Wave scattering by metamaterial wedges and interfaces

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SUMMARY
We outline specific features of numerical simulations of metamaterial wedges and interfaces. We study the effect of different positioning of a grid in the Yee method, which is necessary to obtain consistent convergence in modelling of interfaces with metamaterials characterized by negative dielectric permittivity and negative magnetic permeability. We demonstrate however that, in the framework of the continuous-medium approximation, wave scattering on the wedge may result in a resonant excitation of waves with infinitely large spatial frequencies, leading to non-convergence of the simulation results that depend on the discretization step. Copyright © 2006 John Wiley & Sons, Ltd.

KEY WORDS: metamaterial; left-handed media; Yee scheme; wave scattering; singularities

1. INTRODUCTION

Recent theoretical [1–4] and experimental [5–7] studies have shown the possibility of creating novel types of microstructured materials that demonstrate the property of negative refraction. In particular, the composite materials created by arrays of wires and split-ring resonators were shown to possess both negative real parts of magnetic permeability and dielectric permittivity for microwaves. These materials are often referred to as left-handed metamaterials, double-negative materials, negative-index materials, or materials with negative refraction. Properties of such materials were first analysed theoretically by Veselago a long time ago [8], but they were demonstrated experimentally only recently. As was shown by Veselago [8], left-handed metamaterials possess a number of peculiar properties, including negative refraction for interface scattering, inverse light pressure, reverse Doppler effect, etc.

Many suggested and demonstrated applications of negative-index metamaterials utilize unusual features of wave propagation and scattering at the interfaces. In particular, the effect of
negative refraction can be used to realize focusing with a flat slab, the so-called planar lens [8], in a sharp contrast with the well-known properties of conventional lenses with a positive refractive index where curved surfaces are needed to form an image. Moreover, the resolution of the negative-index flat lens can be better than a wavelength due to the effect of amplification of evanescent modes [9].

Direct numerical simulations provide the unique means for a design of microwave and optical devices based on the negative-index materials. However, any realistic simulation should take into account metamaterial dispersion and losses [10–13] as well as a non-linear response [14]. Such numerical simulations are often carried out within the framework of the effective medium approximation, when the metamaterial is characterized by the effective dielectric permittivity and magnetic permeability. This simplification allows for modelling of large-scale wave dynamics using the well-known finite-difference time-domain (FDTD) numerical methods [15].

In this paper, we discuss the main features and major difficulties in applying the standard FDTD numerical schemes for simulating wave scattering by wedges and interfaces of finite-extent negative-index metamaterials, including a key issue of positioning of a discretization grid in the numerical Yee scheme [16] necessary to obtain consistent convergence in modelling waves at an interface between conventional dielectric and metamaterial with negative dielectric permittivity and negative magnetic permeability. In particular, we demonstrate that, in the framework of the continuous-medium approximation, wave scattering on the wedge may result in a resonant excitation of surface waves with infinitely large spatial frequencies, leading to non-convergence of the simulation results that depend on the discretization step.

2. BASIC EQUATIONS

We consider a two-dimensional problem for the propagation of TE-polarized electromagnetic waves in the plane \((x, z)\), where the medium properties are isotropic and characterized by the dielectric permittivity \(\varepsilon\) and magnetic permeability \(\mu\). In the absence of losses, \(\mathbb{1}_m \varepsilon = \mathbb{1}_m \mu = 0\). The response of negative-index materials is known to be strongly frequency dependent [1]. However, in the linear regime the wave propagation at different wavelengths can be described independently. The stationary form of Maxwell’s equations for the complex wave envelopes is well known

\[
\frac{\partial H_y}{\partial x} - \frac{\partial H_z}{\partial z} = \frac{i \omega}{c} \varepsilon(x, z) E_y, \quad \frac{\partial E_y}{\partial z} = -\frac{i \omega}{c} \mu(x, z) H_x, \quad \frac{\partial E_y}{\partial x} = \frac{i \omega}{c} \mu(x, z) H_z \tag{1}
\]

