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Fourth Order Schemes for Time-Harmonic Wave Equations with Discontinuous Coefficients

Guy Baruch[1], Gadi Fibich[1], Semyon Tsynkov[2] and Eli Turkel[1,*]

[1] *School of Mathematical Sciences, Tel Aviv University, Ramat Aviv, Tel Aviv 69978, Israel.*
[2] *Department of Mathematics, North Carolina State University, Box 8205, Raleigh, NC 27695, USA.*

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Abstract. We consider high order methods for the one-dimensional Helmholtz equation and frequency-Maxwell system. We demand that the scheme be higher order even when the coefficients are discontinuous. We discuss the connection between schemes for the second-order scalar Helmholtz equation and the first-order system for the electromagnetic or acoustic applications.

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1 Introduction

We consider the one-dimensional linear Helmholtz equation:

$$\frac{d^2E}{dz^2}+k_0^2\nu(z)E=0, \quad z\in[0,Z_{\max}], \tag{1.1}$$

where the material coefficient $\nu(z)$ is assumed piecewise-constant. In this case, the solution $E(z)$ and its first derivative dE/dz are continuous everywhere [1], whereas the second and higher derivatives undergo jumps at the points of discontinuity of $\nu(z)$. A more complicated, nonlinear, version of Eq. (1.1) that arises in the context of nonlinear optics was analyzed and solved numerically in [1].

*Corresponding author. *Email addresses:* `guybar@post.tau.ac.il` (G. Baruch), `fibich@post.tau.ac.il` (G. Fibich), `tsynkov@math.ncsu.edu` (S. Tsynkov), `turkel@post.tau.ac.il` (E. Turkel)

Along with the second-order equation (1.1), we consider the first-order one-dimensional Maxwell equations in frequency space:

$$i\omega\epsilon E=\frac{dH}{dz},\qquad i\omega\mu H=\frac{dE}{dz}, \tag{1.2}$$

where ϵ is piecewise constant and μ is constant. Eq. (1.1) with

$$k_0^2\nu(z)=\omega^2\epsilon\mu=\frac{\omega^2}{c^2}$$

can be easily obtained from system (1.2) by differentiating its second equation with respect to z and then substituting the derivative dH/dz from the first equation.

It has been recognized since the pioneering work of Kreiss and Oliger [7] that wave propagation equations require schemes with higher order accuracy due to phase errors and long time error accumulation. They found that the optimum scheme was between fourth- and sixth-order accurate. When the coefficients are only piecewise continuous it becomes much more difficult to construct higher order methods that retain their global accuracy. One approach to this difficulty has been the use of fictitious points as in the immersed interface and embedded boundary methods schemes first introduced by Zhang and LeVeque [15]. Later papers include [2, 8, 9, 16]. An analysis of the effect of discontinuous coefficients on the phase and amplitude errors was done by Gustafsson and Wahlund [4].

Our goal is to construct and test high order discrete approximations of (1.1) and (1.2) that keep the global higher order accuracy even in the presence of discontinuities in the coefficients. We will also examine connections between the resulting schemes similar to the previously identified relations [3] between a system and a scalar equation.

2 Fourth-order compact scheme for the Helmholtz equation

In this section we introduce the finite volume schemes for Eq. (1.1) based on its integral form. Let $a,b\in[0,Z_{\max}]$, $a<b$. We integrate (1.1) between the points a and b with respect to z:

$$\frac{dE(b)}{dz}-\frac{dE(a)}{dz}+k_0^2\int_a^b\nu(z)E\,dz=0. \tag{2.1}$$

Eq. (2.1) can be interpreted as the integral conservation law that corresponds to (1.1). For sufficiently smooth solutions, the two formulations are equivalent, see [1].

Following the approach in [1], we approximate the Helmholtz equation on a uniform grid with size h by applying the integral relation (2.1) between the midpoints of every two neighboring cells, i.e., for $[a,b]=[z_{m-\frac{1}{2}},z_{m+\frac{1}{2}}]$, $m=1,2,\dots,M$. In addition, we assume that $\nu(z)$ may be discontinuous only at the grid nodes and denote by $\nu_{m+\frac{1}{2}}$ the value of ν

in the cell $[z_m, z_{m+1}]$. Then,

$$\left.\frac{dE}{dz}\right|_{z_{m-\frac{1}{2}}}^{z_{m+\frac{1}{2}}} + k_0^2 \nu_{m-\frac{1}{2}} \int_{z_{m-\frac{1}{2}}}^{z_m} E dz + k_0^2 \nu_{m+\frac{1}{2}} \int_{z_m}^{z_{m+\frac{1}{2}}} E dz = 0. \tag{2.2}$$

By virtue of Eq. (1.1), $E(z)$ is infinitely differentiable within each cell. Hence, it can be approximated with fourth-order accuracy using cubic Birkhoff-Hermite interpolating polynomials [10], which leads to a fourth-order approximation of the integrals in (2.2). To approximate the derivatives in (2.2) with fourth-order accuracy, we employ a key idea of compact schemes: to use the original differential equation to obtain higher order derivatives that can cancel the leading terms of the truncation error. This idea has been implemented, e.g., by Harari and Turkel [5] and Singer and Turkel [11]. We shall use some elements of this *equation-based* approach but adapt it for material discontinuities [1].

