the numerical wavenumber $k^{N}$ approximates the exact wavenumber $k$ in the same order. However, with more parameters in the difference formula (3.3), we can better suppress the pollution effect.

Remark 3.4. For the optimal 9-point finite difference scheme proposed in [13], we have

$$
\begin{equation*}
\left(k^{N}\right)^{2}=k^{2}+\left[\frac{d}{4}+\frac{e}{2}-\frac{1}{12}+\left(\frac{b}{4}-\frac{5}{24}\right) \sin ^{2}(2 \theta)\right] k^{4} h^{2}+\mathcal{O}\left(k^{5} h^{3}\right), \quad k h \rightarrow 0 \tag{3.16}
\end{equation*}
$$

where $b, d, e$ are parameters of the optimal 9-point formula.
Next, we present the relation of the numerical wavenumber $k^{N}$ and the exact wavenumber $k$. Since $h=\frac{2 \pi}{G k}$, we conclude that

$$
\begin{equation*}
\frac{k^{N}}{k}=\frac{G}{2 \pi} \sqrt{\frac{R}{L}} \tag{3.17}
\end{equation*}
$$

Moreover, the normalized numerical phase velocity (cf. [20,22,35]) is

$$
\begin{equation*}
\frac{V_{p h}^{N}}{v}=\frac{G}{2 \pi} \sqrt{\frac{R}{L}}, \tag{3.18}
\end{equation*}
$$

and the normalized numerical group velocity is

$$
\begin{equation*}
\frac{V_{g r}^{N}}{v}=\frac{G}{4 \pi} \frac{v}{V_{p h}^{N}}\left\{\frac{\left(\frac{1}{h} \frac{\partial R}{\partial k}\right) L-R\left(\frac{1}{h} \frac{\partial L}{\partial k}\right)}{L^{2}}\right\} . \tag{3.19}
\end{equation*}
$$

We choose optimal parameters $\gamma_{i}\left(i \in \mathbb{N}_{5}\right)$ and $b_{j}\left(j \in \mathbb{N}_{7}\right)$ by minimizing the numerical dispersion. To do this, we set

$$
\begin{equation*}
J\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; G, \theta\right):=\frac{G}{2 \pi} \sqrt{\frac{R}{L}}-1 \tag{3.20}
\end{equation*}
$$

for $\sum_{j=1}^{5} \gamma_{j}=1, \sum_{j=1}^{7} b_{j}=1$ and $(G, \theta) \in I_{G} \times I_{\theta}$, where $I_{G}$ and $I_{\theta}$ are two intervals. In general, one can choose $I_{\theta}:=\left[0, \frac{\pi}{2}\right]$ and $I_{G}:=\left[G_{\min }, G_{\max }\right]=[4,400]$. We remark that the interval $\left[0, \frac{\pi}{2}\right]$ can be replaced by $\left[0, \frac{\pi}{4}\right]$ because of the symmetry, and $G_{\min } \geq 2$ based on the Nyquist sampling limit (cf. [22]).

It follows from (3.17) that minimizing the error between the numerical wavenumber $k^{N}$ and the exact wavenumber $k$ is equivalent to minimizing the norm $\left\|J\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G} \times I_{\theta}}$. To do this, we first set $J\left(\gamma_{1}, \ldots\right.$, $\left.\gamma_{5}, b_{1}, \ldots, b_{7} ; G, \theta\right)=0$, which yields the equation

$$
\frac{G^{2}}{4 \pi^{2}} \frac{R}{L}=1
$$

Thus, we have that

$$
\begin{align*}
& G^{2}\left\{4\left(P_{1} Q_{1}-Q_{1}-P_{1}+1\right) \gamma_{2}+\left[3-2\left(P_{1}+Q_{1}\right)+\frac{1}{2}\left(P_{2}+Q_{2}\right)\right] \gamma_{3}\right. \\
& \left.\quad+\frac{1}{2}\left[2 P_{2} Q_{2}-4\left(P_{1}+Q_{1}\right)-P_{2}-Q_{2}+8\right] \gamma_{4}+\frac{1}{2}\left[P_{1} Q_{2}+P_{2} Q_{1}-5\left(P_{1}+Q_{1}\right)+8\right] \gamma_{5}\right\} \\
& \quad+4 \pi^{2}\left\{\frac{1}{2}\left(P_{1}+Q_{1}-2\right) b_{2}+\frac{1}{2}\left(P_{2}+Q_{2}-2\right) b_{3}+\left(P_{1} Q_{1}-1\right) b_{4}+\left(P_{2} Q_{2}-1\right) b_{5}\right. \\
& \left.\quad+\frac{1}{2}\left(R_{1}+R_{2}-2\right) b_{6}+\frac{1}{2}\left(R_{3}+R_{4}-2\right) b_{7}\right\}=-4 \pi^{2}+2 G^{2}\left(2-P_{1}-Q_{1}\right) \tag{3.21}
\end{align*}
$$