where \(H_y, H_z,\) and \(E_y\) are the components of the magnetic and electric fields, respectively, \(\omega\) is angular frequency, and \(c\) is the speed of light in vacuum. The system of coupled equations (1) can be reduced to a single Helmholtz-type equation for the electric field envelope,

\[
\mu(x, z) \frac{\partial}{\partial x} \left( \frac{1}{\mu(x, z)} \frac{\partial E_y}{\partial x} \right) + \mu(x, z) \frac{\partial}{\partial z} \left( \frac{1}{\mu(x, z)} \frac{\partial E_y}{\partial z} \right) + \frac{\omega^2}{c^2} n^2(x, z) E_y = 0 \tag{2}
\]

where \(n^2(x, z) = \varepsilon(x, z) \mu(x, z),\) and \(n(x, z)\) is the refractive index of the medium.
3. WAVE SCATTERING BY A NEGATIVE-INDEX SLAB

The concept of perfect sub-wavelength imaging of a point source through reconstitution of the evanescent waves by a flat lens has remained highly controversial [17] because it is severely constrained by anisotropy and losses of the metamaterials. Nevertheless, several numerical studies showed that nearly perfect imaging should be expected even under realistic conditions when both dispersion and losses are taken into account, although the sub-wavelength resolution can be archived only by using sub-wavelength-thin lenses which should be separated from the source by distance equal to a small fraction of the wavelength [18–20, 10–13]. In this section, we consider the numerical simulations of the wave scattering by a slab of the negative-index material, i.e., the problem close to that of the perfect lens imaging, and discuss the convergence of the Yee numerical discretization scheme.

3.1. Geometry and discretization

We start our analysis by considering wave propagation through a slab made of the negative-index material, as schematically illustrated in Figure 1, with homogeneous properties in the $(y, z)$ plane characterized by two functions, the electric permittivity $\varepsilon = \varepsilon(x)$ and magnetic permeability $\mu = \mu(x)$. To solve this problem numerically, we employ the well-known numerical Yee method [15] and perform the discretization of the electric and magnetic fields on a square grid $(x_m = h m, z_n = h n)$ presenting the fields in the form

$$
E_y|_{m,n} = \langle E_y \rangle_{m,n}, \quad H_z|_{m+1/2,n} = \langle H_z \rangle_{m+1/2,n}, \quad H_x|_{m,n+1/2} = \langle H_x \rangle_{m,n+1/2}
$$

where we use the notation

$$
\langle \bullet \rangle_{m,n} = \int_{x_{m-1/2}}^{x_{m+1/2}} \int_{z_{n-1/2}}^{z_{n+1/2}} \bullet \, dx \, dz
$$

Then, we replace the continuum model by a closed set of the discrete equations for the field amplitudes obtained by averaging Equations (1) over the cells of discretization mesh, taking into account the continuity of the tangential field components at the interface [15],

$$
\begin{align*}
\frac{H_z|_{m+1/2,n} - H_z|_{m-1/2,n}}{h} - \frac{H_x|_{m,n+1/2} - H_x|_{m,n-1/2}}{h} = & \frac{i \omega}{c} \langle \varepsilon \rangle_{m,n} E_y|_{m,n} \\
\frac{H_y|_{m,n+1} - H_y|_{m,n}}{h} - \frac{\mu^{-1} H_z|_{m,n+1/2}}{h} = & \frac{-i \omega}{c} H_x|_{m,n+1/2} \\
\frac{E_y|_{m,n} - E_y|_{m+1,n}}{h} = & \frac{i \omega}{c} \langle \mu \rangle_{m+1/2,n} H_z|_{m+1/2,n}
\end{align*}
$$