The differential equation (1.1) inside the grid cells can be used to evaluate the one-sided second derivatives at the grid nodes as follows:

$$E''_{m+} \stackrel{\text{def}}{=} \left.\frac{d^2E}{dz^2}\right|_{z=z_m+} = -k_0^2 \nu_{m+\frac{1}{2}} E_m, \tag{2.3a}$$

$$E''_{(m+1)-} \stackrel{\text{def}}{=} \left.\frac{d^2E}{dz^2}\right|_{z=z_{m+1}-} = -k_0^2 \nu_{m+\frac{1}{2}} E_{m+1}. \tag{2.3b}$$

We use formulae (2.3) to approximate each of the three terms on the left-hand side of (2.2) with fourth-order accuracy.

To approximate the fluxes $E'_{m\pm\frac{1}{2}}$ in (2.2), we use the Taylor expansion:

$$E'_{m+\frac{1}{2}} = \frac{E_{m+1} - E_m}{h} - \frac{h^2}{24} E^{(3)}_{m+\frac{1}{2}} + \mathcal{O}(h^4).$$

Then, using

$$E^{(3)}_{m+\frac{1}{2}} = -\nu_{m+\frac{1}{2}} k_0^2 E'_{m+\frac{1}{2}},$$

we obtain:

$$E'_{m+\frac{1}{2}} = \left(1 + \frac{\nu_{m+\frac{1}{2}} (hk_0)^2}{24}\right) \frac{E_{m+1} - E_m}{h} + \mathcal{O}(h^4).$$

We repeat the calculation for $E'_{m-\frac{1}{2}}$. Altogether, the flux difference, i.e., the first term in (2.2), is approximated as

$$\left.\frac{dE}{dz}\right|_{z_{m-\frac{1}{2}}}^{z_{m+\frac{1}{2}}} = \frac{E_{m+1} - E_m}{h} \left(1 + \nu_{m+\frac{1}{2}} \frac{(hk_0)^2}{24}\right) - \frac{E_m - E_{m-1}}{h} \left(1 + \nu_{m-\frac{1}{2}} \frac{(hk_0)^2}{24}\right) + \mathcal{O}(h^4).$$

To approximate the two integral terms in (2.2), we use cubic interpolating polynomials and approximate the integrand $E(z)$ with fourth-order accuracy.

Lemma 2.1. *Let $E(z)\in C^6[z_m,z_{m+1}]$. Given its values $\{E_m,E_{m+1}\}$, as well as the values of its one-sided second derivatives $\{E''_{m+},E''_{(m+1)-}\}$, we can approximate $E(z)$ with fourth-order accuracy:*

$$E(z_m+\zeta h)=P_3(\zeta)+\mathcal{O}(h^4),\qquad \zeta\in[0,1] \tag{2.4a}$$

using the cubic Hermite-Birkhoff polynomial:

$$\begin{aligned}P_3(\zeta)=&\left(E_m-\frac{h^2}{6}E''_{m+}\right)(1-\zeta)+\frac{h^2}{6}E''_{m+}(1-\zeta)^3\\&+\left(E_{m+1}-\frac{h^2}{6}E''_{(m+1)-}\right)\zeta+\frac{h^2}{6}E''_{(m+1)-}\zeta^3.\end{aligned} \tag{2.4b}$$

Moreover, the polynomial $P_3(\zeta)$ is unique.

Lemma 2.1 has been proven in [1]. Substituting expressions (2.3) into formula (2.4b), we obtain a fourth-order approximation of $E(z)$ on $[z_m,z_{m+1}]$:

$$\begin{aligned}E(z_m+\zeta h)=&\left(1+\frac{(hk_0)^2}{6}\nu_{m+\frac{1}{2}}\right)E_m(1-\zeta)-\frac{(hk_0)^2}{6}\nu_{m+\frac{1}{2}}E_m(1-\zeta)^3\\&+\left(1+\frac{(hk_0)^2}{6}\nu_{m+\frac{1}{2}}\right)E_{m+1}\zeta-\frac{(hk_0)^2}{6}\nu_{m+\frac{1}{2}}E_{m+1}\zeta^3+\mathcal{O}(h^4).\end{aligned}$$

Substituting this expression for $E(z)$ into the second integral of (2.2) we have

$$\int_{z_m}^{z_{m+\frac{1}{2}}}Edz=\frac{3h}{8}\left(1+\nu_{m+\frac{1}{2}}\frac{(hk_0)^2}{16}\right)E_m+\frac{h}{8}\left(1+\nu_{m+\frac{1}{2}}\frac{7(hk_0)^2}{48}\right)E_{m+1}+\mathcal{O}(h^5).$$