Note that $P_{1}, P_{2}, Q_{1}, Q_{2}, R_{1}, R_{2}, R_{3}$ and $R_{4}$ are functions of $G$ and $\theta$. We choose $\theta=\theta_{m}:=\frac{(m-1) \pi}{4(l-1)} \in I_{\theta}, m=1,2, \ldots, l$, and $\frac{1}{G}=\frac{1}{G_{n}}:=\frac{1}{G_{\text {max }}}+(n-1) \frac{\frac{1}{G_{\text {min }}}-\frac{1}{G_{\max }}}{r-1} \in\left[\frac{1}{G_{\text {max }}}, \frac{1}{G_{\text {min }}}\right], n=1,2, \ldots, r$. Then, Eq. (3.21) leads to the linear system

$$
\left[\begin{array}{cccccccccc}
S_{1,1}^{1} & S_{1,1}^{2} & S_{1,1}^{3} & S_{1,1}^{4} & S_{1,1}^{5} & S_{1,1}^{6} & S_{1,1}^{7} & S_{1,1}^{8} & S_{1,1}^{9} & S_{1,1}^{10}  \tag{3.22}\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
S_{1, r}^{1} & S_{1, r}^{2} & S_{1, r}^{3} & S_{1, r}^{4} & S_{1, r}^{5} & S_{1, r}^{6} & S_{1, r}^{7} & S_{1, r}^{8} & S_{1, r}^{9} & S_{1, r}^{10} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
S_{m, n}^{1} & S_{m, n}^{2} & S_{m, n}^{3} & S_{m, n}^{4} & S_{m, n}^{5} & S_{m, n}^{6} & S_{m, n}^{7} & S_{m, n}^{8} & S_{m, n}^{9} & S_{m, n}^{10} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
S_{l, r}^{1} & S_{l, r}^{2} & S_{l, r}^{3} & S_{l, r}^{4} & S_{l, r}^{5} & S_{l, r}^{6} & S_{l, r}^{7} & S_{l, r}^{8} & S_{l, r}^{9} & S_{l, r}^{10}
\end{array}\right]\left[\begin{array}{c}
\gamma_{2} \\
\gamma_{3} \\
\gamma_{4} \\
\gamma_{5} \\
b_{2} \\
b_{3} \\
b_{4} \\
b_{5} \\
b_{6} \\
b_{7}
\end{array}\right]=\left[\begin{array}{c}
S_{1,1}^{11} \\
\vdots \\
S_{1, r}^{11} \\
\vdots \\
S_{m, n}^{11} \\
\vdots \\
S_{l, r}^{11}
\end{array}\right],
$$

where

$$
\begin{aligned}
& S_{m, n}^{1}:= 4 G_{n}^{2}\left[1-\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)-\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)+\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right], \\
& S_{m, n}^{2}:= G_{n}^{2}\left\{3-2\left[\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right]+\frac{1}{2}\left[\cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)\right]\right\}, \\
& S_{m, n}^{3}:= \frac{1}{2} G_{n}^{2}\left\{8+2 \cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)-\cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right)-\cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)\right. \\
&\left.-4\left[\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right]\right\}, \\
& S_{m, n}^{4}:= \frac{1}{2} G_{n}^{2}\left\{8+\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)+\cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right. \\
&\left.-5\left[\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right]\right\}, \\
& S_{m, n}^{5}:= 2 \pi^{2}\left[\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)-2\right], \\
& S_{m, n}^{6}:= 2 \pi^{2}\left[\cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right)+\cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)-2\right], \\
& S_{m, n}^{7}:= 4 \pi^{2}\left[\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)-1\right], \\
& S_{m, n}^{8}:= 4 \pi^{2}\left[\cos \left(\frac{4 \pi}{G_{n}} \sin \theta_{m}\right) \cos \left(\frac{4 \pi}{G_{n}} \cos \theta_{m}\right)-1\right], \\
& S_{m, n}^{9}:= 2 \pi^{2}\left[\cos \left(\frac{2 \pi}{G_{n}}\left(2 \sin \theta_{m}-\cos \theta_{m}\right)\right)+\cos \left(\frac{2 \pi}{G_{n}}\left(\sin \theta_{m}+2 \cos \theta_{m}\right)\right)-2\right], \\
& S_{m, n}^{10}:= 2 \pi^{2}\left[\cos \left(\frac{2 \pi}{G_{n}}\left(\sin \theta_{m}-2 \cos \theta_{m}\right)\right)+\cos \left(\frac{2 \pi}{G_{n}}\left(2 \sin \theta_{m}+\cos \theta_{m}\right)\right)-2\right], \\
& S_{m, n}^{11}:=-4 \pi^{2}+2 G_{n}^{2}\left[2-\cos \left(\frac{2 \pi}{G_{n}} \sin \theta_{m}\right)-\cos \left(\frac{2 \pi}{G_{n}} \cos \theta_{m}\right)\right] .
\end{aligned}
$$

The coefficient matrix has $l \times r$ rows and 10 columns, thus (3.22) is an overdetermined system, which can be solved by least-squares method. Moreover, we observe that the optimal parameters given in [22] are roughly chosen, as only one group of parameters were obtained and used to the computation for different frequencies, velocities and step sizes. This may yield much numerical dispersion for large wavenumbers and variable $k(x, y)$ (see examples in Section 4). To reduce the numerical dispersion and improve the accuracy of the difference scheme, we propose the following rule.