Whereas the general form of the discrete equations (4) is well known [15], we point out a number of specific features arising in numerical simulations of the waves scattering at the interfaces with the negative-index media. Since the real parts of both $\varepsilon$ and $\mu$ change sign at these interfaces, the corresponding averaged values may become small or even vanish for a certain layer position with respect to the numerical grid. In this case, Equations (4) may become (almost) singular, leading to poor convergence. In this paper, we suggest that consistent convergence can be achieved by artificially shifting the layer boundary with respect to the grid in order to ensure that the averaged values do not vanish. This shift will not exceed $h/2$, assuring convergence as the step size is decreased.
Because the tangential component \( E_y \) of the electric field should be continuous at the interface, it seems that a natural choice is to align the boundary position with the grid points \( x_m \), where \( E_y \) is defined, and we use this configuration in the numerical simulations presented below. However, we note that such a selection leads to singularities for averaged values if \( \epsilon_1 = -\epsilon_2 \) or \( \mu_1 = -\mu_2 \), which coincides with the flat-lens condition. Therefore, it is necessary to take into account losses in the metamaterial, described by non-zero imaginary parts of the complex values \( \epsilon_2 \) and \( \mu_2 \), or to choose a different boundary alignment to the grid for the numerical simulations of perfect lenses [1].

3.2. Wave spectrum and convergence of discrete solutions

In order to illustrate the convergence of the proposed numerical scheme, we compare the solutions of discrete and continuous equations. We note that wave scattering from an infinite layer is fully characterized by the properties of spatial modes, which wavevector components along the layer \( k_z \) are conserved. These modes have the form

\[
E(x, z) = \delta(x; k_z) \exp(ik_z z), \quad H(x, z) = \mathcal{H}(x; k_z) \exp(ik_z z)
\]  

Substituting Equations (5) into Equations (1) and (4), we obtain a set of corresponding continuous and discrete eigenmode equations. For every \( k_z \), the mode profiles can be determined analytically, e.g. using the transfer-matrix method [21]. The wave spectrum can contain solutions corresponding to the guided modes of a negative-index layer [22], and extended (or propagating) modes that should also be taken into account as well, in order to describe scattering of arbitrary fields.

We solve the discrete eigenmode equations numerically for the slab geometry with periodic boundary conditions, and compare the spectrum of eigenvalues \( k_z \) with exact solutions of the continuous model. In Figure 2(a), we show a part of the spectrum of the discrete eigenvalues (crosses), which indeed coincides with the exact values (circles). The rate of convergence can be judged from Figure 2(b), where the differences between the approximate and exact solutions are shown in logarithmic scale.
4. WAVE SCATTERING BY A WEDGE OF NEGATIVE-INDEX MATERIAL

One of the fundamental problems in the theory of negative-index metamaterials is the wave scattering by wedges [23], where convergence of numerical methods can be slow due to the appearance of singularities [24]. In this section, we demonstrate that the nature of such singularities has to be taken into account when performing finite-difference numerical simulations.

4.1. Singularity parameter

The behaviour of the electric and magnetic fields at the wedges between homogeneous materials characterized by different values of $\epsilon$ and $\mu$ was described analytically in the pioneering paper of Meixner [24], and further refined in the subsequent studies (see, e.g. References [25, 26] and references therein). In the case of the TE wave scattering by a negative-index wedge, as schematically illustrated in Figure 3, the amplitudes of magnetic fields exhibit singular behaviour at the wedge of the order of $\rho^{-1}$, where $\rho$ is the distance from the wedge. For a $\pi/2$ wedge angle, corresponding to the corner of a rectangular slab, the coefficient $\gamma$ is found as [24]

$$\frac{\mu_1 - \mu_2}{\mu_1 + \mu_2} = \pm 2 \cos(\gamma\pi/2)$$

Figure 2. (a) Spectrum of wavenumbers $k_z$ for a negative-index layer: exact (circles) and discrete (crosses, for $N = 512$) solutions; and (b) absolute differences between the exact and discrete values of $k_z$ vs the number of points ($N$) along $x$ for the marked points 1,2,3 in (a). Bottom: Mode profiles marked 1,2,3 in (a). The computational domain is $0 < x < 6.4$, $d_2 = 1.4$ is the width of the negative-index layer with $\epsilon_2 = -1.2$ and $\mu_2 = -1.5$, and $\epsilon_1 = \mu_1 = 1$. The wavenumber in vacuum is normalized as $c/\omega = 1$. 