Similarly, we obtain

$$\int_{z_{m-\frac{1}{2}}}^{z_m}Edz=\frac{3h}{8}\left(1+\nu_{m-\frac{1}{2}}\frac{(hk_0)^2}{16}\right)E_m+\frac{h}{8}\left(1+\nu_{m-\frac{1}{2}}\frac{7(hk_0)^2}{48}\right)E_{m-1}+\mathcal{O}(h^5).$$

Finally, by combining the approximations for all the individual terms in (2.2) we arrive at the following fourth-order scheme:

$$\begin{aligned}&\left(\frac{1}{h^2}+\frac{1}{6}k_0^2\nu_{m-\frac{1}{2}}+\frac{7}{384}h^2k_0^4\nu^2_{m-\frac{1}{2}}\right)E_{m-1}\\&+\left(\frac{-2}{h^2}+\frac{k_0^2}{3}(\nu_{m-\frac{1}{2}}+\nu_{m+\frac{1}{2}})+\frac{3}{128}h^2k_0^4(\nu^2_{m-\frac{1}{2}}+\nu^2_{m+\frac{1}{2}})\right)E_m\\&+\left(\frac{1}{h^2}+\frac{1}{6}k_0^2\nu_{m+\frac{1}{2}}+\frac{7}{384}h^2k_0^4\nu^2_{m+\frac{1}{2}}\right)E_{m+1}=0,\end{aligned} \tag{2.5}$$

or equivalently,

$$\begin{aligned}&\frac{1}{h^2}(E_{m-1}-2E_m+E_{m+1})+\frac{k_0^2}{6}\left(\nu_{m-\frac{1}{2}}E_{m-1}+2(\nu_{m-\frac{1}{2}}+\nu_{m+\frac{1}{2}})E_m+\nu_{m+\frac{1}{2}}E_{m+1}\right)\\&+\frac{h^2k_0^4}{384}\left(7\nu^2_{m-\frac{1}{2}}E_{m-1}+9(\nu^2_{m-\frac{1}{2}}+\nu^2_{m+\frac{1}{2}})E_m+7\nu^2_{m+\frac{1}{2}}E_{m+1}\right)=0.\end{aligned} \tag{2.6}$$

The fourth-order radiation boundary conditions for scheme (2.6), as well as their two-way version that prescribes the given impinging wave, are discussed in [1].

For the constant coefficient case: $\nu_{m+\frac{1}{2}}=\nu_{m-\frac{1}{2}}\equiv\nu$, scheme (2.6) reduces to

$$\begin{aligned}&\frac{E_{m-1}-2E_m+E_{m+1}}{h^2}+k_0^2\nu\frac{E_{m-1}+4E_m+E_{m+1}}{6}\\&\quad+h^2k_0^4\nu^2\frac{7E_{m-1}+18E_m+7E_{m+1}}{384}=0.\end{aligned} \tag{2.7}$$

A three-point fourth-order compact approximation of the Helmholtz equation (1.1) was derived in [11]:

$$\frac{E_{m-1}-2E_m+E_{m+1}}{h^2}+k_0^2\nu\frac{E_{m-1}+10E_m+E_{m+1}}{12}=0. \tag{2.8}$$

Define

$$\boldsymbol{L}=\frac{d^2}{dz^2}+k_0^2\nu,$$

the Helmholtz operator. Then, using a Taylor series expansion (2.7) yields

$$\left(1+\frac{h^2}{12}\boldsymbol{L}\right)\boldsymbol{L}E=\mathcal{O}(h^6)$$

while (2.8) yields

$$\left(1+\frac{h^2}{12}\frac{d^2}{dz^2}\right)\boldsymbol{L}E=\mathcal{O}(h^6).$$

Hence, both are fourth-order accurate.

The issue of symmetry for the discretization (2.6) deserves a special comment. We see that if $\nu_{m-\frac{1}{2}}\neq\nu_{m+\frac{1}{2}}$, then, technically speaking, (2.6) is not symmetric, although for the case of constant coefficients the symmetry is restored, see formulae (2.7)-(2.8). We also see, however, that the asymmetry of (2.6) resides only in its non-differentiated terms, whereas the discretization of E'' is still symmetric. Hence, even though we did not study this question in detail, we expect that the spectral properties of the finite difference operator will not suffer much, and if there are complex eigenvalues their imaginary parts will be $\mathcal{O}(h^2)$. We additionally note that the original differential operator

$$\boldsymbol{L}E\equiv E''+k_0^2\nu E$$

is symmetric, but only on the class of twice continuously differentiable functions. However, the solution of $\boldsymbol{L}E=0$ does not belong to this class.