Rule 3.5 (Refined Choice Strategy).
Step 1. Estimate the interval $I_{G}:=\left[G_{\min }, G_{\max }\right]$.
Step 2. Choose $\gamma_{i}\left(i \in \mathbb{N}_{5}\right)$ and $b_{j}\left(j \in \mathbb{N}_{7}\right)$ such that

$$
\begin{align*}
& \left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7}\right) \\
& \quad=\arg \min \left\{\left\|J\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G} \times I_{\theta}}: \sum_{j=1}^{5} \gamma_{j}=1, \sum_{j=1}^{7} b_{j}=1\right\} . \tag{3.23}
\end{align*}
$$

In general, we can estimate $I_{G}$ by using a priori information before choosing parameters. For example, if the frequency $f \in\left[f_{\min }, f_{\max }\right]$ and the velocity $v \in\left[v_{\min }, v_{\max }\right]$ then for a given step size $h$ we have $G_{\min }:=\frac{v_{\min }}{h f_{\max }}$ and $G_{\max }:=\frac{v_{\max }}{h f_{\min }}$. In Tables 1 and 2, we present some groups of refined optimal parameters.

Fig. 2 shows the normalized phase and group velocity curves for the rotated 9-point difference scheme (the rotated 9 p), the 25 -point difference scheme (3.10) with parameters (3.12) (the global 25 p) and the 25 -point difference scheme (3.10) with refined optimal parameters in Tables 1 and 2 (the refined 25 p), respectively. It is easy to find that both the global 25 p and the refined 25 p have much improvement over the rotated 9 p. Additionally, the refined 25 p has much less

Table 1
Refined optimal parameters.

| $I_{G}$ | $[2,2.5]$ | $[2.5,3]$ | $[3,4]$ | $[4,5]$ |
| :--- | ---: | :--- | ---: | ---: |
| $\gamma_{1}$ | 0.047999963330863 | 0.147293330179725 | 0.183180998407207 | 0.242239308507107 |
| $\gamma_{2}$ | -0.005925928525878 | 0.055379772312106 | 0.137353578227016 | 0.160596541280590 |
| $\gamma_{3}$ | 0.413091635341205 | 0.373678865083601 | 0.3601198863699911 | 0.327023199880231 |
| $\gamma_{4}$ | 0.060680766447008 | 0.033859215177640 | 0.018241197835580 | 0.011791633533360 |
| $\gamma_{5}$ | 0.484153563406802 | 0.389788817246928 | 0.301104339160286 | 0.258349316798712 |
| $b_{1}$ | 0.220260676569402 | 0.282263140398365 | 0.309536538872974 | 0.341944671328177 |
| $b_{2}$ | 0.432457082691776 | 0.441814591036386 | 0.472535719623776 | 0.469476235857888 |
| $b_{3}$ | 0.042688088077091 | 0.026873864763897 | 0.022287994431260 | 0.017876897372456 |
| $b_{4}$ | 0.249255472098946 | 0.216439606315222 | 0.174143429821568 | 0.154237668357416 |
| $b_{5}$ | 0.003945393848657 | 0.001727236334600 | $-2.386237853810076 e-4$ | $-1.979300495582987 e-4$ |
| $b_{6}$ | 0.025756984442826 | 0.015441838603192 | 0.010867906476688 | 0.008331249852036 |
| $b_{7}$ | 0.025636302271301 | 0.015439722548337 | 0.010867034559120 | 0.008331207281584 |

Table 2
Refined optimal parameters (continue).

| $I_{G}$ | $[5,6]$ | $[6,8]$ | $[8,10]$ | $[10,400]$ |
| :--- | :--- | :--- | :---: | :---: |
| $\gamma_{1}$ | 0.271782609062930 | 0.284158049895963 | 0.299001074252186 | 0.297046004487648 |
| $\gamma_{2}$ | 0.168528263975194 | 0.180982896912852 | 0.184118800813270 | 0.199464088268622 |
| $\gamma_{3}$ | 0.310427677250485 | 0.304028496720736 | 0.295761877237356 | 0.297395880484200 |
| $\gamma_{4}$ | 0.009649524814674 | 0.007447303978096 | 0.006627125174128 | 0.004284766350832 |
| $\gamma_{5}$ | 0.239611924896718 | 0.223383252492354 | 0.214491122523060 | 0.201809260408696 |
| $b_{1}$ | 0.357993213516404 | 0.365234692044752 | 0.373254845373659 | 0.374319397679971 |
| $b_{2}$ | 0.465956594566756 | 0.470297541934252 | 0.468262706183388 | 0.474948027209072 |
| $b_{3}$ | 0.016031996569628 | 0.015198470230312 | 0.014388012687780 | 0.015492621083616 |
| $b_{4}$ | 0.145493965355276 | 0.136125397562404 | 0.131767373961080 | 0.125185968578920 |
| $b_{5}$ | $-1.621668629146452 \mathrm{e}-4$ | $-2.746678031531637 \mathrm{e}-4$ | $-2.541135299981671 \mathrm{e}-4$ | $-2.455072713816700 \mathrm{e}-4$ |
| $b_{6}$ | 0.007343200878844 | 0.006709277150948 | 0.006290587218416 | 0.005149658844840 |
| $b_{7}$ | 0.007343195976008 | 0.006709288880488 | 0.006290588105672 | 0.005149833874960 |

numerical dispersion than the global 25 p. Therefore, we expect that the refined 25 p will be the best choice to control the numerical dispersion and to suppress non-physical oscillations. This will be illustrated by numerical experiments in the next section.