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Int. J. Numer. Model. 2006; 19:105–117
where $\mu_1$ and $\mu_2$ are magnetic permeabilities of the two neighbouring media. In the case of conventional dielectric or magnetic media with $\mu_j > 0$, Equation (6) has solutions with real $\gamma$. However, when $\mu$ changes its sign at the interface with a negative-index medium, the coefficient $\gamma$ becomes complex playing role of a singularity parameter. This happens when

$$-3\mu_1 < \mu_2 < -\frac{\mu_1}{3}$$

so that $|\mu_1 - \mu_2|/|\mu_1 + \mu_2| > 2$; see Figure 4.

For real $\gamma$ (taking the solution with $0 < \gamma < 1$, according to Reference [24]), the field amplitudes decay monotonically away from the corner. In this case, numerical simulations may be based on the simplest discretization, although the convergence rate can be improved by taking into account the singular behaviour in the discrete equations.
However, the case of complex $\gamma$ corresponds to the fields that oscillate infinitely fast near the corner because

$$\rho^{\gamma-1} = \rho^{\Re(\gamma-1)} \exp[i \Im(\gamma) \log(\rho)]$$

The second multiplier indicates the excitation of infinitely large spatial harmonics. However, such a situation is unphysical because the effective-medium approximation of the negative-index materials is valid for slowly varying fields only. Therefore, in numerical simulations it is necessary to take into account the physical effects that suppress such oscillations. In particular, we discuss the effect of losses in Section 4.3.

4.2. Numerical results

We now analyse convergence of the numerical finite-difference solutions for the problem of wave scattering by a finite-extent negative-index slab. We align the boundaries of the negative-index domain with the grid, as shown schematically in Figure 1(b). Since the electric field components $E_y$ are continuous at the interfaces, it is possible to obtain the discrete equations that have the form of Equations (4).

In order to construct the full solutions for scattering problem, we decompose the field into a set of eigenmodes of the negative-index layer ($z > 0$) and free space ($z < 0$). More specifically, for
where \( j \) is the number of eigenmodes. Here the summation is performed over the propagating modes \( (\mathcal{I} m k_z = 0) \) which transport energy away from the interface, and evanescently decaying modes with \( \mathcal{I} m k_z < 0 \). In free space at \( z = 0 \), the field is composed of incident and reflected plane waves

\[
\begin{align*}
E_i |_{m,n} & = \sum_j A_j \mathcal{E}_{m,n}(k^{(j)}_z) \exp(i k^{(j)}_z z), \\
H_i |_{m,n} & = \sum_j A_j \mathcal{H}_{m,n}(k^{(j)}_z) \exp(i k^{(j)}_z z)
\end{align*}
\]

(8)

Here \( N \) is the number of points in the \( x \) direction, and the discrete wavenumber is \( K^{(j)} = \pm \sin^{-1}[h^2 \alpha^2/4c^2 - \sin^2(j\pi/N)]^{1/2}/h \) [15]. The sign of \( K^{(j)} \) is chosen with a proper wave asymptotic behaviour, i.e. we choose \( \Re(K^{(j)}) > 0 \), if \( K^{(j)} \) is real, and \( \Im(K^{(j)}) > 0 \) if \( K^{(j)} \) is complex. The magnetic field at \( z < 0 \) is found from Equation (1), with homogeneous parameters \( \langle \epsilon \rangle = \epsilon_1, \langle \mu \rangle = \mu_1, \langle \mu^{-1} \rangle = \mu_1^{-1} \). Then, we substitute Equations (8) and (9) into the first of Equation (4), and using the condition of the continuity of the electric field, obtain a set of equations for all \( m = 1, \ldots, N \) that are used to calculate the amplitudes \( F_j^{(\text{refl})} \) and \( A_j \) of the