3 Extensions of the fourth-order Helmholtz scheme

Several extensions can be contemplated for the fourth-order scheme (2.6). One of those is the extension to higher orders of accuracy. In order to achieve that, we can use one-sided derivatives of orders higher than second in the context of Birkhoff-Hermite interpolation. For example, given the field values $\{E_m, E_{m+1}\}$, as well as the values of its one-sided *second and fourth* derivatives $\{E''_{m+}, E''_{(m+1)-}, E^{(4)}_{m+}, E^{(4)}_{(m+1)-}\}$, one can approximate $E(z)$ with sixth-order accuracy using a quintic polynomial:

$$E(z_m+\zeta h) = P_5(\zeta) + \mathcal{O}(h^6),$$

where

$$\begin{aligned}P_5(\zeta) = &\left(E_m - \frac{h^2}{6}E''_{m+} + \frac{7h^4}{360}E^{(4)}_{m+}\right)(1-\zeta)\\ &+\left(\frac{h^2}{6}E''_{m+} - \frac{h^4}{36}E^{(4)}_{m+}\right)(1-\zeta)^3 + \frac{1}{120}E^{(4)}_{m+}(1-\zeta)^5\\ &+\left(E_{m+1} - \frac{h^2}{6}E''_{(m+1)-} + \frac{7h^4}{360}E^{(4)}_{(m+1)-}\right)\zeta\\ &+\left(\frac{h^2}{6}E''_{(m+1)-} - \frac{h^4}{36}E^{(4)}_{(m+1)-}\right)\zeta^3 + \frac{1}{120}E^{(4)}_{(m+1)-}\zeta^5.\end{aligned}$$

Similarly to (2.3), the fourth derivatives are obtained from the differential equation (1.1):

$$E^{(4)}_{m+} = -k_0^2\nu_{m+\frac{1}{2}}E''_{m+} = k_0^4\nu^2_{m+\frac{1}{2}}E_m, \qquad E^{(4)}_{(m+1)-} = k_0^4\nu^2_{m-\frac{1}{2}}E_{m-1}.$$

Then, substituting $P_5(\zeta)$ for $E(z)$ into the second and third terms of (2.2) and evaluating the integrals with respect ζ, we can obtain a sixth-order discrete approximation of the integrals in (2.2).

To approximate the fluxes $E'_{m\pm\frac{1}{2}}$ in (2.2) with sixth-order accuracy, we again use the Taylor expansion:

$$\frac{E_{m+1}-E_m}{h} = E'_{m+\frac{1}{2}} + \frac{h^2}{24}E^{(3)}_{m+\frac{1}{2}} + \frac{h^4}{1920}E^{(5)}_{m+\frac{1}{2}} + \mathcal{O}(h^6).$$

Since Eq. (1.1) implies that

$$E^{(3)}_{m+\frac{1}{2}} = -\nu_{m+\frac{1}{2}}k_0^2E'_{m+\frac{1}{2}} \quad \text{and} \quad E^{(5)}_{m+\frac{1}{2}} = (\nu_{m+\frac{1}{2}}k_0^2)^2E'_{m+\frac{1}{2}},$$

we obtain

$$\frac{E_{m+1}-E_m}{h} = \left(1 - \frac{1}{24}\nu_{m+\frac{1}{2}}(hk_0)^2 + \frac{1}{1920}\left(\nu_{m+\frac{1}{2}}(hk_0)^2\right)^2\right)E'_{m+\frac{1}{2}} + \mathcal{O}(h^6).$$

Therefore,

$$E'_{m+\frac{1}{2}} = \left(1 + \frac{1}{24}\nu_{m+\frac{1}{2}}(hk_0)^2 + \frac{7}{5760}\left(\nu_{m+\frac{1}{2}}(hk_0)^2\right)^2\right)\frac{E_{m+1}-E_m}{h} + \mathcal{O}(h^6).$$

Altogether, we obtain the following $\mathcal{O}(h^6)$ approximation for Eq. (1.1):

$$0=L_1(\nu_{m-\frac{1}{2}})E_{m-1}-\Big(L_0(\nu_{m-\frac{1}{2}})+L_0(\nu_{m+\frac{1}{2}})\Big)+L_1(\nu_{m+\frac{1}{2}})E_{m+1}, \tag{3.1a}$$

where

$$L_0(\nu)=1-\frac{1}{3}\nu(hk_0)^2-\frac{1}{45}\left(\nu(hk_0)^2\right)^2-\frac{11}{5120}\left(\nu(hk_0)^2\right)^3, \tag{3.1b}$$

$$L_1(\nu)=1+\frac{1}{6}\nu(hk_0)^2+\frac{7}{360}\left(\nu(hk_0)^2\right)^2+\frac{31}{15360}\left(\nu(hk_0)^2\right)^3. \tag{3.1c}$$

Note that as Eq. (1.1) is one-dimensional, the foregoing technique can be extended further, and the schemes of accuracy higher than $\mathcal{O}(h^6)$ can be built in a similar way.

Another possible extension of the scheme of Section 2 can be aimed at accommodating the material coefficient $\nu(z)$ with jump discontinuities at the points other than grid nodes, e.g., at $z^*=z_m+\lambda h$, $\lambda\in(0,1/2)$. To do that, one should first split the integral in (2.1) as

$$\int_{z_{m-\frac{1}{2}}}^{z_{m+\frac{1}{2}}}=\int_{z_{m-\frac{1}{2}}}^{z^*}+\int_{z^*}^{z_{m+\frac{1}{2}}}.$$

Then, one can construct a Birkhoff-Hermite approximation of the field on $[z_{m-\frac{1}{2}},\, z^*]$, using the values at z_{m-1} and z_m. Similarly, one can use the values at z_{m+1} and z_{m+2} to approximate the field on $[z^*,\, z_{m+\frac{1}{2}}]$. Note that this approach will not involve extrapolation across the discontinuity, and hence the approximations will remain fourth-order. The proof of Lemma 2.1 given in [1] can be easily modified to show this.