### 3.3. A generalization

In practice, we usually compute on the nonuniform grids. In this subsection, we generalize the consistent 25 -point scheme to a nonuniform case, and show how to optimize the corresponding parameters in the interior domain.

To construct the finite difference scheme, we consider the network of grid points ( $x_{m}, y_{n}$ ), where $x_{m}:=x_{0}+(m-1) \Delta x$ and $y_{n}:=y_{0}+(n-1) \Delta y$, with $\Delta x, \Delta y$ being the step size of the variable $x, y$ respectively. We denote

$$
\begin{equation*}
\left.\tilde{\mathcal{L}}_{\Delta x, x} u\right|_{(m, n+j)}:=\frac{A_{m+\frac{1}{2}, n+j}\left(u_{m+1, n+j}-u_{m, n+j}\right)-A_{m-\frac{1}{2}, n+j}\left(u_{m, n+j}-u_{m-1, n+j}\right)}{(\Delta x)^{2}} \tag{3.24}
\end{equation*}
$$

for $j \in \mathbb{Z}_{2}:=\{-1,0,1\}$. It is easy to find that simply replacing the step size $h$ with $\Delta x$ in $\tilde{\sim}_{\sim}$ the left hand side of the Eq. (3.1) yields the left hand side of the above equation. Similarly, we introduce the notions $\left.\tilde{\mathscr{L}}_{2 \Delta x, x} u\right|_{(m, n+j)}$ for $j \in \mathbb{Z}_{3}$. Then we approximate the first term of the left hand side of (1.2) as

$$
\left.\left.\frac{\partial}{\partial x}\left(A \frac{\partial u}{\partial x}\right)\right|_{x=x_{m}, y=y_{n}} \approx \tilde{\mathscr{L}}_{\Delta x, x} u\right|_{x=x_{m}, y=y_{n}}+\left.\tilde{\mathscr{L}}_{2 \Delta x, x} u\right|_{x=x_{m}, y=y_{n}}
$$

where notions $\left.\tilde{\mathscr{L}}_{\Delta x, x} u\right|_{x=x_{m}, y=y_{n}},\left.\tilde{\mathscr{L}}_{2 \Delta x, x} u\right|_{x=x_{m}, y=y_{n}}$ are introduced following the way of definitions of $\left.\tilde{\mathscr{L}}_{h, x} u\right|_{x=x_{m}, y=y_{n}}$, $\left.\tilde{\mathcal{L}}_{2 h, x} u\right|_{x=x_{m}, y=y_{n}}$ respectively (see, Section 3.1). The approximation of the second term is dealt with similarly, that is,

$$
\left.\left.\frac{\partial}{\partial y}\left(B \frac{\partial u}{\partial y}\right)\right|_{x=x_{m}, y=y_{n}} \approx \tilde{\mathscr{L}}_{\Delta y, y} u\right|_{x=x_{m}, y=y_{n}}+\left.\tilde{\mathscr{L}}_{2 \Delta y, y} u\right|_{x=x_{m}, y=y_{n}}
$$

Let $\tilde{\mathscr{L}}_{\Delta x, \Delta y}:=\tilde{\mathscr{L}}_{\Delta x, x}+\tilde{\mathscr{L}}_{\Delta y, y}+\tilde{\mathscr{L}}_{2 \Delta x, x}+\tilde{\mathscr{L}}_{2 \Delta y, y}$. We obtain the following 25-point finite difference approximation for the Helmholtz-PML equation (1.2)

$$
\begin{equation*}
\left.\tilde{\mathscr{L}}_{\Delta x, \Delta y} u\right|_{x=x_{m}, y=y_{n}}+\left.l_{h}\left(C k^{2} u\right)\right|_{x=x_{m}, y=y_{n}}=f_{m, n} . \tag{3.25}
\end{equation*}
$$



Fig. 2. (a) Normalized phase velocity curve for the optimal 9p, (b) Normalized group velocity curve for the optimal 9p, (c) Normalized phase velocity curve for the global 25 p, (d) Normalized group velocity curve for the global 25 p, (e) Normalized phase velocity curve for the refined 25 p, (f) Normalized group velocity curve for the refined 25 p.

Remark 3.6. If $\sum_{j=1}^{5} \gamma_{j}=1$ and $\sum_{j=1}^{7} b_{j}=1$, then the 25 -point finite difference approximation (3.25) is consistent with the Helmholtz-PML equation (1.2).