Figure 6. (a) Amplitudes of reflected plane waves vs the number of points; and (b,c) electric field profiles for \( N = 64 \) and \( N = 256 \). Parameters are the same as in Figure 2.
reflected and transmitted waves

\[ \sum_j A_j \mathcal{E}_y |_{m,0}(k^j_z) = \sum_{j=-N/2+1}^{N/2} (F^{(in)}_j + F^{(refl)}_j) \exp(i2\pi jm/N) \]

\[ \sum_j A_j \mathcal{H}_x |_{m,-1/2}(k^j_z) + \mathcal{H}_x |_{m,1/2}(k^j_z) \]

\[ = -\frac{2c}{\omega \mu_1 h} \sum_{j=-N/2+1}^{N/2} (F^{(in)}_j - F^{(refl)}_j) \sin(K^j h) \exp(i2\pi jm/N). \] (10)

These equations are solved using the standard linear algebra package.

We now present results of our numerical simulations for the scattering of normally incident plane waves, with \( F^{(in)}_0 = 1, F^{(in)}_{\neq 0} = 0 \). First, we consider scattering by a negative-index slab with \( \mu_2 < -3 \). In this case, we observe a steady convergence of numerical solutions, as shown in Figure 5. This demonstrates that even simplest finite-difference numerical schemes can be successfully employed to model the scattering process when the singularity parameter \( \gamma \) is real, in full agreement with earlier studies of wave scattering at dielectric wedges [26].
However, the situation changes dramatically when \( \gamma \) is complex, i.e. for \( \mu_2 = -1.5 \). According to the analytical solution, in this case the magnetic field should oscillate infinitely fast in the vicinity of the corner, corresponding to excitation of infinitely large spatial harmonics. However, such behaviour cannot be described by discrete equations, and we find that in this regime solutions of finite-difference equation do not converge, as demonstrated in Figure 6.

### 4.3. Effects of losses

The analytical description of the edge singularities discussed above is only valid for lossless media, i.e. when all \( \epsilon \) and \( \mu \) are real. However, the negative-index metamaterials always have non-vanishing losses, and we have studied whether this important physical effect can regularize the field oscillations at the corner. However, our results demonstrate that even substantial losses may not be sufficient enough to suppress such oscillations, as presented in the example of Figure 7.

### 4.4. Singularities and perfect lenses

Finally, we consider the problem of wave scattering from the corners of perfect lenses, where \( \Re(\epsilon_2) \approx -1 \) and \( \Re(\mu_2) \approx -1 \) (we take \( \epsilon_1 = \mu_1 = 1 \)). This is a special case, where the singularity becomes an essential singularity if losses are neglected. We find that introducing sufficiently large losses does indeed regularize the field oscillations at the corners, leading to
convergence of numerical simulations, as demonstrated for the example of Figure 8. However, this only occurs when the value of losses exceeds a certain threshold; if the losses are too weak then non-convergent behaviour is again observed, as shown in Figure 9. The threshold value of losses for achieving convergence of the numerical scheme is increased for larger $\Re (\mu_2) + 1$.

We note that this is completely different from the temporal dynamics at an infinitely extended slab, where convergence to a steady state is eventually achieved with arbitrarily small losses [12].

5. CONCLUSIONS

We have discussed a number of specific features manifested in numerical simulations of wedges and interfaces of metamaterials, i.e. composite materials with negative dielectric permittivity and negative magnetic permeability. We have demonstrated that a numerical discretization grid in the Yee method may have a dramatic effect on the convergence in numerical modelling of surface waves at interfaces and wedges. In the framework of the continuous-medium approximation, wave scattering on the wedge may result in a resonant excitation of surface waves with infinitely large spatial frequencies, leading to non-convergence of the numerical simulation results that depend strongly on the value of the discretization step. We find that sufficiently high losses may suppress oscillations and allow to obtain converging solutions to the...
scattering problem, however in the case of smaller losses it may be necessary to take into account the metamaterial properties beyond the effective-medium approximation, such as the effect of spatial dispersion.

ACKNOWLEDGEMENTS

The authors thank Alexander Zharov and Pavel Belov for useful discussions and suggestions. This work has been supported by the Australian Research Council.

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