4 Maxwell first-order system

We now consider the first-order system (1.2). We use a staggered mesh with E at the nodes and H half way in between and consider the following finite difference approximation:

$$i\omega\epsilon\left[\left(\alpha+\beta h^2\right)E_j+\left(1-\alpha+\gamma h^2\right)E_{j-1}\right]=\frac{H_{j+1/2}-H_{j-1/2}}{h}, \tag{4.1a}$$

$$i\omega\mu\left[\left(1-\alpha+\gamma h^2\right)H_{j+1/2}+\left(\alpha+\beta h^2\right)H_{j-1/2}\right]=\frac{E_j-E_{j-1}}{h}. \tag{4.1b}$$

The left-hand side (LHS) of the first equation is centered at $j-1/2$ and the right-hand side at j. For the second equation we reverse the orientation and center the LHS at j and the RHS at $j-1/2$. Each operator is a one-sided operator and so can be inverted trivially.

We now try and duplicate the formulae we derived for the Helmholtz equation starting from (4.1). We first consider the case where both μ and ϵ are constant. We take another difference of the second equation (4.1b) and divide by h. We then get:

$$i\omega\mu\left[\left(\alpha+\beta h^2\right)\left(\frac{H_{j+1/2}-H_{j-1/2}}{h}\right)+\left(1-\alpha+\gamma h^2\right)\left(\frac{H_{j+3/2}-H_{j+1/2}}{h}\right)\right]$$
$$=\frac{E_{j+1}-2E_j+E_{j-1}}{h^2}.$$

Using the first equation (4.1a) we get:

$$-\omega^2\epsilon\mu\left[\left(1-\alpha+\gamma h^2\right)\left(\alpha+\beta h^2\right)\left(E_{j-1}+E_{j+1}\right)+\left(\left(1-\alpha+\gamma h^2\right)^2+\left(\alpha+\beta h^2\right)^2\right)E_j\right]$$
$$=\frac{E_{j+1}-2E_j+E_{j-1}}{h^2}. \tag{4.2}$$

In the notation of the Helmholtz equation

$$\omega^2\epsilon\mu=\frac{\omega^2}{c^2}=k_0^2\nu.$$

Matching this to the previous formula for the Helmholtz equation (2.7) we derive:

$$\left(1-\alpha+\gamma h^2\right)\left(\alpha+\beta h^2\right)=\frac{1}{6}+\frac{7}{384}h^2k_0^2\nu, \tag{4.3a}$$
$$\left(1-\alpha+\gamma h^2\right)^2+\left(\alpha+\beta h^2\right)^2=\frac{2}{3}+\frac{18}{384}h^2k_0^2\nu, \tag{4.3b}$$

or

$$\alpha-\alpha^2=\frac{1}{6}, \quad (1-\alpha)\beta+\alpha\gamma=\frac{7}{384}k_0^2\nu, \quad \alpha\beta+(1-\alpha)\gamma=\frac{9}{384}k_0^2\nu.$$

So,

$$\alpha=\frac{1}{2}+\sqrt{\frac{1}{12}}, \quad 1-\alpha=\frac{1}{2}-\sqrt{\frac{1}{12}}, \quad \beta=\frac{7-16\alpha}{1-2\alpha}\frac{k_0^2\nu}{384}, \quad \gamma=\frac{9-16\alpha}{1-2\alpha}\frac{k_0^2\nu}{384}, \tag{4.4}$$

and we recover the fourth-order approximation to the Helmholtz equation (2.7). We stress that each part of the discretization is only first-order. We can consider the first-order system as a LU decomposition into two bi-diagonal matrices of the tridiagonal matrix of the Helmholtz equation. Similar ideas were explored in [3] and [6]. We now redo the calculations for the case where μ is constant but ϵ is only piecewise constant. We consider the low order scheme with $\beta=\gamma=0$ in (4.1). We now compare (4.2) with (2.6) ignoring the $\mathcal{O}(h^2)$ terms. The matching conditions (4.3) are replaced by

$$\alpha(1-\alpha)=\frac{1}{6}, \quad (1-\alpha)^2=\frac{1}{3}, \quad \alpha^2=\frac{1}{3}. \tag{4.5}$$

However, there is no solution to these equations and hence nothing identical to that we achieved for the Helmholtz equation even to first-order accuracy! Note, that for the constant coefficient case we only need to satisfy the sum of the last two equations in (4.5) rather than each equation individually which yields (4.4).