When $\Delta x=h, \Delta y=\gamma h$ ( $\gamma$ is a positive constant), performing the classical dispersion analysis to the finite difference method (3.25), yields

$$
\begin{equation*}
k^{N}=\frac{1}{h} \sqrt{\frac{\tilde{R}}{\tilde{L}}}, \tag{3.26}
\end{equation*}
$$

where

$$
\begin{aligned}
\tilde{L}:= & b_{1}+\frac{b_{2}}{2}\left(P_{1}+\tilde{Q}_{1}\right)+\frac{b_{3}}{2}\left(P_{2}+\tilde{Q}_{2}\right)+b_{4} P_{1} \tilde{Q}_{1}+b_{5} P_{2} \tilde{Q}_{2}+\frac{b_{6}}{2}\left(\tilde{R}_{1}+\tilde{R}_{2}\right)+\frac{b_{7}}{2}\left(\tilde{R}_{3}+\tilde{R}_{4}\right), \\
\tilde{R}:= & 2 \gamma_{1}\left[\left(1+\frac{1}{\gamma^{2}}\right)-P_{1}-\frac{1}{\gamma^{2}} \tilde{Q}_{1}\right]+2 \gamma_{2}\left[\frac{1}{\gamma^{2}} P_{1}+\tilde{Q}_{1}-\left(1+\frac{1}{\gamma^{2}}\right) P_{1} \tilde{Q}_{1}\right]+\frac{\gamma_{3}}{2}\left[\left(1+\frac{1}{\gamma^{2}}\right)-P_{2}-\tilde{Q}_{2}\right] \\
& +\frac{\gamma_{4}}{2}\left[\frac{1}{\gamma^{2}} P_{2}+\tilde{Q}_{2}-\left(1+\frac{1}{\gamma^{2}}\right) P_{2} \tilde{Q}_{2}\right]+\frac{\gamma_{5}}{2}\left[\left(1-P_{2}\right) \tilde{Q}_{1}+\frac{1}{\gamma^{2}}\left(1-\tilde{Q}_{2}\right) P_{1}\right],
\end{aligned}
$$

in which

$$
\begin{aligned}
& \tilde{Q}_{1}:=\cos (\gamma k h \cos \theta)=\cos \left(\frac{2 \pi}{G} \gamma \cos \theta\right), \quad \tilde{Q}_{2}:=\cos (2 \gamma k h \cos \theta)=\cos \left(\frac{4 \pi}{G} \gamma \cos \theta\right), \\
& \tilde{R}_{1}:=\cos (k h(2 \sin \theta-\gamma \cos \theta))=\cos \left(\frac{2 \pi}{G}(2 \sin \theta-\gamma \cos \theta)\right), \\
& \tilde{R}_{2}:=\cos (k h(\sin \theta+2 \gamma \cos \theta))=\cos \left(\frac{2 \pi}{G}(\sin \theta+2 \gamma \cos \theta)\right), \\
& \tilde{R}_{3}:=\cos (k h(\sin \theta-2 \gamma \cos \theta))=\cos \left(\frac{2 \pi}{G}(\sin \theta-2 \gamma \cos \theta)\right), \\
& \tilde{R}_{4}:=\cos (k h(2 \sin \theta+\gamma \cos \theta))=\cos \left(\frac{2 \pi}{G}(2 \sin \theta+\gamma \cos \theta)\right) .
\end{aligned}
$$

As $h=\frac{2 \pi}{G k}$, we conclude that

$$
\begin{equation*}
\frac{k^{N}}{k}=\frac{G}{2 \pi} \sqrt{\frac{\tilde{R}}{\tilde{L}}} \tag{3.27}
\end{equation*}
$$

Similarly, we choose optimal parameters $\gamma_{i}\left(i \in \mathbb{N}_{5}\right)$ and $b_{j}\left(j \in \mathbb{N}_{7}\right)$ by minimizing the numerical dispersion. To do this, we define the functional

$$
\begin{equation*}
J_{\gamma}\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; G, \theta\right):=\frac{G}{2 \pi} \sqrt{\frac{\tilde{R}}{\tilde{L}}}-1 . \tag{3.28}
\end{equation*}
$$

It follows from (3.27) that minimizing the error between the numerical wavenumber $k^{N}$ and the exact wavenumber $k$ is equivalent to minimizing the norm $\left\|J_{\gamma}\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G}, I_{\theta}}$. The corresponding refined choice strategy can be obtained by replacing $\left\|J\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G} \times I_{\theta}}$ in Rule 3.5 with $\left\|J_{\gamma}\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G} \times I_{\theta}}$.