Hence, for the case of discontinuous coefficients we can no longer find a high order discretization to the Maxwell equations using only a bidiagonal approximation to each individual equation. Instead, we replace the approximation (4.1) with a tridiagonal approximation for each equation. When combined to form the Helmholtz equation, these will lead to a five point stencil and so will no longer be identical to (2.5). To derive this approximation we again begin with the integral form of the equation similar to what was done in (2.1). We use a staggered mesh with E defined at j while H is defined at $j+\frac{1}{2}$. We begin with the constant coefficient case. Integrating (1.2) over one cell we get:

$$i\omega\int_{-\frac{h}{2}}^{\frac{h}{2}}\epsilon(z)E(z)dz=\int_{-\frac{h}{2}}^{\frac{h}{2}}\frac{dH}{dz}dz=H_{j+1/2}-H_{j-1/2}, \tag{4.6a}$$

$$i\omega\mu\int_{-h}^{0}H(z)dz=\int_{-h}^{0}\frac{dE}{dz}dz=E_j-E_{j-1}. \tag{4.6b}$$

To obtain a numerical scheme we need to approximate the integrals using values of E at grid points and H at halfway in between grid points. The integrals on the left hand side are non-standard since for example, the first integral is from $-h/2$ to $h/2$ but the function is only given at $E(h)$,$E(0)$ and $E(-h)$. Nevertheless, we can get a numerical approximation to higher order by either using a Taylor series expansion or else an appropriate interpolation polynomial as an extension to Newton-Cotes formulae. The result is

$$i\omega\frac{\epsilon_{j+1}E_{j+1}+22\epsilon_jE_j+\epsilon_{j-1}E_{j-1}}{24}=\frac{H_{j+\frac{1}{2}}-H_{j-\frac{1}{2}}}{h}, \tag{4.7a}$$

$$i\omega\mu\frac{H_{j+3/2}+22H_{j+1/2}+H_{j-1/2}}{24}=\frac{E_{j+1}-E_j}{h}. \tag{4.7b}$$

This is equivalent to the TY scheme [12–14], which is a fourth-order compact implicit scheme for the Maxwell equations.

We check what happens at the discontinuity when we use a fourth-order compact implicit (TY) scheme and evaluate ϵ at the point of discontinuity by

$$\epsilon_j=\frac{\epsilon^l+\epsilon^r}{2},$$

where l and r denote values to the left and right of the discontinuity. Then

$$\begin{aligned}&\frac{1}{24}\epsilon_{j-1}E_{j-1}+\frac{22}{24}\epsilon_jE_j+\frac{1}{24}\epsilon_{j+1}E_{j+1}\to\frac{\epsilon^l}{24}E_{j-1}+\frac{11(\epsilon^l+\epsilon^r)}{24}E_j+\frac{\epsilon^r}{24}E_{j+1}\\&=\epsilon^l\left(\frac{1}{2}E^l_j-\frac{1}{24}E^{l'}_jh+\frac{1}{24}E^{l''}_j\frac{h^2}{2}\right)+\epsilon^r\left(\frac{1}{2}E^r_j+\frac{1}{24}E^{r'}_jh+\frac{1}{24}E^{r''}_j\frac{h^2}{2}\right)+\mathcal{O}(h^3).\end{aligned}$$

We estimate the integrals using derivatives:

$$
\begin{aligned}
&\int_{-\frac{h}{2}}^{\frac{h}{2}} \epsilon(z)E(z)\,dz = \int_{-\frac{h}{2}}^{0} \epsilon(z)E(z)\,dz + \int_{0}^{\frac{h}{2}} \epsilon(z)E(z)\,dz \\
&= \epsilon^l \int_{-\frac{h}{2}}^{0} \left(E_j^l + E_j^{l'} z + E_j^{l''} \frac{z^2}{2} \right) dz + \epsilon^r \int_{0}^{\frac{h}{2}} \left(E_j^r + E_j^{r'} z + E_j^{r''} \frac{z^2}{2} \right) dz + \mathcal{O}(h^3).
\end{aligned}
\tag{4.8}
$$

The error is given by

$$
\begin{aligned}
&h\left(\frac{1}{24}\epsilon_{j-1}E_{j-1} + \frac{22}{24}\epsilon_j E_j + \frac{1}{24}\epsilon_{j+1}E_{j+1} \right) - \int_{-\frac{h}{2}}^{\frac{h}{2}} \epsilon(z)E(z)\,dz \\
&= \frac{\epsilon^l}{12} E_j^{l'} h^2 - \frac{\epsilon^r}{12} E_j^{r'} h^2 + \mathcal{O}(h^3) = \frac{E_j' h^2}{12} \left(\epsilon^l - \epsilon^r \right) + \mathcal{O}\left(h^3\right).
\end{aligned}
\tag{4.9}
$$

In a continuous region, where $\epsilon^l = \epsilon^r$, the leading term vanishes and gives a high order approximation to the integral. However, at a point of discontinuity it reduces the accuracy to second-order.

To regain higher order we need to evaluate the integral on each side of the discontinuity. This can be done for a general location of the discontinuity in the interval. However, to simplify matters we consider the same case as for the Helmholtz equation when the discontinuity occurs at a nodal point (where E is defined). We only consider ϵ^l and ϵ^r on the two sides of the discontinuity. ϵ at the discontinuity is not defined. We substitute

$$
E' \approx \frac{-3E_j + 4E_{j+1} - E_{j+2}}{2h}, \quad E'' = -\omega^2 \epsilon \mu E
$$

into (4.8). Let j be the point of discontinuity. Since E is continuous we have:

$$
\begin{aligned}
&\int_{-\frac{h}{2}}^{\frac{h}{2}} \epsilon(z)E(z)\,dz = \epsilon^l \int_{-\frac{h}{2}}^{0} \left(E_j^l + E_j^{l'} z + E_j^{l''} \frac{z^2}{2} \right) dz + \epsilon^r \int_{0}^{\frac{h}{2}} \left(E_j^r + E_j^{r'} z + E_j^{r''} \frac{z^2}{2} \right) dz \\
&= \epsilon^l \left[\frac{h}{2} E_j - E_j' \frac{h^2}{8} - \omega^2 \epsilon^l \mu E_j \frac{h^3}{48} \right] + \epsilon^r \left[\frac{h}{2} E_j + E_j' \frac{h^2}{8} - \omega^2 \epsilon^r \mu E_j \frac{h^3}{48} \right] + \mathcal{O}(h^4) \\
&= \frac{\epsilon^r + \epsilon^l}{2} E_j h + \frac{\epsilon^r - \epsilon^l}{8} E_j' h^2 - \frac{h^3 \omega^2 \mu}{48} \left(\epsilon^{r2} + \epsilon^{l2} \right) E_j.
\end{aligned}
\tag{4.10}
$$

We approximate E_j' by a Taylor series and find:

$$
\begin{aligned}
\frac{\epsilon^r E(h) + \epsilon^l E(-h)}{8} &= \frac{\epsilon^r + \epsilon^l}{8} E_j + \frac{\epsilon^r - \epsilon^l}{8} E_j' h + \frac{h^2}{16} \left(\epsilon^l E_j^{l''} + \epsilon^r E_j^{r''} \right) + \mathcal{O}\left(h^3\right) \\
&= \frac{\epsilon^r + \epsilon^l}{8} E_j + \frac{\epsilon^r - \epsilon^l}{8} E_j' h - \frac{h^2 \omega^2 \mu}{16} \left(\epsilon^{r2} + \epsilon^{l2} \right) E_j + \mathcal{O}\left(h^3\right).
\end{aligned}
$$

The final formula is

$$\int_{-\frac{h}{2}}^{\frac{h}{2}} \epsilon(z)E(z)dz = h\left[\frac{\epsilon^l E_{j-1}}{8} + \left[\frac{3}{8}(\epsilon^r + \epsilon^l) + \frac{\omega^2 h^2 \mu}{24}\left(\epsilon^{r2} + \epsilon^{l2}\right)\right]E_j + \frac{\epsilon^r E_{j+1}}{8}\right],$$

which is accurate to within h^3. This is put into (4.6a). For (4.6b) μ is continuous and so we can use (4.7a) which is compact.

4.1 Compact third-order not aligned to node

We consider the case where the discontinuity falls in between two nodes:

$$i\omega F(z) = \frac{dH(z)}{dz}, \qquad F(z) = \epsilon E,$$

where $F(z)$ is smooth to the left and right of the discontinuity $z = L$ between 0 and $h/2$, with ϵ piecewise constant. We integrate the equation and split the integral into two parts. We now consider a wider stencil:

$$i\omega\left(\int_{-\frac{h}{2}}^{L} F(z)dz + \int_{L}^{\frac{3h}{2}} F(z)dz\right) = H\left(+\frac{3h}{2}\right) - H\left(-\frac{h}{2}\right).$$

Using a Taylor series expansion of F to third-order and integrating we get

$$\begin{aligned} & i\omega\left[F(0)(L+h/2) + \frac{F'(0)}{2}\left(L^2 - h^2/4\right) + \frac{F''(0)}{6}\left(L^3 + h^3/8\right)\right] \\ & + i\omega\left[F(h)(3h/2 - L) + \frac{F'(h)}{2}\left((3h/2)^2 - L^2\right) + \frac{F''(h)}{6}\left((3h/2)^3 - L^3\right)\right] \\ & = H(+3h/2) - H(-h/2). \end{aligned} \tag{4.11}$$

We wish to express F, F', and F'' using as few nodal points as possible. For $F(0)$ we simply take F_j. Next we use the properties of the Maxwell equations in the smooth zone. Define

$$C_1 = i\omega\epsilon\mu, \quad C_2 = -\omega^2\mu\epsilon^2.$$

Then

$$\begin{aligned} & F' = C_1 H, \quad F'' = C_2 F, \quad F''' = C_1 C_2 H, \\ & F'\left(\frac{-h}{2}\right) = F'(0) - \frac{h}{2}F''(0) + \frac{h^2}{8}F'''\left(\frac{-h}{2}\right). \end{aligned}$$