Rule 3.7 (Refined Choice Strategy II).
Step 1. Estimate the interval $I_{G}:=\left[G_{\min }, G_{\max }\right]$.
Step 2. Choose $\gamma_{i}\left(i \in \mathbb{N}_{5}\right)$ and $b_{j}\left(j \in \mathbb{N}_{7}\right)$ such that

$$
\begin{align*}
& \left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7}\right) \\
& \quad=\arg \min \left\{\left\|J_{\gamma}\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; \cdot, \cdot\right)\right\|_{\infty, I_{G} \times I_{\theta}}: \sum_{j=1}^{5} \gamma_{j}=1, \quad \sum_{j=1}^{7} b_{j}=1\right\} . \tag{3.29}
\end{align*}
$$

To implement Rule 3.7, we set $J_{\gamma}\left(\gamma_{1}, \ldots, \gamma_{5}, b_{1}, \ldots, b_{7} ; G, \theta\right)=0$ to obtain the equation

$$
\begin{aligned}
& G^{2}\left\{2\left(1+\frac{1}{\gamma^{2}}\right)\left(P_{1} \tilde{Q}_{1}-\tilde{Q}_{1}-P_{1}+1\right) \gamma_{2}+\frac{1}{2}\left[3\left(1+\frac{1}{\gamma^{2}}\right)-4 P_{1}-\frac{4}{\gamma^{2}} \tilde{Q}_{1}+P_{2}+\frac{1}{\gamma^{2}} \tilde{Q}_{2}\right] \gamma_{3}\right. \\
& \quad+\frac{1}{2}\left[\left(1+\frac{1}{\gamma^{2}}\right) P_{2} \tilde{Q}_{2}-\frac{4}{\gamma^{2}} \tilde{Q}_{1}-4 P_{1}-\frac{1}{\gamma^{2}} P_{2}-\tilde{Q}_{2}+4\left(1+\frac{1}{\gamma^{2}}\right)\right] \gamma_{4} \\
& \left.\quad+\frac{1}{2}\left[\frac{1}{\gamma^{2}} P_{1} \tilde{Q}_{2}+P_{2} \tilde{Q}_{1}-\left(\frac{4}{\gamma^{2}}+1\right) \tilde{Q}_{1}-\left(4+\frac{1}{\gamma^{2}}\right) P_{1}+4\left(1+\frac{1}{\gamma^{2}}\right)\right] \gamma_{5}\right\} \\
& \quad+4 \pi^{2}\left\{\frac{1}{2}\left(P_{1}+\tilde{Q}_{1}-2\right) b_{2}+\frac{1}{2}\left(P_{2}+\tilde{Q}_{2}-2\right) b_{3}+\left(P_{1} \tilde{Q}_{1}-1\right) b_{4}\right.
\end{aligned}
$$

Table 3
The error in the C-norm for $k=200$.

| $N$ | 129 | 257 | 513 | 1025 |
| :--- | :--- | :--- | :--- | :--- |
| Rotated 9p | 1.0258 | 0.4747 | 0.1298 | 0.0331 |
| Global 25p | 0.4326 | 0.0785 | 0.0210 | 0.0108 |
| Refined 25p | 0.4331 | 0.0788 | 0.0202 | 0.0052 |

$$
\begin{align*}
& \left.+\left(P_{2} \tilde{Q}_{2}-1\right) b_{5}+\frac{1}{2}\left(\tilde{R}_{1}+\tilde{R}_{2}-2\right) b_{6}+\frac{1}{2}\left(\tilde{R}_{3}+\tilde{R}_{4}-2\right) b_{7}\right\} \\
= & -4 \pi^{2}+2 G^{2}\left\{\left(1+\frac{1}{\gamma^{2}}\right)-P_{1}-\frac{1}{\gamma^{2}} \tilde{Q}_{1}\right\} . \tag{3.30}
\end{align*}
$$

Solving Eq. (3.30) by the least square method as we did with Eq. (3.21) yields the refined optimal parameters for the finite difference scheme (3.25).

## 4. Numerical experiments

In this section, we give three numerical experiments to test our method proposed in the last section. The first one is an example for the Helmholtz equation, we show the advantage of the refined 25 p over the rotated 9 p and the global 25 p by comparing the accuracy of these three schemes. The second one is a homogeneous model. We investigate the refined 25 p's ability to portray the wave with a large step $h$ by making comparisons among the rotated 9 p, the global 25 p and the refined 25 p. Finally, a concave model is given to test the refined 25 p for heterogeneous medium.

### 4.1. A numerical example for the Helmholtz equation

Consider the Helmholtz equation

$$
\begin{equation*}
-\Delta u-k^{2} u=0, \quad \text { in } \Omega:=(0,1) \times(0,1), \tag{4.1}
\end{equation*}
$$

with boundary conditions

$$
\begin{equation*}
i k u+\frac{\partial u}{\partial n}=g, \quad \text { on } \Gamma:=\partial \Omega . \tag{4.2}
\end{equation*}
$$

The function $g$ depends on the parameter $\theta$, and is given by

$$
g(x):= \begin{cases}\mathrm{i}\left(k-k_{2}\right) \exp \left(\mathrm{i} k_{1} x_{1}\right), & \text { if } x \in \Gamma_{1}:=(0,1) \times(0,0), \\ \mathrm{i}\left(k+k_{1}\right) \exp \left(\mathrm{i}\left(k_{1}+k_{2} x_{2}\right)\right), & \text { if } x \in \Gamma_{2}:=(1,1) \times(0,1), \\ \mathrm{i}\left(k+k_{2}\right) \exp \left(\mathrm{i}\left(k_{1} x_{1}+k_{2}\right)\right), & \text { if } x \in \Gamma_{3}:=(1,0) \times(1,1), \\ \mathrm{i}\left(k-k_{1}\right) \exp \left(\mathrm{i} k_{2} x_{2}\right), & \text { if } x \in \Gamma_{4}:=(0,0) \times(1,0),\end{cases}
$$

with $\left(k_{1}, k_{2}\right):=k(\cos \theta, \sin \theta)$. The exact solution of this problem is

$$
u(x):=\exp \left(\mathrm{i}\left(k_{1} x_{1}+k_{2} x_{2}\right)\right) .
$$

This problem was used for measuring the efficiency of numerical methods in [25]. We use it to compare the accuracy of the rotated 9 p , the global 25 p and the refined 25 p. The error is measured in C-norm, which is defined as follows. For any complex vector $\mathbf{z}=\left[z_{1}, z_{2}, \ldots, z_{M}\right]$,

$$
\|\mathbf{z}\|_{C}:=\max _{1 \leq j \leq M}\left|z_{j}\right|,
$$

where $\left|z_{j}\right|$ is the complex modulus of $z_{j}$. The parameters in Tables 1 and 2 are used as refined optimal parameters. Additionally, the 25 -point finite difference schemes use the fourth order interpolation polynomials for the numerical boundary conditions (cf. [34]).

In Table 3, we present errors of these three schemes in C-norm for $k=200$ and $\theta=\frac{\pi}{4}$ with different gridpoints $N$ per line. We find that, to obtain a certain accuracy, the refined 25p and the global 25p only need less than half of the grids that the rotated 9p needs, which is consistent with the dispersion analysis in Section 3.2. Also, we see that both the rotated 9p and the refined 25 p are second order, while the global 25 p seems a little slower than the second order, which may be caused by the pollution effect.

To further compare the three schemes in terms of accuracy, in Table 4, we show the error in the C-norm for the case of $\theta=\frac{\pi}{4}$ and $N=1025$ with $k=100,200,300,400$. From this table, we see that there is much improvement in accuracy for the global 25 p and the refined 25 p over the rotated 9 p, especially for large wavenumbers. Additionally, there is an improvement for the refined 25 p over the global 25p, though it is not so sharp.

All of the experiments above are done with $\theta=\frac{\pi}{4}$. We finally test these schemes' dependence on $\theta$. Table 5 shows the corresponding results for $k=400$ and $N=1025$, with $\theta$ varying among [ $0, \pi / 4]$. It is clear that, the refined 25 p and the

Table 4
The error in the C-norm for $N=1025$.

| $k$ | 100 | 200 | 300 | 400 |
| :--- | :--- | :--- | :--- | :--- |
| Rotated 9p | 0.0043 | 0.0331 | 0.1108 | 0.2599 |
| Global 25p | 0.0049 | 0.0108 | 0.0175 | 0.0251 |
| Refined 25p | 0.0013 | 0.0052 | 0.0115 | 0.0202 |

Table 5
The error in the C-norm for $k=400$ and $N=1025$.

| $\theta$ | 0 | $\frac{\pi}{16}$ | $\frac{\pi}{8}$ | $\frac{3 \pi}{16}$ | $\frac{\pi}{4}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Rotated 9p | 0.3519 | 0.4017 | 0.1419 | 0.1260 | 0.2599 |
| Global 25p | 0.0313 | 0.0407 | 0.0326 | 0.0275 | 0.0251 |
| Refined 25p | 0.0313 | 0.0403 | 0.0313 | 0.0247 | 0.0202 |

global 25 p's dependence on the wave direction $\theta$ are much less than the rotated 9 p and their accuracy is much higher than that of the rotated 9 p. The refined 25 p also has an improvement in accuracy over the global 25 p. In practice, we usually do not know the wave's exact propagation direction, so we had better choose the refined 25 p.

From this example, we know that the refined 25 p exactly possess advantages over both the rotated 9 p and the global 25 p, which demonstrates that our proposed refined 25 p is useful and promising.

### 4.2. Constant wavenumber

To test the optimal 25-point schemes for the Helmholtz-PML equation (1.2), we use a 2-D homogeneous model, as shown in Fig. 4(a). The velocity of the medium is $1500 \mathrm{~m} / \mathrm{s}$. A point source $\delta\left(x-x_{s}, y-y_{s}\right) R\left(\omega, f_{0}\right)$ is located at the point $\left(x_{s}, y_{s}\right)=(500 \mathrm{~m}, 1000 \mathrm{~m})$, where $R\left(\omega, f_{0}\right)$ is the Ricker wavelet with

$$
R\left(t, f_{0}\right)=\left(1-2 \pi^{2} f_{0}^{2} t^{2}\right) \exp \left(-\pi^{2} f_{0}^{2} t^{2}\right)
$$

whose dominant frequency is $f_{0}=25 \mathrm{~Hz}$. The grid size is 10 m , the time sampling is 8 ms and the highest frequency we compute is 60 Hz .