For a Yee type scheme F is evaluated at 0, while H is evaluated at $h/2$. Hence,

$$
\begin{aligned}
&\int_{-\frac{h}{2}}^{L} F(z)\,dz \\
&= F(0)\,(L+h/2) + \frac{F'(0)}{2}\left(L^2-h^2/4\right) + \frac{F''(0)}{6}\left(L^3+h^3/8\right) \\
&= F(0)\,(L+h/2) + \frac{1}{2}\left(F'(-\frac{h}{2}) + \frac{h}{2}F''(0) - \frac{h^2}{8}F'''(\frac{-h}{2})\right)\left(L^2-h^2/4\right) + \frac{F''(0)}{6}\left(L^3+h^3/8\right) \\
&= F_0\,(L+h/2) + \frac{1}{2}\left(C_1 H_{-\frac{1}{2}} + \frac{h}{2}C_2 F_0 - \frac{h^2}{8}C_1 C_2 H_{-\frac{1}{2}}\right)\left(L^2-h^2/4\right) + C_2\frac{F_0}{6}\left(L^3+h^3/8\right) \\
&= \left[L+\frac{h}{2}+C_2\frac{h}{4}\left(L^2-h^2/4\right)+\frac{C_2}{6}\left(L^3+h^3/8\right)\right]F_0 + \frac{C_1}{2}\left[L^2-\frac{h^2}{4}-C_2\frac{h^2}{8}L^2\right]H_{-\frac{1}{2}}. \qquad (4.12)
\end{aligned}
$$

Repeating this procedure for the integral from L to $3h/2$ we find the scheme has the form:

$$
i\omega\left(\alpha H_{j-\frac{1}{2}} + \beta F_j + \gamma H_{j+\frac{1}{2}} + \delta F_{j+1}\right) = H_{j+\frac{3}{2}} - H_{j-\frac{1}{2}}.
$$

Combinations of the electric and magnetic fields appear in the left hand side of the magnetic equation and so this differs from the TY scheme [12–14] even for smooth coefficients.

5 Numerical simulations

We computationally assess the performance of the fourth-order (2.5) and sixth-order scheme (3.1) for the Helmholtz equation. At the interface we have a material discontinuity:

$$
\nu(z) = \begin{cases} 1, & \text{for } z\in[-\infty,0), \\ 4, & \text{for } z\in(0,+\infty]. \end{cases} \qquad (5.1)
$$

The value of the linear wavenumber is $k_0=1$. We consider the wave e^{iz} that propagates from $z=-\infty$ in the positive z direction. It is partially reflected back at the interface $z=0$ giving rise to the left traveling wave Re^{-iz} for $z<0$, and partially transmitted, which yields a right traveling wave Te^{2iz} for $z>0$. The values of R and T can be determined by a straightforward calculation that involves matching the field E and its derivative dE/dz at both sides of the interface $z=0$.

The simulation region is $z\in[-1,1]$. At the boundary $z=-1$, the boundary condition should prescribe the incoming wave e^{iz} and enable the reflectionless propagation of the outgoing wave Re^{-iz}. Likewise, at the boundary $z=1$ the boundary condition should enable the reflectionless propagation of the outgoing wave Te^{2iz}. Hence, we set:

$$
\left(\frac{d}{dz}+i\right)E\bigg|_{z=-1} = 2ie^{-i} \quad \text{and} \quad \left(\frac{d}{dz}-2i\right)E\bigg|_{z=1} = 0. \qquad (5.2)
$$

Table 1: Error of the fourth-order scheme (2.5), the sixth-order scheme (3.1), and a similar second-order scheme applied to the analysis of the two layer configuration (5.1). The last column provides the functional dependence of the error on the grid size h, obtained by a least squares fit. For $h=0.01$, the error of the sixth-order discretization is limited by the machine precision.

approximation	grid size h				error(h)
	0.33	0.1	0.033	0.01	
second-order	$1.2\cdot 10^{-2}$	$1.4\cdot 10^{-3}$	$1.5\cdot 10^{-4}$	$1.4\cdot 10^{-5}$	$0.14\cdot h^2$
fourth-order	$1.0\cdot 10^{-3}$	$7.8\cdot 10^{-6}$	$9.4\cdot 10^{-8}$	$7.6\cdot 10^{-10}$	$0.078\cdot h^4$
sixth-order	$4.9\cdot 10^{-5}$	$3.4\cdot 10^{-8}$	$4.6\cdot 10^{-11}$	—	$0.034\cdot h^6$

Boundary conditions (5.2) are implemented directly for the discretization as in [1].

The numerical solutions are compared with the closed form continuous solutions in the maximum norm. The results are displayed in Table 1. They corroborate the design fourth and sixth-order convergence of the schemes, respectively. In the paper, we have provided a formal accuracy analysis plus computational evidence, see Table 1, for the fourth-order convergence. In [1], the fourth-order convergence has been rigorously justified for a linear equation with piecewise constant coefficients.

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