For $201 \times 201$ mesh points, we generate synthetic seismograms by the extended 25 p, the optimal 9-point difference scheme (the optimal 9 p) proposed in [13], the global 25 p and the refined 25 p. Figs. $4(\mathrm{~b})$ and 3 show the synthetic seismograms for each formulation. Seen from Fig. 4(b), we find many non-physical oscillations appearing in the synthetic seismogram obtained by the extended 25p. From Fig. 3(b)-(d), we see that the synthetic seismogram based on the optimal 9p suffers from much more non-physical oscillations than the global 25 p, while there are almost no non-physical oscillations in the synthetic seismogram generated by the refined 25 p. In addition, the maximum value in Fig. 3(b)-(d) appears at the same time of 0.6720 s . According to the velocity of the wave, the wave propagates a distance of 1008 m , which is an appropriate result in practice. Moreover, snapshots at the time $t=256 \mathrm{~ms}$ generated by the optimal 9 p and the refined 25 p are shown in Fig. 3(e) and (f) respectively. As the model is a homogeneous model, the exact snapshot is a perfect circle without any reflections when the wave does not arrive at the boundaries. However, we see that the snapshot generated by the optimal 9 p suffers from many false reflections, while the snapshot based on the refined 25 p is very clear.

Now, we come to our conclusion that the refined 25 p is the best choice as it has simulated the wave propagation better and suppresses false reflections much more effectively when compared with the optimal 9 p and the global 25p.

### 4.3. Concave model

The concave model is shown in Fig. 5(a). There are three velocities in this model: from the top, $v=1500 \mathrm{~m} / \mathrm{s}, 2000 \mathrm{~m} / \mathrm{s}$, $2500 \mathrm{~m} / \mathrm{s}$. The grid size is taken as $\Delta x=\Delta y:=10 \mathrm{~m}$ and the interval of time sampling $\Delta t:=8 \mathrm{~ms}$. The source is located at the point ( $1000 \mathrm{~m}, 800 \mathrm{~m}$ ). As in the homogeneous model above, the Ricker wavelet with domain frequency 25 Hz is used as the source.

For $201 \times 201$ mesh points, we generate snapshots for the wavefield by the optimal 9 p and the refined 25 p. The monofrequency wavefield (real part) for $f=25 \mathrm{~Hz}$ obtained by the refined 25p is present in Fig. 5(b). The PML's absorption is efficient, and almost no boundary reflections exist. Additionally, the upward incident waves, the downward incident waves and transmissive waves are all clear. We also note that in the middle velocity layer, the incident waves are interfered with the reflected waves returned from the middle velocity layer's interfaces, and this phenomena obeys Snell's law. In Fig. 5(c), we show the snapshot for the time being 400 ms , generated by the optimal 9-point scheme, and Fig. 5(d) shows the corresponding snapshot generated by the refined 25p. Comparing Fig. 5(d) with Fig. 5(c), we find that Fig. 5(d) is clearer than Fig. 5(c), indicating that the refined 25p has less numerical dispersion than the optimal 9p.

## 5. Conclusion

In this section, we summarize and comment on the difference methods. In Section 2, we proved that, though it is a popular scheme for the Helmholtz equation, the extended 25-point finite difference scheme with its optimal parameters


Fig. 3. (a) Ricker wavelet, (b) Synthetic seismograms generated by the optimal 9p, (c) Synthetic seismograms generated by the global 25 p, (d) Synthetic seismograms generated by the refined 25p, (e) Snapshot generated by the optimal 9p at the time $t=256 \mathrm{~ms}$, (f) Snapshot generated by the refined 25 p at the time $t=256 \mathrm{~ms}$.
given in [22] is not pointwise consistent with the Helmholtz-PML equation. To deal with this problem, a consistent 25-point difference scheme was constructed and the refined choice strategy for choosing optimal parameters based on minimizing the numerical dispersion were proposed in Section 3. Additionally, normalized numerical phase and group velocity curves showed that the refined 25 -point finite difference scheme has the smallest numerical dispersion and anisotropy, compared with the extended 25 -point finite difference scheme and the optimal 9-point finite difference scheme. Finally, numerical experiments in Section 4 were presented to confirm that the refined 25-point finite difference scheme is the best scheme for the Helmholtz-PML equation. The applications ranged from constant wavenumbers to varying wavenumbers. Compared to the optimal 9 -point finite difference scheme and the global 25 -point finite difference scheme, the refined 25 -point


Fig. 4. (a) The homogeneous model, (b) Synthetic seismograms generated by the extended 25 p.





Fig. 5. (a) Concave model, (b) Monofrequency wavefield (real part) for $f=25 \mathrm{~Hz}$ obtained by the refined 25 p , (c) Snapshot generated by the optimal 9 p at the time $t=400 \mathrm{~ms}$, (d) Snapshot generated by the refined 25 p at the time $t=400 \mathrm{~ms}$.
finite difference scheme possesses the ability of portraying waves well with large steps while suppressing non-physical oscillations most effectively, especially for large wavenumbers.

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